Final Project: Wine Data Unsupervised Learning

GitHub link:
Goal:
Provide an Unsupervised Learning problem resolution to Wine Data set to perform EDA and model analysis.
Methods:

We will perform cluster analysis, an unsupervised learning task. We will accept that this dataset has no classes and search for patterns based on the attributes. The clustering will be performed with k-means approach and use Dimension Reduction by using PCA. Afterwards we will perform a k-means approach and see if the total outcome of unsupervised learning will improve.

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Introduction:

```
In [1]: # Import nessesary Packages:
        import pandas as pd
        import numpy as np
        from itertools import combinations
        import matplotlib as ml
        import matplotlib.pyplot as plt
        %matplotlib inline
        ml.style.use('fivethirtyeight')
        from sklearn import datasets
        from sklearn.model selection import train test split
        from sklearn.metrics import silhouette_samples,silhouette_score
        import seaborn as sns
        from seaborn import heatmap, diverging_palette
        import itertools
        from sklearn.feature_extraction.text import TfidfVectorizer
        from sklearn.decomposition import NMF
        from sklearn.metrics import accuracy_score
        from sklearn.ensemble import RandomForestClassifier
        from sklearn.preprocessing import MinMaxScaler
        from sklearn.cluster import KMeans
        from sklearn.metrics import silhouette_score, calinski_harabasz_score, davi
        es_bouldin_score, silhouette_samples
        from sklearn.preprocessing import MinMaxScaler
        from sklearn.decomposition import PCA
```

Data Description:

The datasets is included, related to white vinho verde wine samples, from the north of Portugal. The dataset was downloaded from UCI Machine Learning Repository link: https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-white.csv (https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality-white.csv). All variables are continuous. The last column of this dataset - quality, is the target data used for other data science tasks (e.g. classification) and will be dropped.

```
In [8]: # importing data and creating dataframe
    def load_dataset():
        url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/wine-q
    uality/winequality-white.csv'
        df = pd.read_csv(url, header=0, sep=';')
        df = df.iloc[:, :-1]
        return df

df = load_dataset()
    df.head(10)
```

Out[8]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	рН	sulphates	alcor
	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	{
	1 6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	Ę
:	2 8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	1(
	3 7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	ξ
	4 7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	ξ
	5 8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	1(
	6.2	0.32	0.16	7.0	0.045	30.0	136.0	0.9949	3.18	0.47	ξ
	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	}
	8 6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	ξ
	9 8.1	0.22	0.43	1.5	0.044	28.0	129.0	0.9938	3.22	0.45	1′

```
In [9]: #Size of Dataset:
    df.shape
```

Out[9]: (4898, 11)

```
In [4]: #Basic information
    df.info()

#Describe the data
    df.describe()
```

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 4898 entries, 0 to 4897
Data columns (total 11 columns):

#	Column	Non-Null Count	Dtype
0	fixed acidity	4898 non-null	float64
1	volatile acidity	4898 non-null	float64
2	citric acid	4898 non-null	float64
3	residual sugar	4898 non-null	float64
4	chlorides	4898 non-null	float64
5	free sulfur dioxide	4898 non-null	float64
6	total sulfur dioxide	4898 non-null	float64
7	density	4898 non-null	float64
8	рН	4898 non-null	float64
9	sulphates	4898 non-null	float64
10	alcohol	4898 non-null	float64

dtypes: float64(11)
memory usage: 421.0 KB

Out[4]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total s dic
count	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.00
mean	6.854788	0.278241	0.334192	6.391415	0.045772	35.308085	138.36
std	0.843868	0.100795	0.121020	5.072058	0.021848	17.007137	42.49
min	3.800000	0.080000	0.000000	0.600000	0.009000	2.000000	9.00
25%	6.300000	0.210000	0.270000	1.700000	0.036000	23.000000	108.00
50%	6.800000	0.260000	0.320000	5.200000	0.043000	34.000000	134.00
75%	7.300000	0.320000	0.390000	9.900000	0.050000	46.000000	167.00
max	14.200000	1.100000	1.660000	65.800000	0.346000	289.000000	440.00

1. EDA - Exploratory Data Analysis:

EDA is done to understand the data and summarize the data set. To detect outliers we will implement the IQR method. We will define the spread difference between the 75th and 25th percentiles of the data.

Exploring Dataset:

```
In [10]: # displaying data types, null values, and possible outliers in each column
         def dataframe_summary():
             # Lists
             var_list = df.columns.to_list()
             dtype_list = []
             null_list = []
             # Looping through columns
             for col in df.columns:
                 dtype_list.append(df[col].dtype)
                 null_list.append(df[col].isnull().sum())
             # outliers IQR
             Q1 = df.quantile(.25)
             Q3 = df.quantile(.75)
             IQR = Q3 - Q1
             k = 1.5
             outlier_list = ((df < (Q1 - k * IQR)) | (df > (Q3 + k * IQR))).sum().to
         _list()
             # stacking lists into dictionary
             dict = {'Variable': var_list, 'Data type': dtype_list, 'Null values': n
         ull_list, 'Outliers': outlier_list}
             return pd.DataFrame(dict).style.hide_index()
         dataframe_summary()
```

Out[10]:

Variable	Data type	Null values	Outliers
fixed acidity	float64	0	119
volatile acidity	float64	0	186
citric acid	float64	0	270
residual sugar	float64	0	7
chlorides	float64	0	208
free sulfur dioxide	float64	0	50
total sulfur dioxide	float64	0	19
density	float64	0	5
рН	float64	0	75
sulphates	float64	0	124
alcohol	float64	0	0

There are no missing values in the dataframe. All attributes are continuous and contain double-precision numbers. We summed up outliers for each variable.

3.0

2.8

0.4

9

8

alcohol

1.00

0.99

100

chlorides free sulfur dioxidel sulfur dioxide density

We will proceed further and visualize outliers with box plots.

```
In [6]:
          # plotting box plots
          def plot_box_plots():
               fig, ax = plt.subplots(nrows=1, ncols=len(df.columns), figsize=(15, 6))
               # visualizing IQR results with box plots
               for i in range(len(df.columns)):
                    df.boxplot(column=df.columns[i], ax=ax[i], vert=True)
               fig.tight_layout()
               plt.show()
          plot_box_plots()
                                                     300
                                                                     1.04
                                            0.35
           14 °
                                                                              3.8
                                                                                                14
                                     60
                                                                                       1.0
                   1.0
                           1.50
                                            0.30
                                                     250
                                                                     1.03
                                                                                                13
                                                                              3.6
           12 0
                           1.25 0
                                            0.25 8
                   8.0
                                                     200
                                                             300
                                                                                       0.8
                                                                                                12
                                                                     1.02
                                                                              3.4
                           1.00
           10
                   0.6
                                                     150
                                                                                                11
                           0.75
                                                             200
                                                                     1.01
                                                                                       0.6
                                                                              3.2
                                            0.15
            8
                                                     100
                                                                                                10
                   0.4
                           0.50
                                     20
```

Only alcohol column has no outliers. The least outliers are visible for: residual sugar and density. The most errors are in: chlorides and volatile acidity.

0.10

0.05

0.00

10

0.25

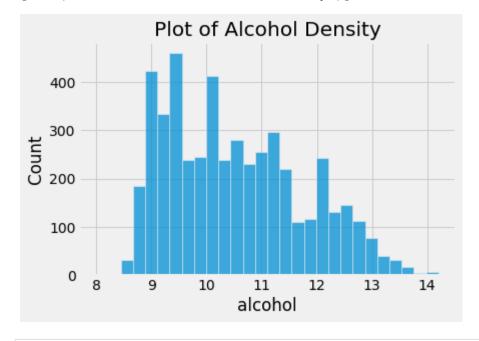
0.00

fixed acidity volatile acidity citric acid residual sugar

0.2

```
In [7]: sns.histplot(
    data = df,
    x = 'alcohol',
    legend = False
).set(title = "Plot of Alcohol Density")
```

Out[7]: [Text(0.5, 1.0, 'Plot of Alcohol Density')]



```
In [11]: # removing duplicate rows
    df = df.drop_duplicates()

# descriptive statistics of dataset
    round(df.describe(), 2)
```

Out[11]:

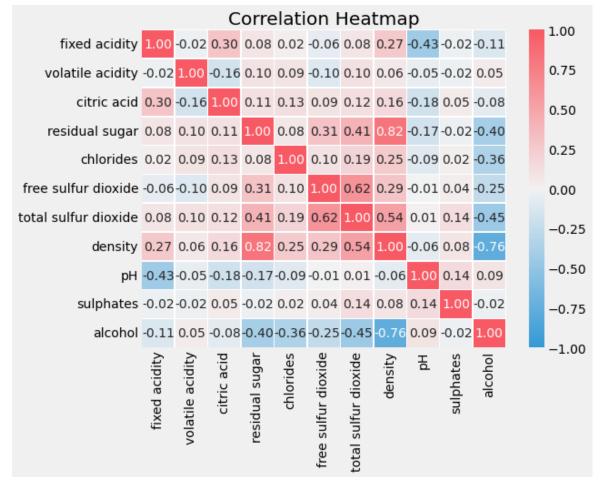
	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	рН	sulp
count	3961.00	3961.00	3961.00	3961.00	3961.00	3961.00	3961.00	3961.00	3961.00	39
mean	6.84	0.28	0.33	5.91	0.05	34.89	137.19	0.99	3.20	
std	0.87	0.10	0.12	4.86	0.02	17.21	43.13	0.00	0.15	
min	3.80	0.08	0.00	0.60	0.01	2.00	9.00	0.99	2.72	
25%	6.30	0.21	0.27	1.60	0.04	23.00	106.00	0.99	3.09	
50%	6.80	0.26	0.32	4.70	0.04	33.00	133.00	0.99	3.18	
75%	7.30	0.33	0.39	8.90	0.05	45.00	166.00	1.00	3.29	
max	14.20	1.10	1.66	65.80	0.35	289.00	440.00	1.04	3.82	

```
In [12]: df.shape
```

Out[12]: (3961, 11)

We can see that size of Dataset reduced from (4898, 11) to (3961, 11). These rows do not bring much value in data modelling. Min value row displays 0.0 for citric acid column. This should be acceptable and not a measurement error.

Heat Map to see correlation between variables:



There are some strong, interesting co-dependencies between some of the features:

```
alcohol vs. density;
total sulfur dioxide (TSO2) vs. free sulfur dioxide (FSO2);
density vs. residual sugar.
```

2. Normalizing Data

Clustering algorithms in geometrical context are distance based. Therefore, rescaling data is a must. We will implement the MinMaxScaler method from sklearn library. The transformation shifts the values as given:

$$X_i' = rac{X_i - min(X)}{max(X) - min(X)},$$

where X_i is the original value, min(X) the minimum value in feature range, and max(X) the maximum value.

```
In [13]: # normalizing data
         def normalizing_data(data):
             # rescaling data
             scaler = MinMaxScaler()
             norm_features = scaler.fit_transform(data)
             return norm_features
         df2 = normalizing_data(data=df)
         df2
Out[13]: array([[0.30769231, 0.18627451, 0.21686747, ..., 0.25454545, 0.26744186,
                 0.12903226],
                [0.24038462, 0.21568627, 0.20481928, ..., 0.52727273, 0.31395349,
                 0.24193548],
                [0.41346154, 0.19607843, 0.24096386, ..., 0.49090909, 0.25581395,
                 0.33870968],
                [0.25961538, 0.15686275, 0.11445783, ..., 0.24545455, 0.27906977,
                 0.22580645],
                [0.16346154, 0.20588235, 0.18072289, ..., 0.56363636, 0.18604651,
                 0.77419355],
                [0.21153846, 0.12745098, 0.22891566, ..., 0.49090909, 0.11627907,
                 0.61290323]])
```

3. Evaluating Clustering Algorithm

Clustering is an unsupervised learning method meaning we do not have the ground truth to compare the results to the true labels to check how well it worked. We can investigate clustering process in two ways:

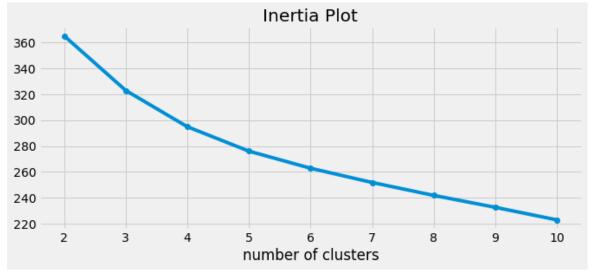
- visually we try to investigate the structure of the data by splitting the dat a points into distinct subgroups;
- with measures we use scores and numbers to describe the performance; we will use: the silhouette score, Caliński-Harabasz score, and Davies-Bouldin index to e valuate the algorithms.

4. k-Means Clustering

This partitional grouping method is the most basic, frequently used, and for general purposes. It involves identifying the dataset's cluster centers that are distinct from one another. The k-means iteratively divides data points into k clusters (centers or groups) by minimizing the variance in each cluster.

We will start the clustering process by choosing the appropriate number of centers. The quality of the cluster assignments is determined by computing the sum of the squared error (SSE) after the centroids converge. The SSE (or inertia) is defined as the sum of the squared Euclidean distances of each point to its closest centroid. Since this is a measure of error, the objective of k-means is to try to minimize this value.

```
In [14]: # finding optimal number of clusters
         def kmeans_optimal_clusters(data):
             from sklearn.cluster import KMeans
             from sklearn.metrics import silhouette_score
             # sum of squared error = clusters inertia
             clusters_inertia = []
             # k-means properties
             kmeans_kwargs = {'init': 'k-means++', 'max_iter': 300}
             # calculate scores for clusters between 2 and 10
             for i in range(2, data.shape[1]):
                  kmeans = KMeans(n_clusters=i, **kmeans_kwargs).fit(data)
                  clusters_inertia.append(kmeans.inertia_)
             # visualize results
             plt.figure(figsize=(10, 4))
             plt.plot(range(2, data.shape[1]), clusters_inertia, marker='o', markers
         ize=6)
             plt.xticks(np.arange(2, data.shape[1]))
             plt.title('Inertia Plot')
             plt.xlabel('number of clusters')
             plt.show()
         kmeans_optimal_clusters(data=df2)
```



```
In [ ]:
```

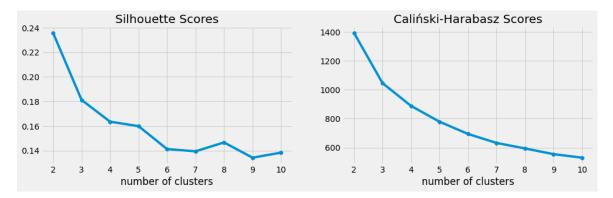
Determining the elbow point in the SSE curve is not always straightforward. This graph has no clear "elbow" visible. Three clusters should be a fair choice. Another way for choosing the best number of clusters is by silhouette scores and Caliński-Harabasz scores.

```
In [15]: # finding optimal number of clusters with silhouette and Caliński-Harabasz
         coefficients
         def kmeans hyperparameter tuning(data):
             from sklearn.cluster import KMeans
             from sklearn.metrics import silhouette_score, calinski_harabasz_score
             from sklearn.model_selection import ParameterGrid
             # grid of clusters for tuning
             parameters = list(range(2, data.shape[1]))
             # instantiating ParameterGrid
             parameter_grid = ParameterGrid({'n_clusters': parameters})
             # k-means properties
             kmeans_kwargs = {'init': 'k-means++', 'max_iter': 300}
             # instantiating k-means model
             kmeans_model = KMeans(**kmeans_kwargs)
             # silhouette coefficients
             silhouette_scores = []
             # Caliński-Harabasz coefficients
             cal_har_scores = []
             # calculating scores for each cluster
             for i, j in zip(parameter_grid, parameters):
                  kmeans_model.set_params(**i)
                 kmeans model.fit(data)
                 # appending lists
                  ss = silhouette_score(data, kmeans_model.labels_)
                  chs = calinski_harabasz_score(data, kmeans_model.labels_)
                 silhouette_scores += [ss]
                  cal_har_scores += [chs]
                 print('Number of Clusters = {}: \tSilhouette Score: {}, \tCaliński-
         Harabasz Score: {}'
                        .format(j, round(ss, 6), round(chs, 6)))
             # visualizing results
             fig = plt.figure(figsize=(15, 4))
             # subplot 1
             plt.subplot(1, 2, 1)
             plt.plot(range(2, data.shape[1]), silhouette_scores, marker='o', marker
         size=6)
             plt.xticks(np.arange(2, data.shape[1]))
             plt.title('Silhouette Scores')
             plt.xlabel('number of clusters')
             # subplot 2
             plt.subplot(1, 2, 2)
             plt.plot(range(2, data.shape[1]), cal_har_scores, marker='o', markersiz
         e=6)
             plt.xticks(np.arange(2, data.shape[1]))
```

```
plt.title('Caliński-Harabasz Scores')
plt.xlabel('number of clusters')
plt.show()

kmeans_hyperparameter_tuning(data=df2)
```

Number	of Clusters = 2:	Silhouette	Score:	0.235842,	Caliński-Ha
rabasz	Score: 1393.438255				
Number	of Clusters = 3:	Silhouette	Score:	0.181216,	Caliński-Ha
rabasz	Score: 1045.651469				
Number	of Clusters = 4:	Silhouette	Score:	0.163513,	Caliński-Ha
rabasz	Score: 888.267938				
Number	of Clusters = 5:	Silhouette	Score:	0.159846,	Caliński-Ha
rabasz	Score: 778.777009				
Number	of Clusters = 6:	Silhouette	Score:	0.141193,	Caliński-Ha
rabasz	Score: 694.226727				
Number	of Clusters = 7:	Silhouette	Score:	0.139364,	Caliński-Ha
rabasz	Score: 632.022064				
Number	of Clusters = 8:	Silhouette	Score:	0.146599,	Caliński-Ha
rabasz	Score: 593.779057				
Number	of Clusters = 9:	Silhouette	Score:	0.134181,	Caliński-Ha
rabasz	Score: 554.487818				
Number	of Clusters = 10:	Silhouette	Score:	0.13829,	Caliński-Ha
rabasz	Score: 529.995671				



From visual analysis we can see a significant decrease from 2 clusters to three. Although, two clusters have the highest score value it might be too simplistic for this kind of data. The best option would be respectively three centers. We will provide this quantity in the training process.

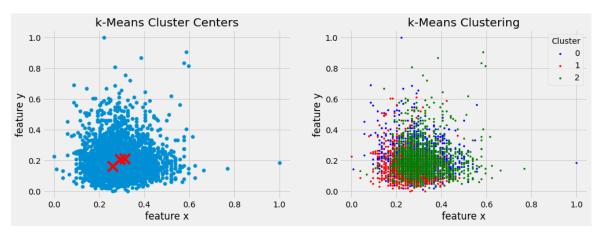
```
In [16]: # performing k-means clustering
         def kmeans_clustering(n_clusters, data):
              # fitting model
              kmeans = KMeans(n_clusters=n_clusters, init='k-means++', max_iter=300)
              pred_y = kmeans.fit_predict(data)
              # new data with predicted clusters
              array = np.append(data, pred_y.reshape(-1, 1), axis=1)
              # number of features
              print('Number of Fitted Variables:', kmeans.n_features_in_)
              # counting instances for each cluster
              print('\n#### Number of Instances Per Cluster ####')
              for i in range(0, n_clusters):
                  print('Cluster {}: {}'.format(i, (array[:,-1] == i).sum()))
              # visualizing results
              plt.figure(figsize=(15, 5))
              # subplot 1
              plt.subplot(1, 2, 1)
              plt.scatter(x=data[:, 0], y=data[:, 1])
              plt.scatter(x=kmeans.cluster_centers_[:, 0], y=kmeans.cluster_centers_
          [:, 1], s=300, c='red', marker='x')
              plt.title('k-Means Cluster Centers')
              plt.xlabel('feature x')
              plt.ylabel('feature y')
              colors = ['blue', 'red', 'green', 'cyan', 'magenta']
              # subplot 2
              plt.subplot(1, 2, 2)
              for i, color in zip(range(0, n_clusters), colors):
                  plt.scatter(x=array[:, 0][(array[:, -1] == i)],                             y=array[:, 1][(arra
         y[:, -1] == i)], marker='.', color=color, label=i)
              plt.title('k-Means Clustering')
              plt.xlabel('feature x')
              plt.ylabel('feature y')
              plt.legend(loc='best', title='Cluster')
              plt.show()
              print('#### Centroid Coordinates [x, y] ####')
              for i in range(0, n_clusters):
                  print('Cluster {}: \t[{}, {}]'.format(i, round(kmeans.cluster_cente
         rs_[i, 0], 3),
                                                     round(kmeans.cluster_centers_[i,
         1], 3)))
              # subplot 3
              plt.figure(figsize=(7, 4))
              # silhouette score for each sample
```

```
silhouette_vals = silhouette_samples(data, pred_y)
   y_lower, y_upper = 0, 0
    for i in range(n_clusters):
        # grouping and sorting silhouette scores
        cluster silhouette vals = silhouette vals[pred y == i]
        cluster_silhouette_vals.sort()
        size_cluster_i = cluster_silhouette_vals.shape[0]
        y upper = y lower + size cluster i
        plt.fill betweenx(y=np.arange(y lower, y upper), x1=0, x2=cluster s
ilhouette_vals, alpha=0.5, edgecolor=None)
        # cluster label at the middle
        plt.text(x=-0.05, y=(y_lower + y_upper) / 2, s=str(i))
        # new y_lower for next plot
        y_lower = y_upper + 10
   # plotting average silhouette score
    avg_score = (silhouette_vals).mean()
    plt.axvline(x=avg score, color='red', linestyle='--', linewidth=2, labe
l='average')
    plt.yticks([])
    plt.xlim([-0.2, 1])
    plt.title('Silhouette Plot For {} Clusters'.format(n_clusters))
    plt.xlabel('Silhouette Score')
    plt.ylabel('Cluster')
    plt.grid(axis='x')
   plt.legend(loc='upper right')
    plt.show()
   print('#### Model Validation ####')
    print('Average Silhouette Score:', silhouette_score(data, kmeans.labels
_))
    print('Caliński-Harabasz Score:', calinski harabasz score(data, kmeans.
labels_))
    print('Davies-Bouldin Index:', davies bouldin score(data, kmeans.labels
_))
kmeans_clustering(n_clusters=3, data=df2)
```

Number of Fitted Variables: 11

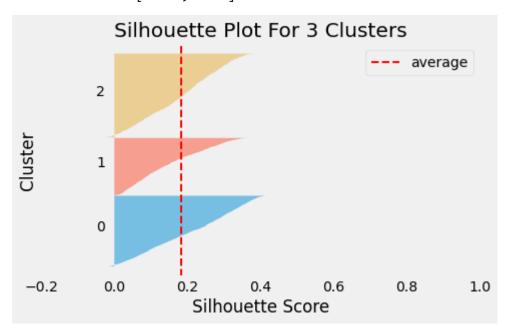
Number of Instances Per Cluster

Cluster 0: 1319 Cluster 1: 1072 Cluster 2: 1570



Centroid Coordinates [x, y]

Cluster 0: [0.293, 0.208] Cluster 1: [0.26, 0.163] Cluster 2: [0.313, 0.21]



Model Validation

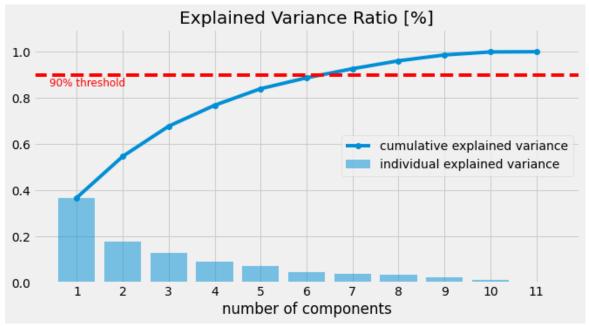
Average Silhouette Score: 0.18126118990661816 Caliński-Harabasz Score: 1045.6321448733058 Davies-Bouldin Index: 1.7659861783764155

The clustering is poor and far from perfect. We can see lots of overlapping within the data points. In geometrical content, each group has its own centroid (cluster center). The centroids are very close each other which also indicates poor grouping.

5. Dimensionality Reduction Using Principal Component Analysis (PCA)

The principal component analysis (PCA) is an unsupervised method which inverses a dataset so that these features are not statistically correlated.

```
In [17]: # finding optimal number of components with explained variance
         def pca_optimal_components(data):
             scaler = MinMaxScaler()
             scaled_data = scaler.fit_transform(data)
             pca = PCA(n_components=None).fit(scaled_data)
             # percentage of variance explained by each of the selected components
             y = np.cumsum(pca.explained_variance_ratio_)
             # visualizing results
             plt.figure(figsize=(10, 5))
             plt.ylim(0.0, 1.1)
             plt.plot(range(1, data.shape[1]+1), y, marker='o', markersize=6, label=
          'cumulative explained variance')
             plt.bar(range(1, data.shape[1]+1), pca.explained_variance_ratio_, alpha
         =0.5, label='individual explained variance')
             plt.title('Explained Variance Ratio [%]')
             plt.xlabel('number of components')
             plt.axhline(y=0.9, color='red', linestyle='--')
             plt.text(x=0.4, y=0.85, s='90% threshold', color='red', fontsize=12)
             plt.xticks(np.arange(1, data.shape[1]+1))
             plt.legend(loc='best')
             plt.show()
         pca_optimal_components(data=df2)
```



The plot shows the variances explained by each variable. It displays that cumulative explained variance is inversed to individual explained variance. The line plot determines which principal components to keep and which ones to discard. Most of the time, we use enough eigenvectors so that they explain 95% to 99% of the variation in the dataset. By examining the above figure, we can conclude that first 6 dimensions contain most of the information.

6. After Dimensionality Reduction

```
In [18]: # performing dimensionality reduction with PCA
         def reduce_dimensionality(n_components, data):
             from sklearn.preprocessing import MinMaxScaler
             from sklearn.decomposition import PCA
             scaler = MinMaxScaler()
             scaled_data = scaler.fit_transform(data)
             pca = PCA(n_components=n_components)
             pca_result = pca.fit_transform(scaled_data)
             return pca_result
         df3 = reduce dimensionality(n components=6, data=df2)
         df3
Out[18]: array([[-0.37376295, -0.1461661 , 0.01459762, 0.0286885 ,
                                                                      0.04700836,
                 -0.05763429],
                [-0.12220269, 0.1014675, -0.08277814, -0.02970811, -0.11097741,
                  0.02710799],
                [-0.05556597, -0.02265431, -0.06342425, -0.05313953, -0.04707583,
                  0.1466882 ],
                [-0.14777124, -0.13990322, -0.008534, -0.0900996, -0.14365979,
                 -0.1279622 ],
                [0.41409829, 0.04268417, -0.1525949, 0.03149197, 0.03856393,
                 -0.03502136],
                [0.26234653, -0.05374422, -0.19160334, -0.0793331, 0.02902432,
                 -0.01109314]])
```

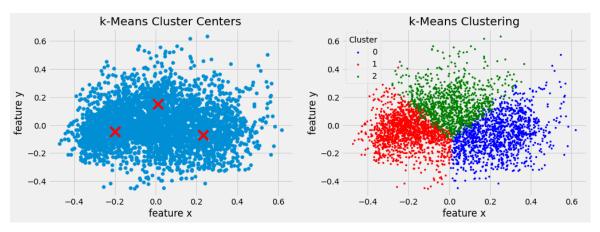
7. Clustering After Reducing Dimensions

In [19]: # 1. k-means clustering kmeans_clustering(n_clusters=3, data=df3)

Number of Fitted Variables: 6

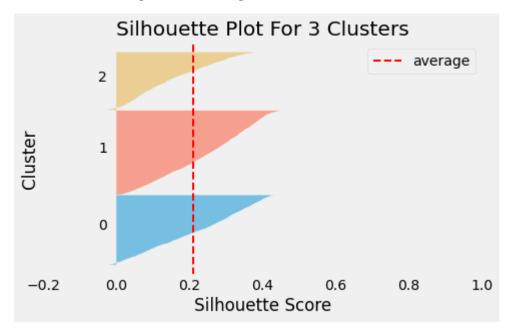
Number of Instances Per Cluster

Cluster 0: 1302 Cluster 1: 1575 Cluster 2: 1084



Centroid Coordinates [x, y]

Cluster 0: [0.233, -0.07] Cluster 1: [-0.2, -0.045] Cluster 2: [0.011, 0.148]



Model Validation

Average Silhouette Score: 0.211239685844038 Caliński-Harabasz Score: 1261.6981910329434 Davies-Bouldin Index: 1.6032056261222243

8. Summary / Conclusion:

We can see final results after dimensionality reduction improved:

Method	Silhouette	Caliński- Harabasz	Davies- Bouldin	Cluster 0	Cluster 1	Cluster 2	
k-Means	0.2116	1261.7120	1.6024	1075	1308	1578	

The scores are higher and clustering process looks more cleaner.

Before:

Model Validation

Average Silhouette Score: 0.18126118990661816 Caliński-Harabasz Score: 1045.6321448733058 Davies-Bouldin Index: 1.7659861783764155

After:

Model Validation

Average Silhouette Score: 0.211239685844038 Caliński-Harabasz Score: 1261.6981910329434 Davies-Bouldin Index: 1.6032056261222243

Conclusion:

This project introduces the k-means and PCA unsupervised algorithms that can be applied for exploratory data analysis and preprocessing on white wine dataset. Right representation of data is crucial for Unsupervised Learning. Important parts of this are Preprocessing and Decomposition methods.

The dimensionality reduction of initial datset is an essential tool to make sense of the data in the absence of supervision information. Applying PCA method improved the clustering process. Any further enhancing should be in removing possible outliers in the dataset. Overall, clustering can be a useful exploration tool for identifying homogeneous groups and pattern recognition within the data. This approach could help us understand more about the data before performing supervised tasks and develop more refine models.

In []: