Project 1 - Unsupervised Learning

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Contents

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1 Environment

First of all, we'd better declare the working environment, including the version of Python and packages used. We use watermark package to printe date and time stamps, version numbers, and hardware information.

```
In [68]: %load_ext watermark
         import matplotlib.cm as cm
         import matplotlib.pyplot as plt
         from matplotlib.patches import Ellipse
         import numpy as np
         import pandas as pd
         from pandas.plotting import scatter_matrix as sm
         from scipy.spatial.distance import cdist
         import seaborn as sns
         from sklearn import preprocessing
         from sklearn.metrics import silhouette_samples, silhouette_score
         from sklearn.cluster import KMeans
         from sklearn.decomposition import PCA
         from sklearn.mixture import GaussianMixture
         from sklearn.metrics.cluster import adjusted_rand_score
         %watermark
```

```
The watermark extension is already loaded. To reload it, use:
  %reload_ext watermark
2018-09-24T21:46:42+08:00

CPython 3.6.5
IPython 6.4.0

compiler   : GCC 4.2.1 Compatible Clang 4.0.1 (tags/RELEASE_401/final)
system     : Darwin
release    : 15.6.0
machine    : x86_64
processor  : i386
CPU cores  : 4
interpreter: 64bit
```

```
In [69]: %watermark -p matplotlib,numpy,pandas,scipy,seaborn,sklearn
```

```
matplotlib 2.2.3
numpy 1.15.1
pandas 0.23.0
scipy 1.1.0
seaborn 0.9.0
sklearn 0.19.1
```

In this project, we will take use some self-defined functions to plot the 2-D K-Means and Gaussian Mixture Model (GMM).

```
In [70]: # k-means weaknesses that mixture models address directly
         # code sourced from:
         #   http://nbviewer.jupyter.org/github/jakevdp/PythonDataScienceHandbook/blob/master/no

         # Predefined parameters
         def plot_kmeans(kmeans, X, n_clusters, rseed=2, ax=None):
             dot_size = 50
             cmap = 'viridis'
             labels = kmeans.fit_predict(X)

             # plot input data
             #ax = ax or plt.gca() # <-- nice trick
             fig, ax = plt.subplots(figsize=(9,7))
             ax.axis('equal')
             ax.scatter(X[:, 0], X[:, 1],
                        c=labels, s=dot_size, cmap=cmap, zorder=2)

             # plot the representation of Kmeans model
             centers = kmeans.cluster_centers_
             radii = [cdist(X[labels==i], [center]).max()
                      for i, center in enumerate(centers)]

             for c, r in zip(centers, radii):
                 ax.add_patch(plt.Circle(c, r, fc='#CCCCCC',edgecolor='slategrey',
                                         lw=4, alpha=0.5, zorder=1))
             return

         # code sourced from:
         # http://nbviewer.jupyter.org/github/jakevdp/PythonDataScienceHandbook/blob/master/note
         def draw_ellipse(position, covariance, ax=None, **kwargs):
             """Draw an ellipse with a given position and covariance"""
             # Convert covariance to principal axes
             if covariance.shape == (2, 2):
                 U, s, Vt = np.linalg.svd(covariance)
                 angle = np.degrees(np.arctan2(U[1, 0], U[0, 0]))
                 width, height = 2 * np.sqrt(s)
             else:
                 angle = 0
                 width, height = 2 * np.sqrt(covariance)

             # Draw the Ellipse
             for nsig in range(1, 4):
                 ax.add_patch(Ellipse(position, nsig * width, nsig * height,
                                      angle, **kwargs))
```

```
def plot_gmm(gmm, X, label=True, ax=None):
    dot_size = 50
    cmap = 'viridis'

    fig, ax = plt.subplots(figsize=(9,7))
    ax = ax or plt.gca()
    labels = gmm.fit(X).predict(X)

    if label:
        ax.scatter(X[:, 0], X[:, 1], c=labels, s=dot_size, cmap=cmap, zorder=2)
    else:
        ax.scatter(X[:, 0], X[:, 1], s=dot_size, zorder=2)
    ax.axis('equal')

    w_factor = 0.2 / gmm.weights_.max()
    for pos, covar, w in zip(gmm.means_, gmm.covariances_, gmm.weights_):
        draw_ellipse(pos, covar, ax=ax, alpha=w * w_factor)
```

2 Import Data

In this project, we use Wine Dataset to cluster different types of wines. This data set contains the results of a chemical analysis of wines grown in a specific area of Italy.

The attributes are (dontated by Riccardo Leardi, riclea@anchem.unige.it): 1. Alcohol 2. Malic acid 3. Ash 4. Alcalinity of ash
5. Magnesium 6. Total phenols 7. Flavanoids 8. Nonflavanoid phenols 9. Proanthocyanins 10. Color intensity 11. Hue 12. OD280/OD315 of diluted wines 13. Proline

Variable `Label` include the true labels of different wine.

```
In [71]: wine = pd.read_csv('wine.data', \
                           names = ['Label', \
                                    'Alcohol', \
                                    'Malic acid', \
                                    'Ash', \
                                    'Alcalinity of ash', \
                                    'Magnesium', \
                                    'Total phenols', \
                                    'Flavanoids', \
                                    'Nonflavanoid phenols', \
                                    'Proanthocyanins', \
                                    'Color intensity', \
                                    'Hue', \
                                    'OD280', \
                                    'Proline'])
        # True labels
        label = wine['Label']
        del wine['Label']
        # Data description
```

```
print("Types of variables:\n",wine.dtypes)

wine.describe()
```

```
Types of variables:
 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                   float64
Proline                   int64
dtype: object
```

Out[71]:

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium
count	178.000000	178.000000	178.000000	178.000000	178.000000
mean	13.000618	2.336348	2.366517	19.494944	99.741573
std	0.811827	1.117146	0.274344	3.339564	14.282484
min	11.030000	0.740000	1.360000	10.600000	70.000000
25%	12.362500	1.602500	2.210000	17.200000	88.000000
50%	13.050000	1.865000	2.360000	19.500000	98.000000
75%	13.677500	3.082500	2.557500	21.500000	107.000000
max	14.830000	5.800000	3.230000	30.000000	162.000000

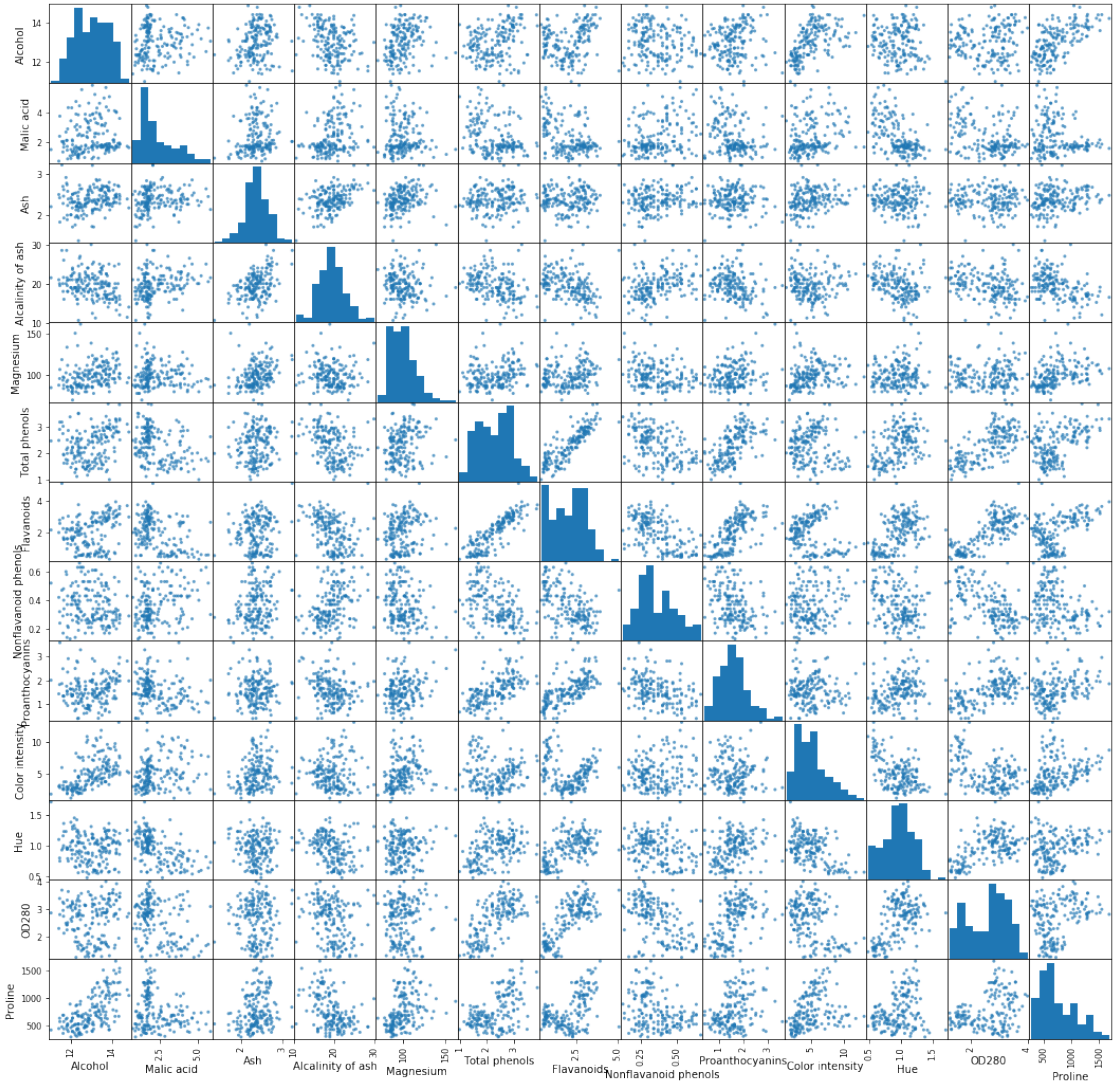
	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins
count	178.000000	178.000000	178.000000	178.000000
mean	2.295112	2.029270	0.361854	1.590899
std	0.625851	0.998859	0.124453	0.572359
min	0.980000	0.340000	0.130000	0.410000
25%	1.742500	1.205000	0.270000	1.250000
50%	2.355000	2.135000	0.340000	1.555000
75%	2.800000	2.875000	0.437500	1.950000
max	3.880000	5.080000	0.660000	3.580000

	Color intensity	Hue	OD280	Proline
count	178.000000	178.000000	178.000000	178.000000
mean	5.058090	0.957449	2.611685	746.893258
std	2.318286	0.228572	0.709990	314.907474
min	1.280000	0.480000	1.270000	278.000000
25%	3.220000	0.782500	1.937500	500.500000
50%	4.690000	0.965000	2.780000	673.500000

```
75%          6.200000     1.120000     3.170000    985.000000
max         13.000000     1.710000     4.000000   1680.000000
```

From the table above we can get that there are 178 instances of wine and 13 attributes and for each attribute, the distribution differ a lot. Then we are going to plot the scatter plot of the dataset `wine` as follow:

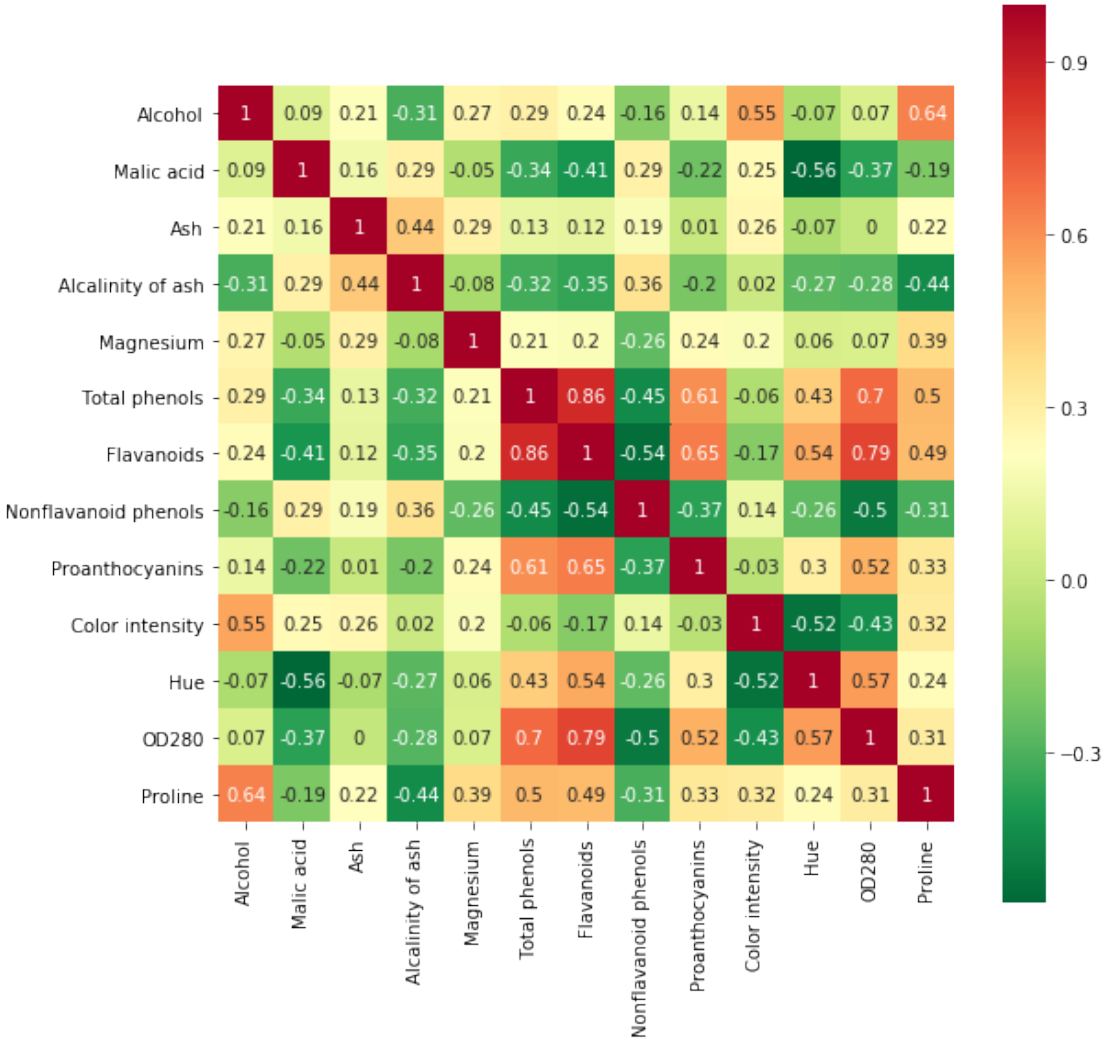
```
In [72]: # Scatter plot
         sm(wine, alpha = 0.7, figsize = (18,18))
         plt.show()
```



From the scatter plot, it's hard for us to cluster the data.

```
In [73]: # Correlation Heatmap
         correlation = wine.corr()
```

```
plt.subplots(figsize = (9,9))
sns.heatmap(correlation.round(2),
            annot = True,
            vmax = 1,
            square = True,
            cmap = 'RdYlGn_r')
plt.show()
```



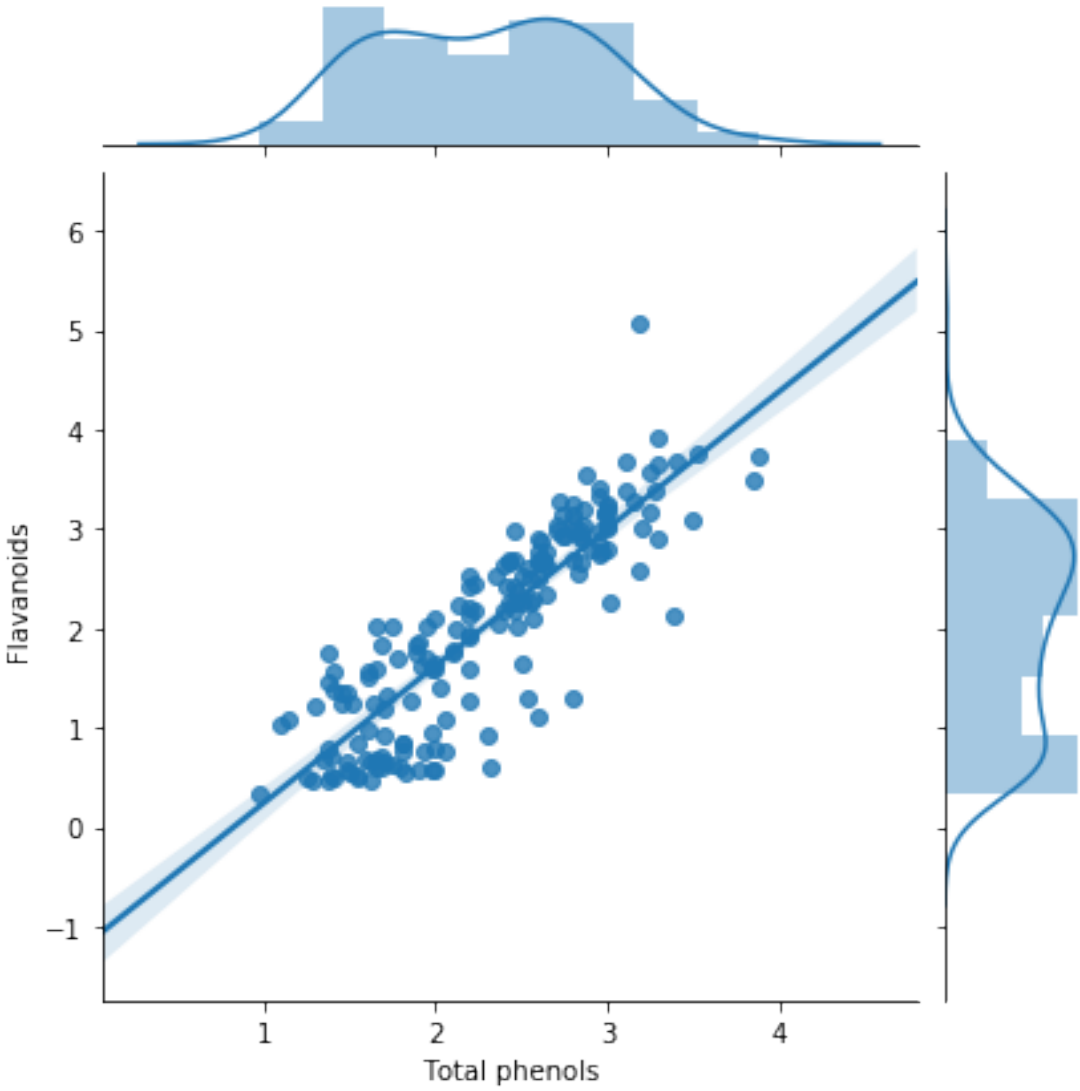
From the heatmap above, we can conclude that the correlation between

- "Flavanoids" and "Total phenols" (`0.86`);
- "OD280" and "Flavanoids" (`0.79`);
- "OD280" and "Total phenols" (`0.7`);

are large.
Then we can plot the regression of "Flavanoids" on "Total phenols" as follow:

In [74]:
```
# regression
sns.jointplot(x=wine.columns[5],
              y=wine.columns[6],
              data=wine,
              kind="reg");
plt.show()
```

```
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWar
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
```



2.1 Normalize data

We are going to normalize data by removing the mean and scaling to unit variance using `preprocessing.StandardScaler` and the table below show the general description statistics of normalized data.

```
In [75]: scaler = preprocessing.StandardScaler()
         scaler.fit(wine)
         X_scaled_array = scaler.transform(wine)
         winenorm = pd.DataFrame(X_scaled_array, columns = wine.columns)
         winenorm.head()
```

Out[75]:

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	\
0	1.518613	-0.562250	0.232053	-1.169593	1.913905	
1	0.246290	-0.499413	-0.827996	-2.490847	0.018145	
2	0.196879	0.021231	1.109334	-0.268738	0.088358	
3	1.691550	-0.346811	0.487926	-0.809251	0.930918	
4	0.295700	0.227694	1.840403	0.451946	1.281985	

	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins	\
0	0.808997	1.034819	-0.659563	1.224884	
1	0.568648	0.733629	-0.820719	-0.544721	
2	0.808997	1.215533	-0.498407	2.135968	
3	2.491446	1.466525	-0.981875	1.032155	
4	0.808997	0.663351	0.226796	0.401404	

	Color intensity	Hue	OD280	Proline
0	0.251717	0.362177	1.847920	1.013009
1	-0.293321	0.406051	1.113449	0.965242
2	0.269020	0.318304	0.788587	1.395148
3	1.186068	-0.427544	1.184071	2.334574
4	-0.319276	0.362177	0.449601	-0.037874

3 K-Means Clustering

In this part, we are going to cluster the `winenorm` dataset using K-Means method. The KMeans algorithm clusters data by trying to separate samples in `n` groups of equal variance, minimizing a criterion known as the **inertia** or within-cluster sum-of-squares (WSS).

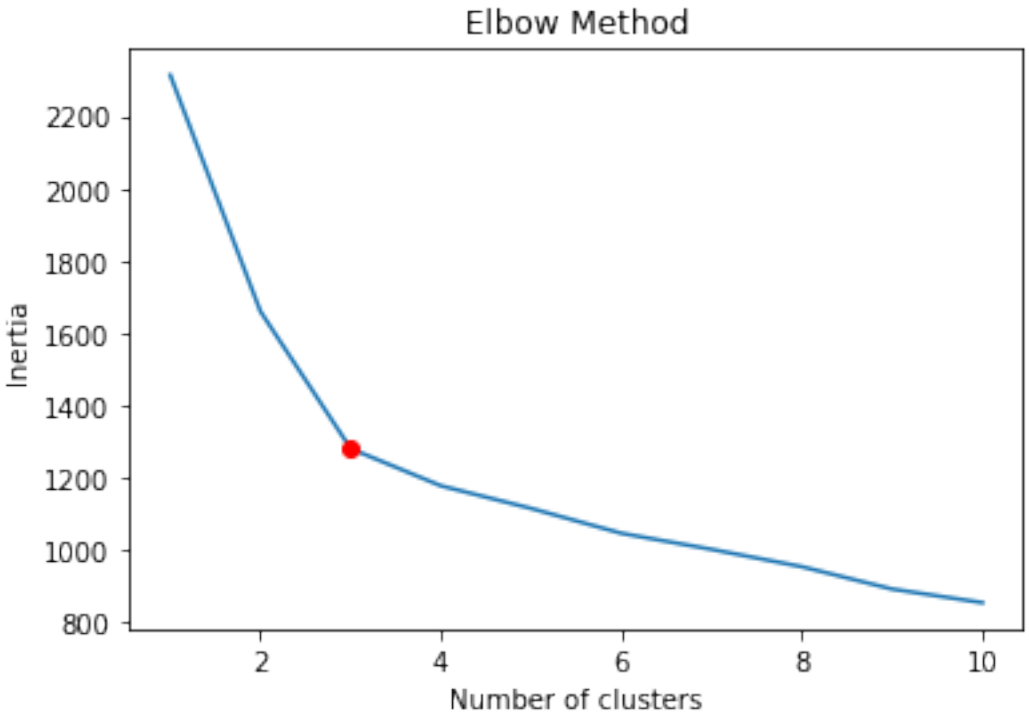
3.1 Choosing number of cluster

3.1.1 Elbow Method

First of all, we are going to choose the number of cluster by elbow method.

Inertia is sum of squared distances of samples to their closest cluster center. And the Elbow method looks at the inertia as a function of the number of clusters. One should choose a number of clusters so that adding another cluster doesn't improve much better the inertia.

```
In [76]: #Elbow Method
         seed = 0
         elbow = dict()
         for k in range(1,11):
             estimator = KMeans(n_clusters = k,random_state=seed)
             res = estimator.fit_predict(winenorm)
             inertia = estimator.inertia_
             elbow[k] = inertia

         elbow_df = pd.Series(elbow)
         ax = elbow_df.plot(title = 'Elbow Method')
         ax.set_xlabel('Number of clusters')
         ax.set_ylabel('Inertia')
         plt.plot(3,elbow_df[3],'ro')

Out[76]: [<matplotlib.lines.Line2D at 0x1a24e66d30>]
```



From the figure above, we can see that when the number of cluster is 3, it's hard to tell whether adding another cluster can improve much better the inertia or not.

3.1.2 Average silhouette method

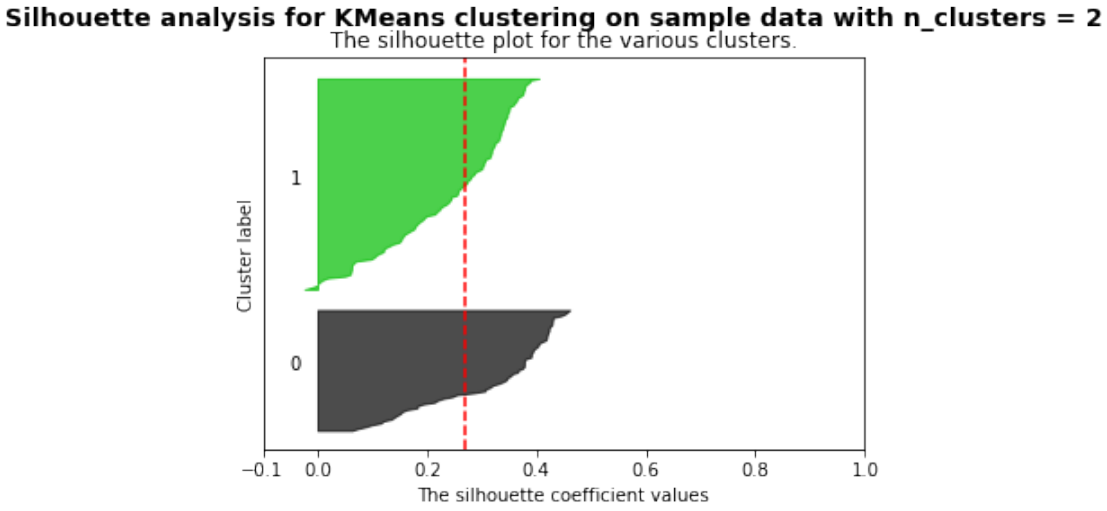
The Silhouette Score is calculated using the mean intra-cluster distance (`a`) and the mean nearest-cluster distance (`b`) for each sample. The Silhouette Coefficient for a sample is `(b - a) / max(a, b)`. It measures the quality of a clustering.

Average silhouette method computes the average silhouette of observations for different values of k. The optimal number of clusters k is the one that maximize the average silhouette over a range of possible values for k (Kaufman and Rousseeuw 1990).

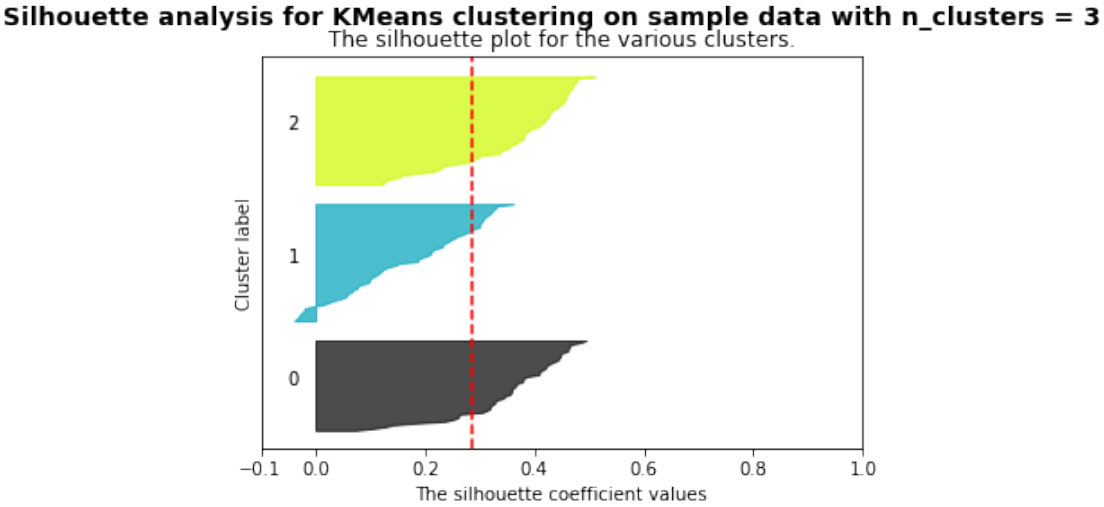
```
In [77]: # Silhouette Score Method
         seed = 0
         dict_silhouette_avg = dict()
         range_n_clusters = range(2,11)

         for n_clusters in range_n_clusters:
             fig, ax = plt.subplots()
             # The silhouette coefficient can range from -1, 1 but in this example all
             # lie within [-0.1, 1]
             ax.set_xlim([-0.1, 1])
             # The (n_clusters+1)*10 is for inserting blank space between silhouette
             # plots of individual clusters, to demarcate them clearly.
             ax.set_ylim([0, winenorm.shape[0] + (n_clusters + 1) * 10])

             estimator = KMeans(n_clusters = n_clusters,random_state=seed)
             cluster_labels = estimator.fit_predict(winenorm)

             # The silhouette_score gives the average value for all the samples.
             # This gives a perspective into the density and separation of the formed
             # clusters
             silhouette_avg = silhouette_score(winenorm,cluster_labels)
             print("For n_clusters =", n_clusters,
                   "The average silhouette_score is :", silhouette_avg)

             dict_silhouette_avg[n_clusters] = silhouette_avg

             # Compute the silhouette scores for each sample
             sample_silhouette_values = silhouette_samples(winenorm,cluster_labels)

             y_lower = 10
             for i in range(n_clusters):
                 # Aggregate the silhouette scores for samples belonging to
                 # cluster i, and sort them
                 ith_cluster_silhouette_values = \
                     sample_silhouette_values[cluster_labels == i]

                 ith_cluster_silhouette_values.sort()

                 size_cluster_i = ith_cluster_silhouette_values.shape[0]
                 y_upper = y_lower + size_cluster_i

                 color = cm.nipy_spectral(float(i) / n_clusters)
                 ax.fill_betweenx(np.arange(y_lower, y_upper),
                                  0, ith_cluster_silhouette_values,
```

```
                                      facecolor=color, edgecolor=color, alpha=0.7)

                # Label the silhouette plots with their cluster numbers at the middle
                ax.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))

                # Compute the new y_lower for next plot
                y_lower = y_upper + 10  # 10 for the 0 samples

            ax.set_title("The silhouette plot for the various clusters.")
            ax.set_xlabel("The silhouette coefficient values")
            ax.set_ylabel("Cluster label")

            # The vertical line for average silhouette score of all the values
            ax.axvline(x=silhouette_avg, color="red", linestyle="--")

            ax.set_yticks([])  # Clear the yaxis labels / ticks
            ax.set_xticks([-0.1, 0, 0.2, 0.4, 0.6, 0.8, 1])

            plt.suptitle(("Silhouette analysis for KMeans clustering on sample data "
                          "with n_clusters = %d" % n_clusters),
                         fontsize=14, fontweight='bold')

            plt.show()

        silhouette_df = pd.Series(dict_silhouette_avg)
        ax = silhouette_df.plot(title = 'Silhouette Score Method')
        ax.set_xlabel('Number of clusters')
        ax.set_ylabel('Silhouette Score')
        plt.plot(3,silhouette_df[3],'ro')
```

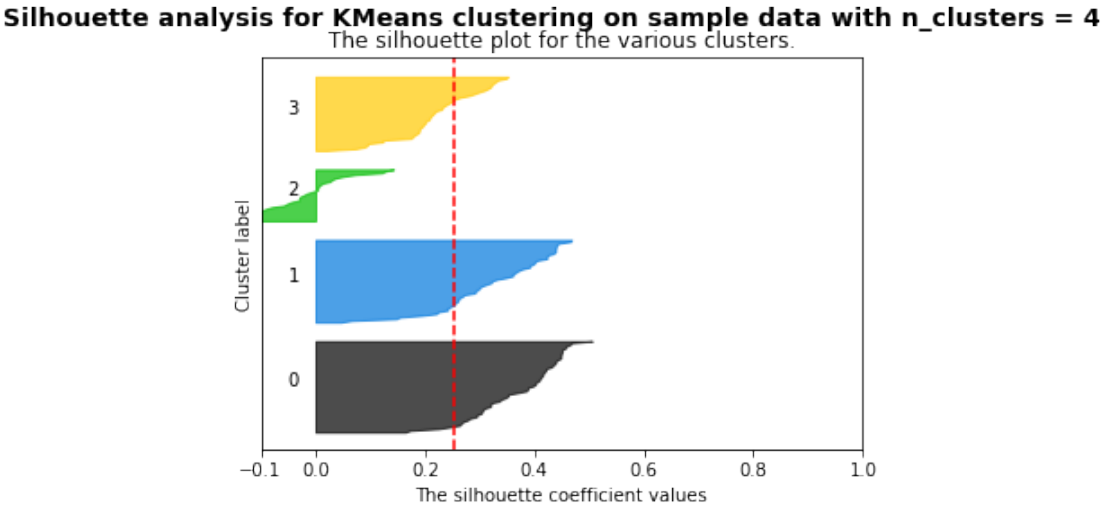
```
For n_clusters = 2 The average silhouette_score is : 0.2683134097105213
```



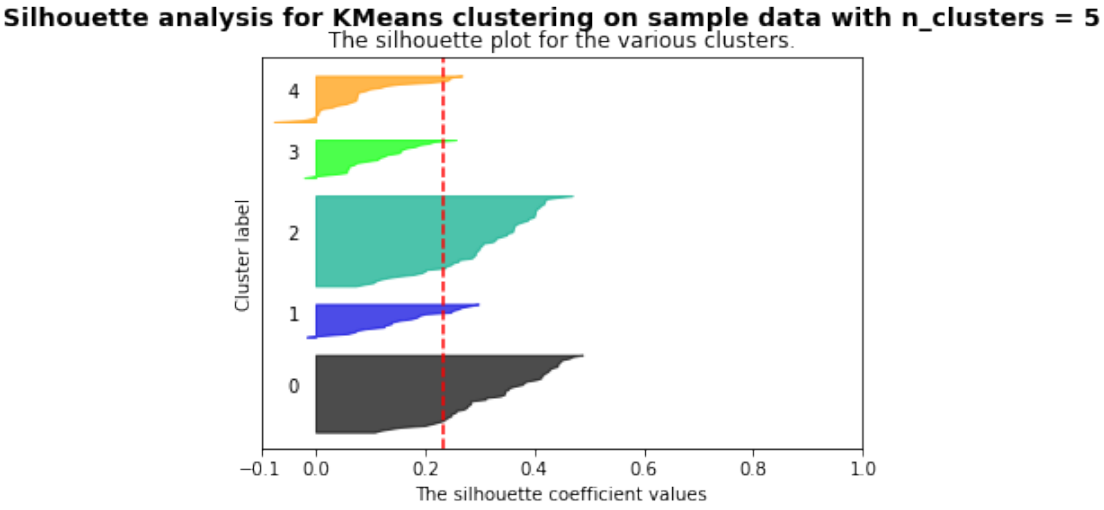
For n_clusters = 3 The average silhouette_score is : 0.28594199657074876



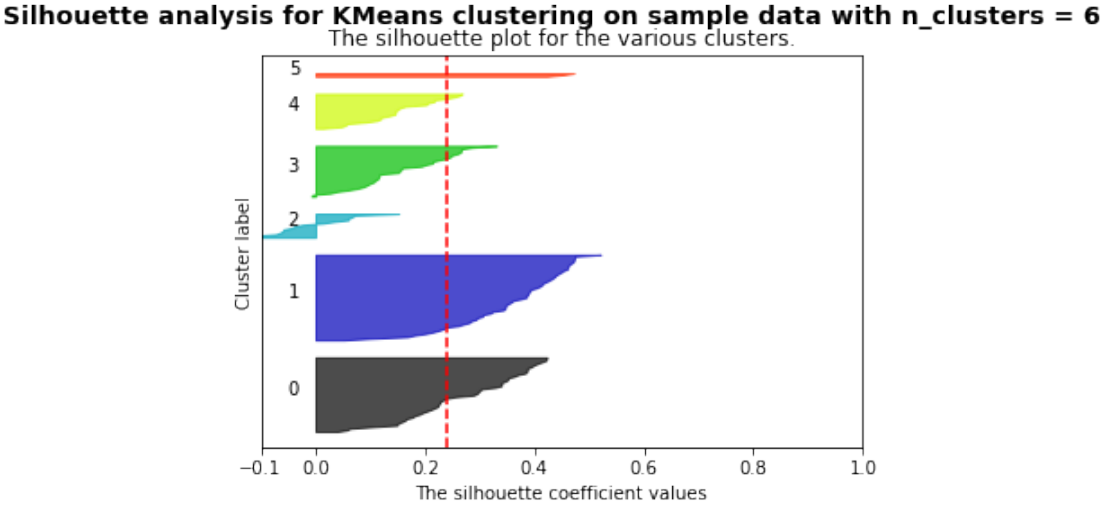
For n_clusters = 4 The average silhouette_score is : 0.25173343011696475



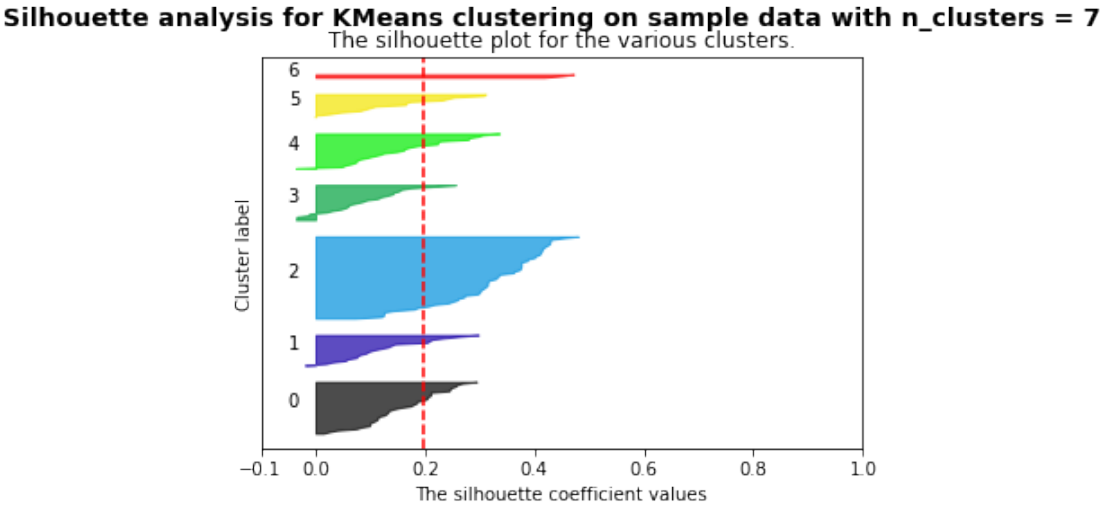
For n_clusters = 5 The average silhouette_score is : 0.23187479572412723



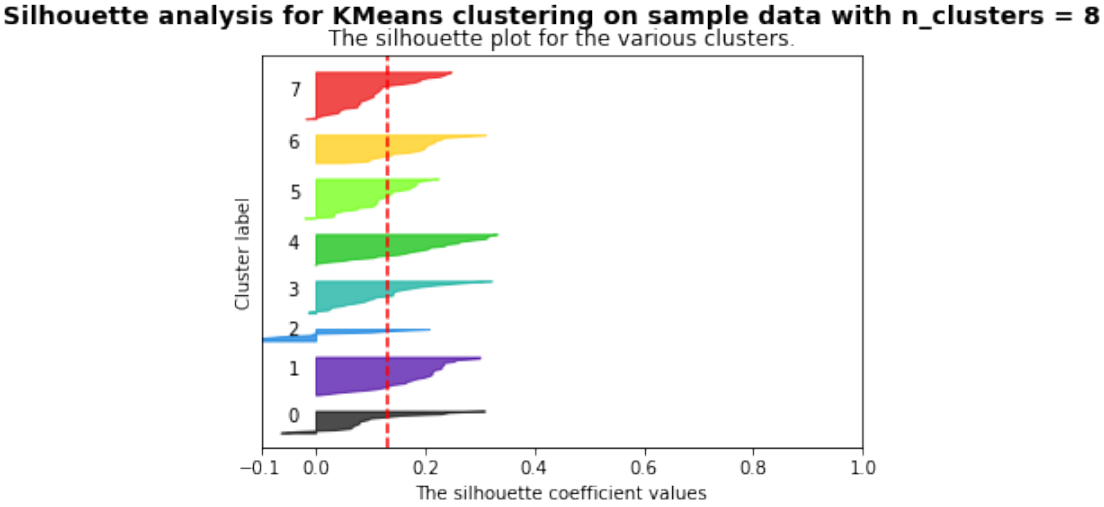

```
For n_clusters = 6 The average silhouette_score is : 0.23964277899912415
```



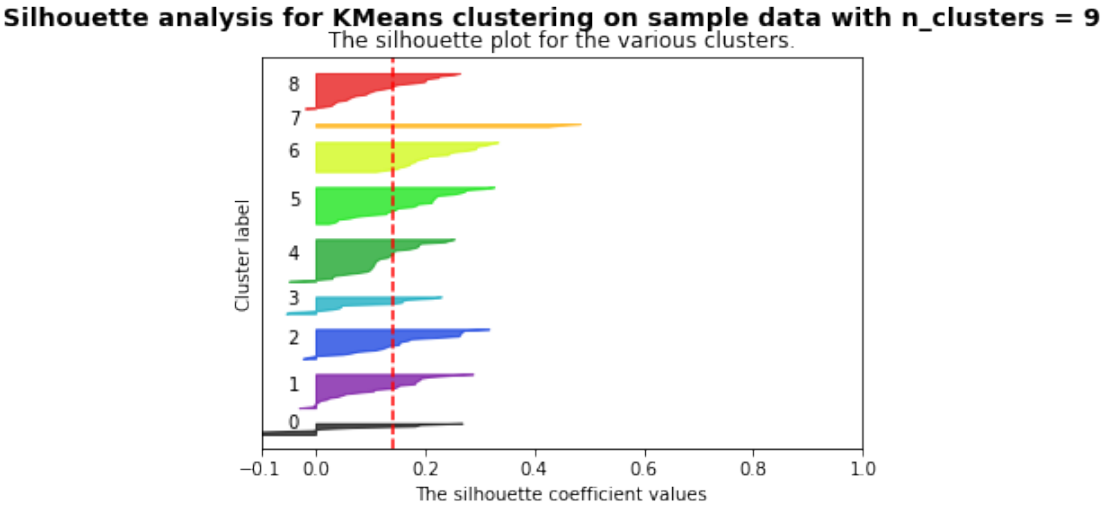

```
For n_clusters = 7 The average silhouette_score is : 0.1977124515910614
```



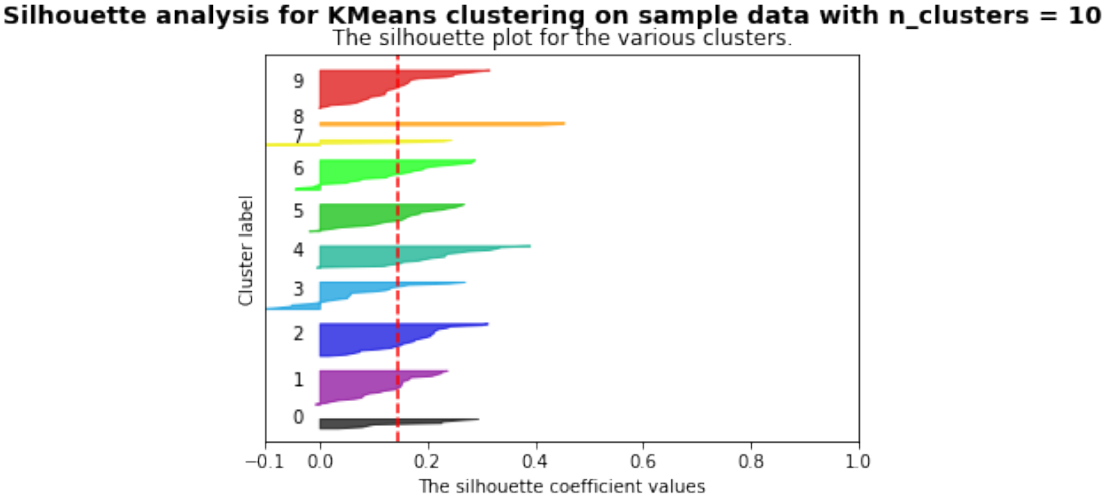

```
For n_clusters = 8 The average silhouette_score is : 0.133114891253478
```



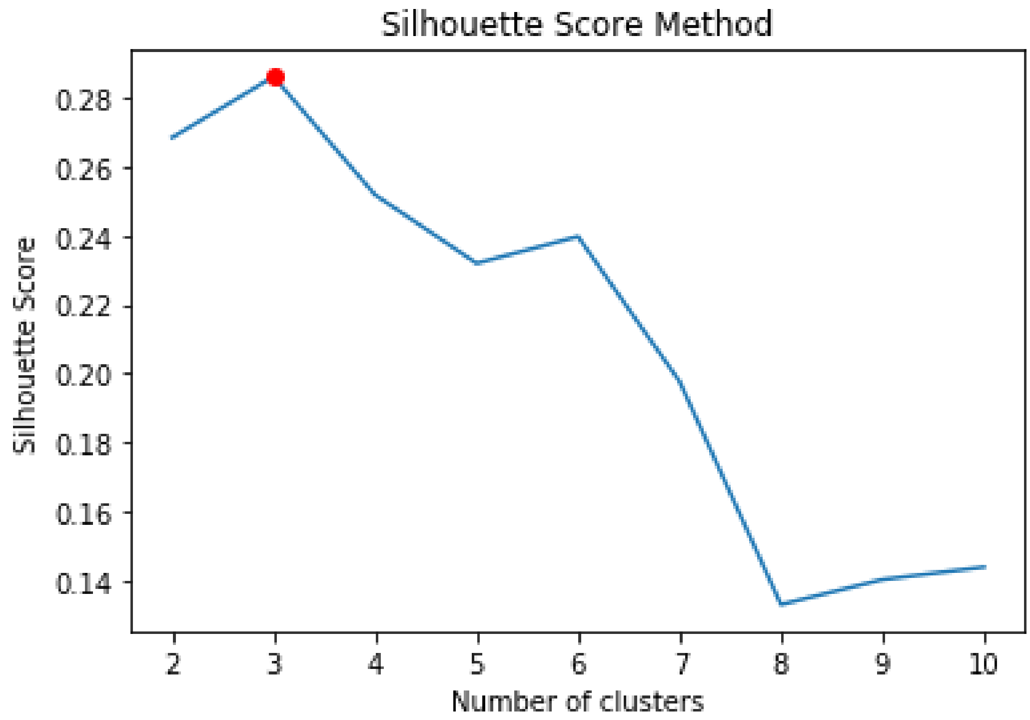

```
For n_clusters = 9 The average silhouette_score is : 0.14035373736325835
```




```
For n_clusters = 10 The average silhouette_score is : 0.14398677296462006
```




```
Out[77]: [<matplotlib.lines.Line2D at 0x1a25c977b8>]
```



From the figure above, we can see that when the number of cluster is 3, average silhouette score is maximized.

Thus we choose the number of cluster to be **3**.

3.2 K-Means

In [78]:
```
KM = KMeans(n_clusters = 3, random_state=seed)
res = KM.fit_predict(winenorm)

label_pred_KM = KM.labels_
print("Labels predicted by K-Means:",label_pred_KM)
print('Length of labels is same as data entry', label_pred_KM.shape)

centroids_KM= KM.cluster_centers_
print("Shape of centroids_KM",centroids_KM.shape)
print("Centroids:",centroids_KM)

inertia_KM = KM.inertia_
print("Inertia:",inertia_KM)
```

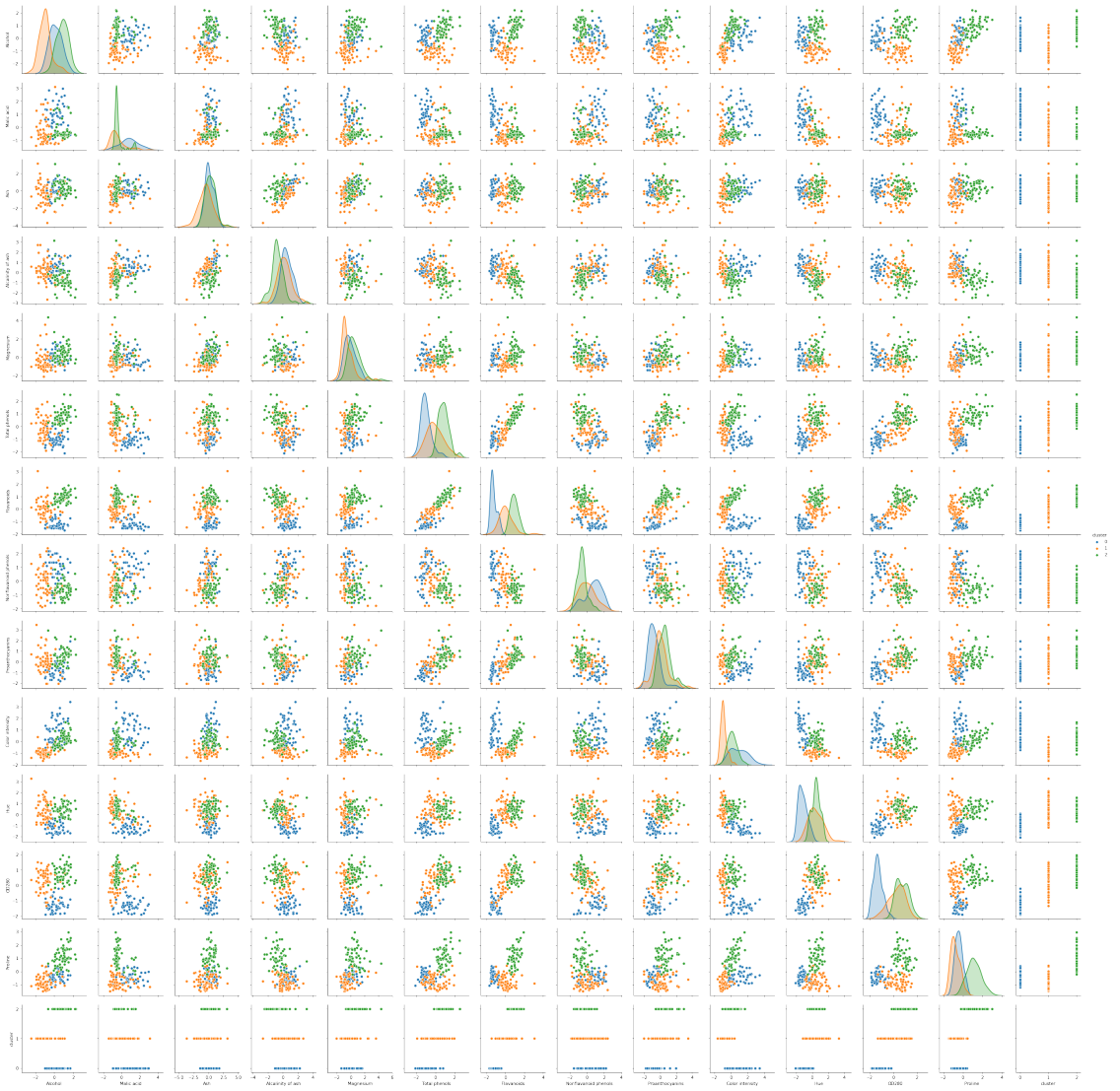
```
Labels predicted by K-Means: [2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 0 1 1 1 1 1 1 1 1 1 1 2
 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0 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]
```

```
Length of labels is same as data entry (178,)
Shape of centroids_KM (3, 13)
Centroids: [[ 0.16490746  0.87154706  0.18689833  0.52436746 -0.07547277 -0.97933029
  -1.21524764  0.72606354 -0.77970639  0.94153874 -1.16478865 -1.29241163
  -0.40708796]
 [-0.93900326 -0.39196582 -0.43920097  0.20898793 -0.46377382 -0.05334831
   0.06690377 -0.01982215  0.06479192 -0.88207529  0.45298189  0.28973833
  -0.75602559]
 [ 0.87809728 -0.30457633  0.31894179 -0.66452366  0.56488825  0.87650546
   0.94363903 -0.58558981  0.58178294  0.16718842  0.48372814  0.76705349
   1.15834713]]
Inertia: 1278.7607763668143
```

We can plot the pairwise relationships of `winenorm` with the colored label predicted bt K-Means method.

```
In [79]: # Pairplot
         winenorm['cluster'] = label_pred_KM.astype(str)
         sns_plot = sns.pairplot(winenorm, hue = "cluster")
```

```
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWar
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kde.py:488
  binned = fast_linbin(X, a, b, gridsize) / (delta * nobs)
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kdetools.p
  FAC1 = 2*(np.pi*bw/RANGE)**2
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/numpy/core/fromnumeric.py:83: Runtim
  return ufunc.reduce(obj, axis, dtype, out, **passkwargs)
```



4 Gaussian Mixture Model

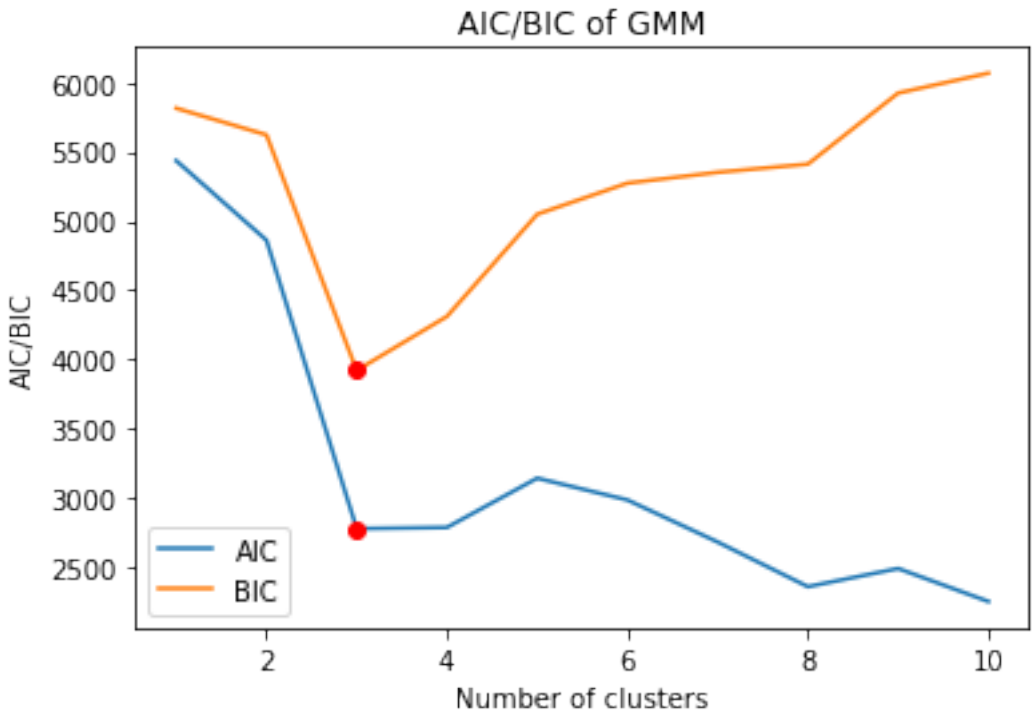
A Gaussian mixture model is a probabilistic model that assumes all the data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters. One can think of mixture models as generalizing k-means clustering to incorporate information about the covariance structure of the data as well as the centers of the latent Gaussians.

In this project, we take use of `GaussianMixture` from `sklearn` package. The `GaussianMixture` object implements the expectation-maximization (EM) algorithm for fitting mixture-of-Gaussian models.

4.1 Choosing number of cluster

We use Akaike information criterion (AIX) AND Bayesian information criterion (BIC) as criteria to select optimal number of clusters. The optimal number of clusters is the number that with minimum AIC/BIC.

```
In [80]: aic = dict()
         bic = dict()
         for k in range(1,11):
                 estimator = GaussianMixture(n_components = k, random_state=seed)
                 res = estimator.fit(winenorm)
                 ic1 = estimator.aic(winenorm)
                 ic2 = estimator.bic(winenorm)
                 aic[k] = ic1
                 bic[k] = ic2

         aic_df = pd.Series(aic)
         bic_df = pd.Series(bic)

         temp = {'AIC' : aic_df,
              'BIC' : bic_df}
         ic_df = pd.DataFrame(temp)
         ax = ic_df.plot(title='AIC/BIC of GMM')
         ax.set_xlabel('Number of clusters')
         ax.set_ylabel('AIC/BIC')
         plt.plot(3,aic_df[3],'ro')
         plt.plot(3,bic_df[3],'ro')

Out[80]: [<matplotlib.lines.Line2D at 0x1a1b6320b8>]
```



From the figure above, we can see that considering both AIC and BIC, the number of clusters should be **3**.

4.2 Gaussian Mixture Model

```
In [81]: GMM = GaussianMixture(n_components = 3, random_state=seed)
         res_GMM = GMM.fit(winenorm)

         weights_GMM = GMM.weights_
         print("Weights:",weights_GMM)
         means_GMM = GMM.means_
         print("Means:",means_GMM)
         covariance_GMM = GMM.covariances_
         print("Type of covariance_GMM:",type(covariance_GMM))
         covariance_GMM.size

         label_pred_GMM = GMM.predict(winenorm)
         print("Labels predicted by GMM:",label_pred_GMM)
         print('Length of labels is same as data entry', label_pred_GMM.shape)
```

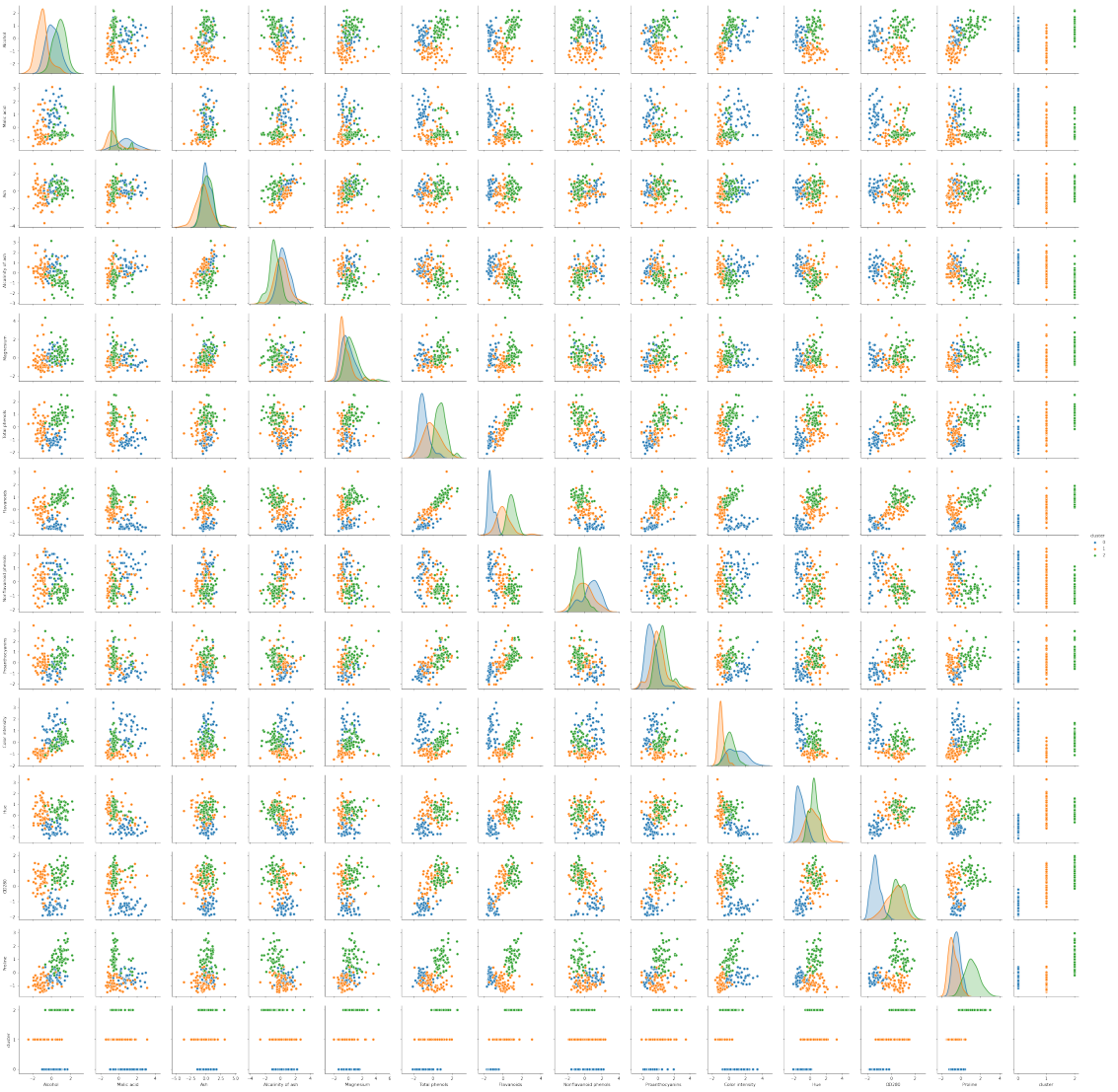
```
Weights: [0.28651685 0.37078652 0.34269663]
Means: [[ 0.16490746  0.87154706  0.18689833  0.52436746 -0.07547277 -0.97933029
  -1.21524764  0.72606354 -0.77970639  0.94153874 -1.16478865 -1.29241163
  -0.40708796  0.        ]
 [-0.93900326 -0.39196582 -0.43920097  0.20898793 -0.46377382 -0.05334831
```

```
   0.06690377 -0.01982215  0.06479192 -0.88207529  0.45298189  0.28973833
  -0.75602559  1.        ]
 [ 0.87809728 -0.30457633  0.31894179 -0.66452366  0.56488825  0.87650546
   0.94363903 -0.58558981  0.58178294  0.16718842  0.48372814  0.76705349
   1.15834713  2.        ]]
Type of covariance_GMM: <class 'numpy.ndarray'>
Labels predicted by GMM: [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 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 1 0 1 1 1 1 1 1 1 1 1 1 1 2
 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 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]
Length of labels is same as data entry (178,)
```

We can plot the pairwise relationships of `winenorm` with the colored label predicted bt GMM method.

```
In [82]: winenorm['cluster'] = label_pred_GMM.astype(str)
         sns_plot = sns.pairplot(winenorm, hue = "cluster")
         #sns_plot.fig.suptitle("Pair ploy",fontsize=14, fontweight='bold')
```

```
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWar
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kde.py:488
  binned = fast_linbin(X, a, b, gridsize) / (delta * nobs)
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kdetools.p
  FAC1 = 2*(np.pi*bw/RANGE)**2
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/numpy/core/fromnumeric.py:83: Runtim
  return ufunc.reduce(obj, axis, dtype, out, **passkwargs)
```



5 Principal component analysis (PCA)

We can take use of PCA to reduce the dimension of dataset.

First of all, we are going to generate the 13 Principal Component (PA) of `winenorm` and check the amount and percentage of of variance explained by each of the selected components.

Then we will compute the singular values corresponding to each of the selected components.

```
In [83]: pca = PCA(random_state=seed)
         pca.fit(winenorm)
         winenorm_pca_array = pca.transform(winenorm)
         winenorm_pca = pd.DataFrame(winenorm_pca_array)
         print("Heads of wine_pca:",winenorm_pca.head())
         var_ratio = pca.explained_variance_ratio_
```

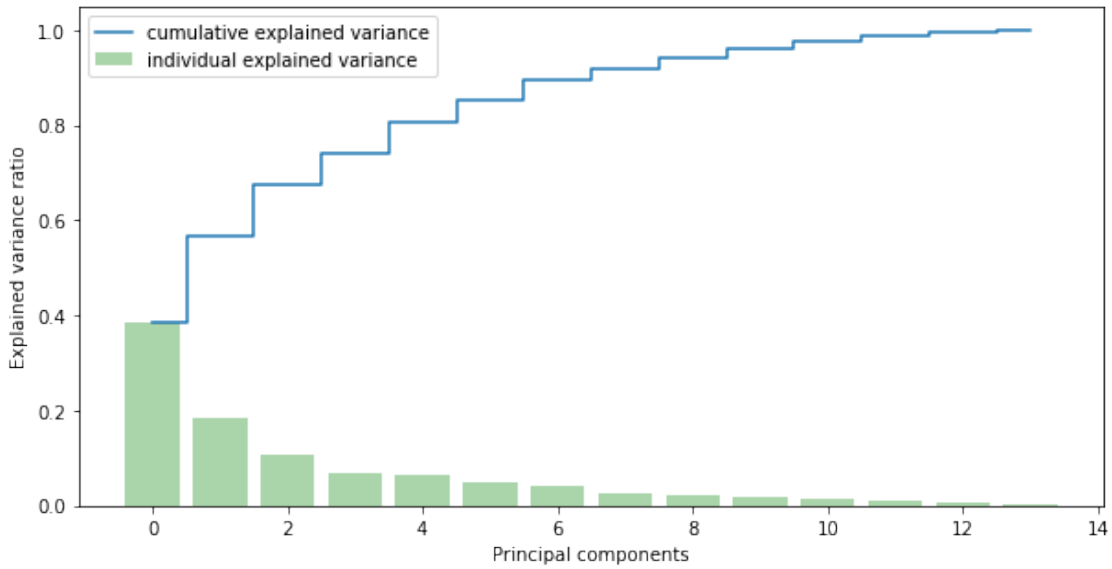
```
        print("Explained variance ratio:",var_ratio)
        sv = pca.singular_values_
        print("Singular Value:",sv)
```

```
Heads of wine_pca:          0         1         2         3         4         5         6   \
0 -3.445737 -1.443130 -0.181606 -0.141619  0.719226 -0.240562  0.571670
1 -2.399645  0.333539 -2.023331 -0.354329 -0.283459 -0.921755 -0.004363
2 -2.686493 -1.030953  0.973409  0.723016 -0.287199  0.496867  0.469883
3 -3.857784 -2.755956 -0.199499  0.592766 -0.306355  0.206030 -0.396391
4 -1.269236 -0.869910  2.039425 -0.427416  0.282081 -0.490755  0.436707

         7         8         9         10        11        12        13
0  0.064579  0.549366  1.007244 -0.510315  0.545838 -0.186642  0.264037
1  1.024387 -0.304723  0.082853 -0.158046  0.389511 -0.017982  0.016434
2 -0.342358 -1.188758 -0.047627 -0.302089  0.001309  0.016720 -0.026927
3  0.643198  0.046618  0.218324  0.734152 -0.236909 -0.463075  0.160431
4  0.416815  0.305063  0.004782 -0.505114 -0.221073  0.077981 -0.459326
Explained variance ratio: [0.38437002 0.18324992 0.10619816 0.06783278 0.06301955 0.04841391
 0.04060422 0.02557596 0.02141561 0.01900477 0.01659105 0.01238654
 0.00812535 0.00321217]
Singular Value: [30.53302679 21.08225212 16.04920758 12.82669951 12.36325291 10.83627938
  9.92386178  7.87609726  7.20709619  6.78932262  6.34354462  5.48113044
  4.43931631  2.79121988]
```

5.1 Plot out the cumulative explained variance ratio

We are going to plot the cumulative explained variance ratio for each PCs.

```
In [84]: plt.figure(figsize=(10, 5))
         plt.bar(range(len(var_ratio)),
                 var_ratio,
                 alpha=0.3333,
                 align='center',
                 label='individual explained variance',
                 color = 'g')
         plt.step(range(len(cum_var_ratio)),
                  cum_var_ratio,
                  where='mid',
                  label='cumulative explained variance')
         plt.ylabel('Explained variance ratio')
         plt.xlabel('Principal components')
         plt.legend(loc='best')
         plt.show()

         cum_var_ratio = np.cumsum(var_ratio)
         print("Cumulative explained ratio:",cum_var_ratio)
```




```
Cumulative explained ratio: [0.38437002 0.56761994 0.67381809 0.74165087 0.80467042 0.85308434
 0.89368856 0.91926452 0.94068013 0.9596849  0.97627595 0.98866249
 0.99678783 1.        ]
```

From the figure above, we can get that

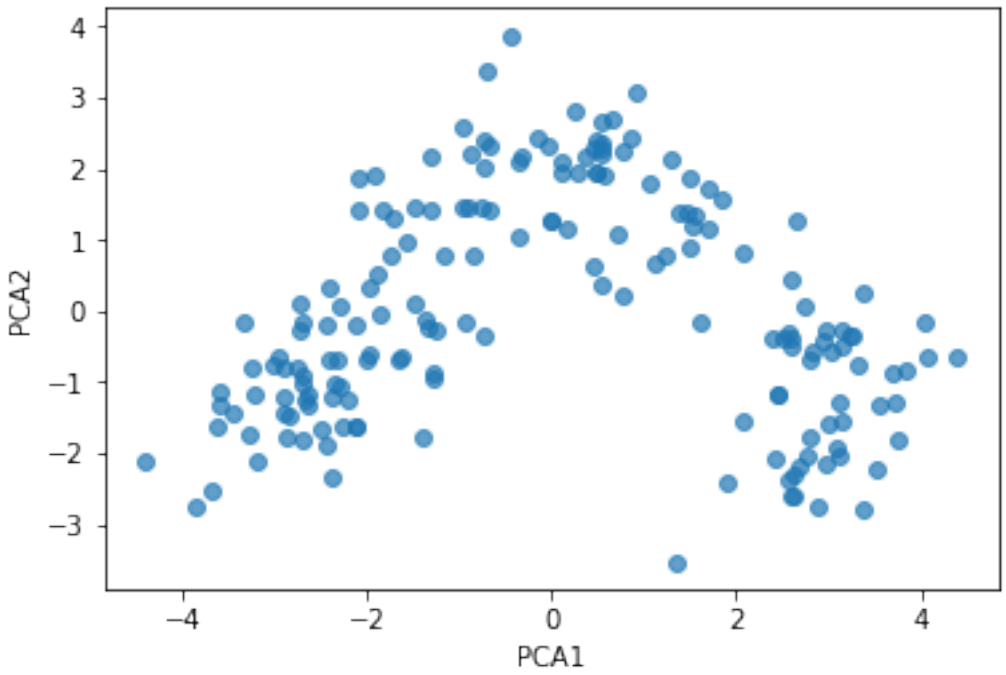
- the first two PCs explain 55.4% of variance;
- the first six PCs explain 85.1% of variance;

5.2 Plot top two principal components

For the convenience of visualization, we choose the top two PCs in this part and plot the scatter plot with colored labels predicted by both K-Mean method and GMM method.

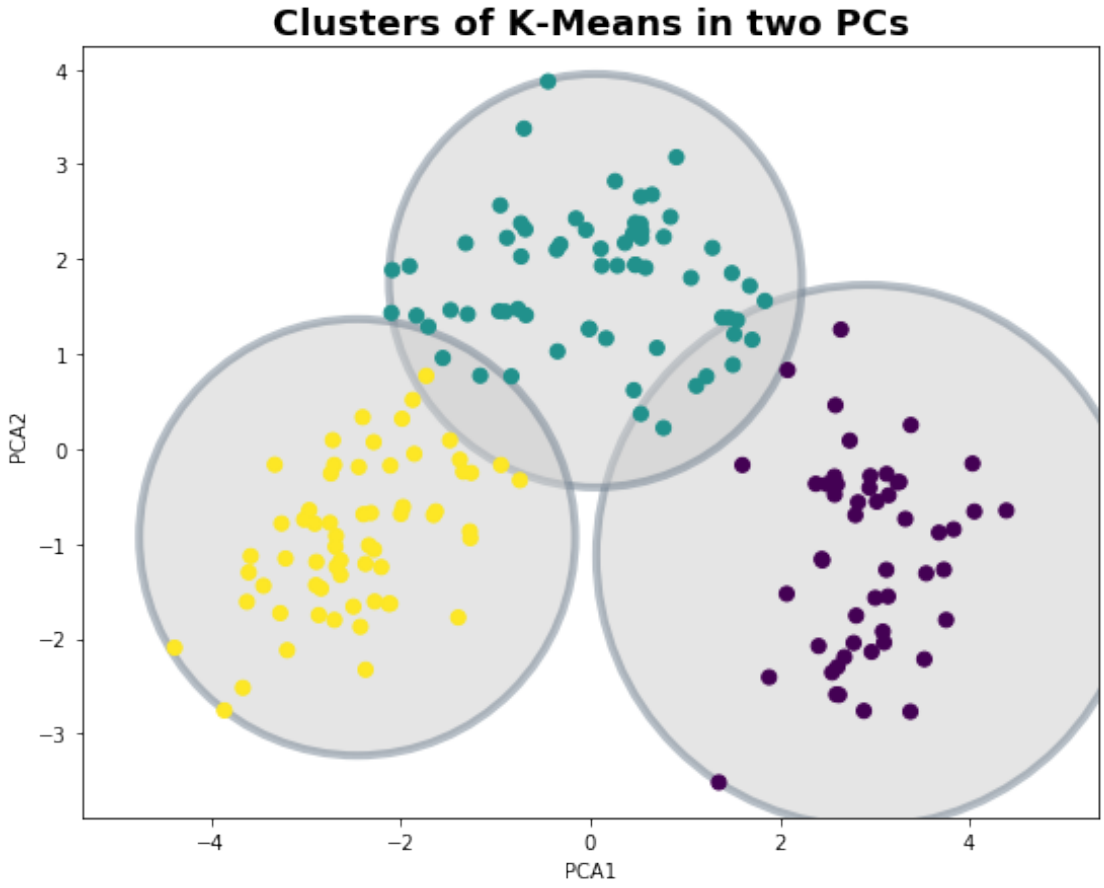
```
In [89]: pca = PCA(n_components=2, random_state=seed)
         pca.fit(winenorm)
         winenorm_pca_array = pca.transform(winenorm)
         winenorm_PCA = pd.DataFrame(winenorm_pca_array)
         plt.scatter(x=winenorm_PCA.iloc[:,0],
                     y=winenorm_PCA.iloc[:,1],
                     alpha = 0.7)
         plt.ylabel('PCA2')
         plt.xlabel('PCA1')
         plt.show()

         # KM
         KM = KMeans(n_clusters = 3, random_state=seed)
```

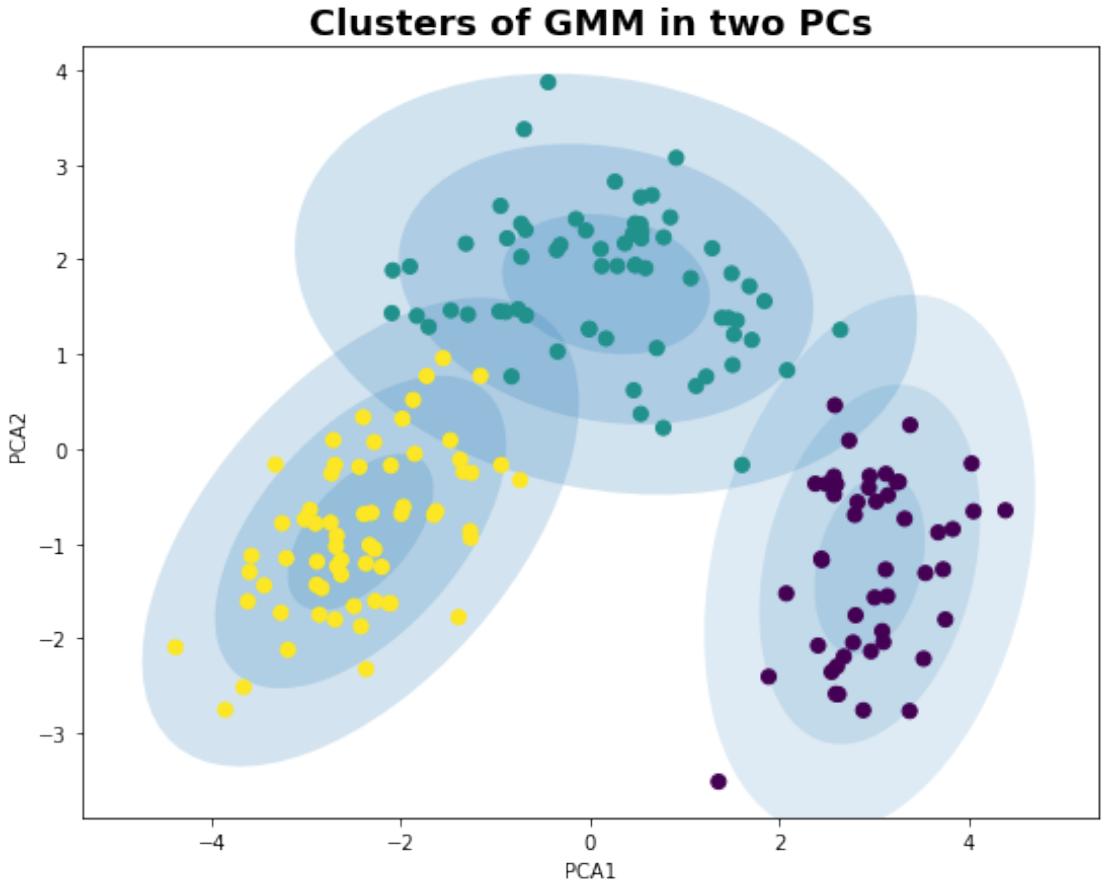
```
res_KM_PCA = KM.fit(winenorm_PCA)
label_pred_KM_PCA = KM.predict(winenorm_PCA)
plot_kmeans(KM, winenorm_PCA.as_matrix(),n_clusters=3)
plt.ylabel('PCA2')
plt.xlabel('PCA1')
plt.title('Clusters of K-Means in two PCs', fontsize=18, fontweight='demi')
# GMM
GMM = GaussianMixture(n_components = 3, random_state=seed)
res_GMM_PCA = GMM.fit(winenorm_PCA)
label_pred_GMM_PCA = GMM.predict(winenorm_PCA)
plot_gmm(GMM, winenorm_PCA.as_matrix())
plt.ylabel('PCA2')
plt.xlabel('PCA1')
plt.title('Clusters of GMM in two PCs', fontsize=18, fontweight='demi')
```




```
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/ipykernel_launcher.py:16: FutureWarn
  app.launch_new_instance()
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/ipykernel_launcher.py:24: FutureWarn
```

```
Out[89]: Text(0.5,1,'Clusters of GMM in two PCs')
```


Clusters of K-Means in two PCs
PCA2
PCA1
4
3
2
1
0
−1
−2
−3
−4
−2
0
2
4



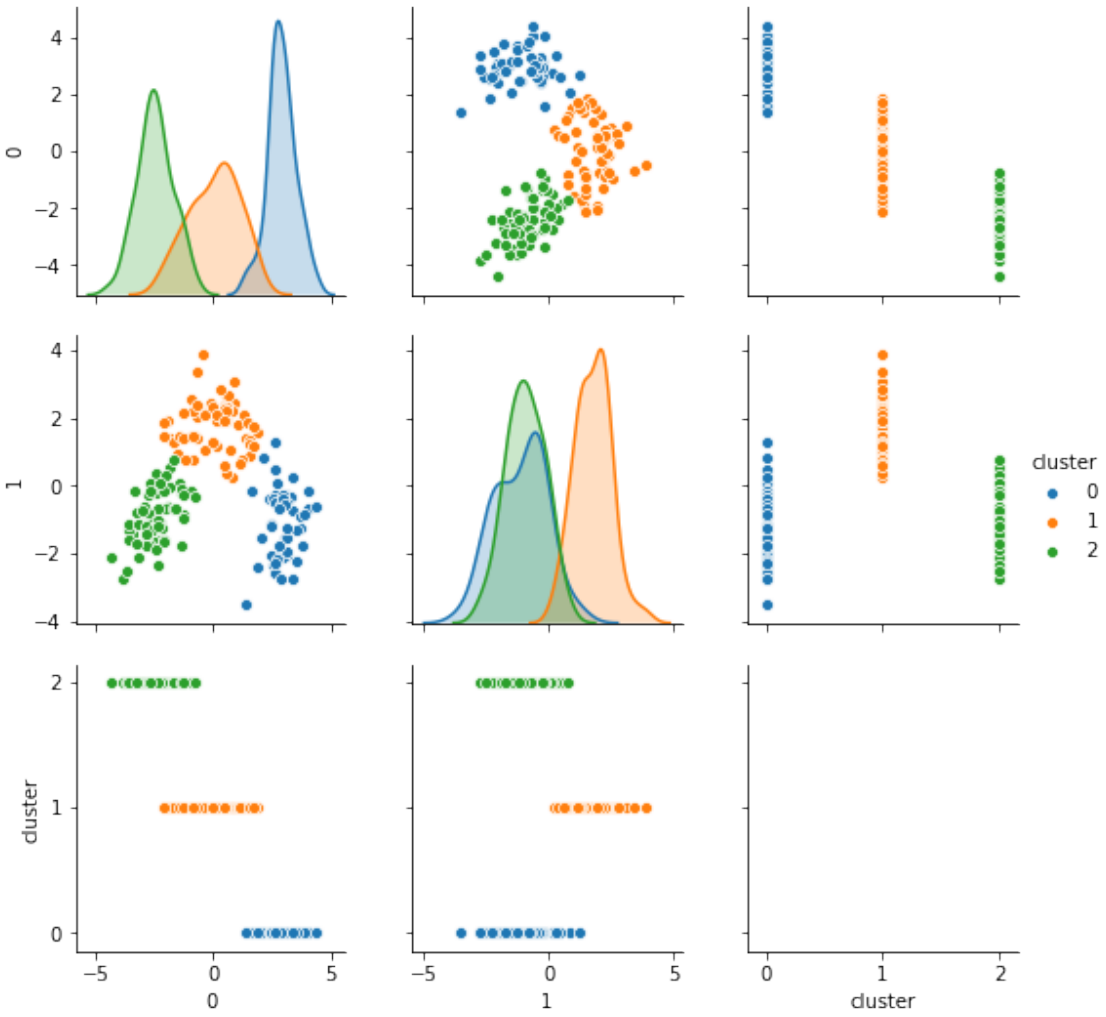
From the above three figures, we can easily figure out how K-Means and GMM method cluster the data.

Then we are going to plot the pair plots for the two PCs.

For the K-Means method:

```
In [90]: # Pairploy
         ## KM
         winenorm_PCA['cluster'] = label_pred_KM_PCA.astype(str)
         sns_plot = sns.pairplot(winenorm_PCA, hue = "cluster")
```

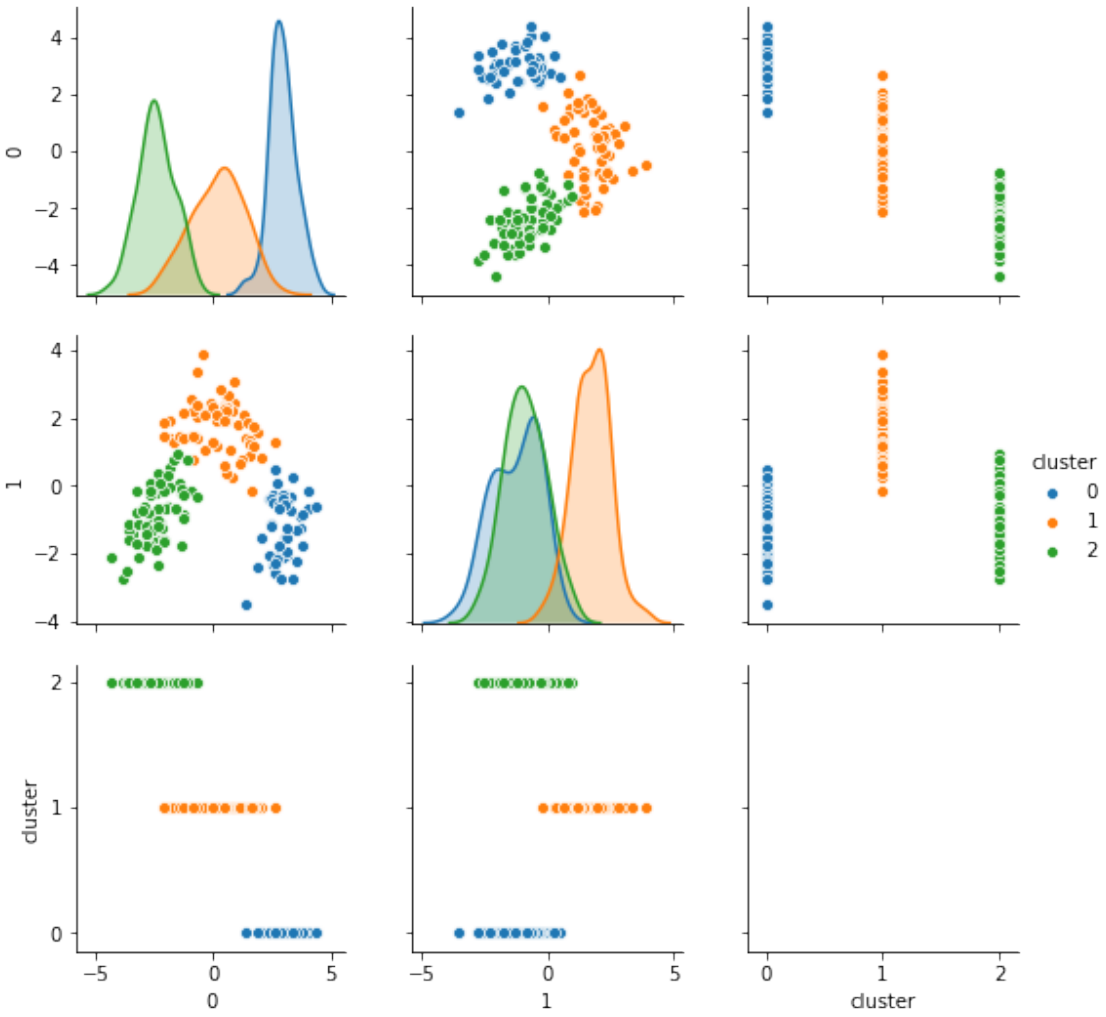
```
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWar
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kde.py:488
  binned = fast_linbin(X, a, b, gridsize) / (delta * nobs)
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kdetools.p
  FAC1 = 2*(np.pi*bw/RANGE)**2
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/numpy/core/fromnumeric.py:83: Runtim
  return ufunc.reduce(obj, axis, dtype, out, **passkwargs)
```



And for the GMM method:

```
In [91]: ## GMM
         winenorm_PCA['cluster'] = label_pred_GMM_PCA.astype(str)
         sns_plot = sns.pairplot(winenorm_PCA, hue = "cluster")
```

```
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWar
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kde.py:488
  binned = fast_linbin(X, a, b, gridsize) / (delta * nobs)
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kdetools.p
  FAC1 = 2*(np.pi*bw/RANGE)**2
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/numpy/core/fromnumeric.py:83: Runtim
  return ufunc.reduce(obj, axis, dtype, out, **passkwargs)
```



6 PCA and Cluster

In this part, we are going to select top six principal components and transform the dataset `winenorm`. Then we are going to run K-Means and GMM model on this dimension reduced dataset.

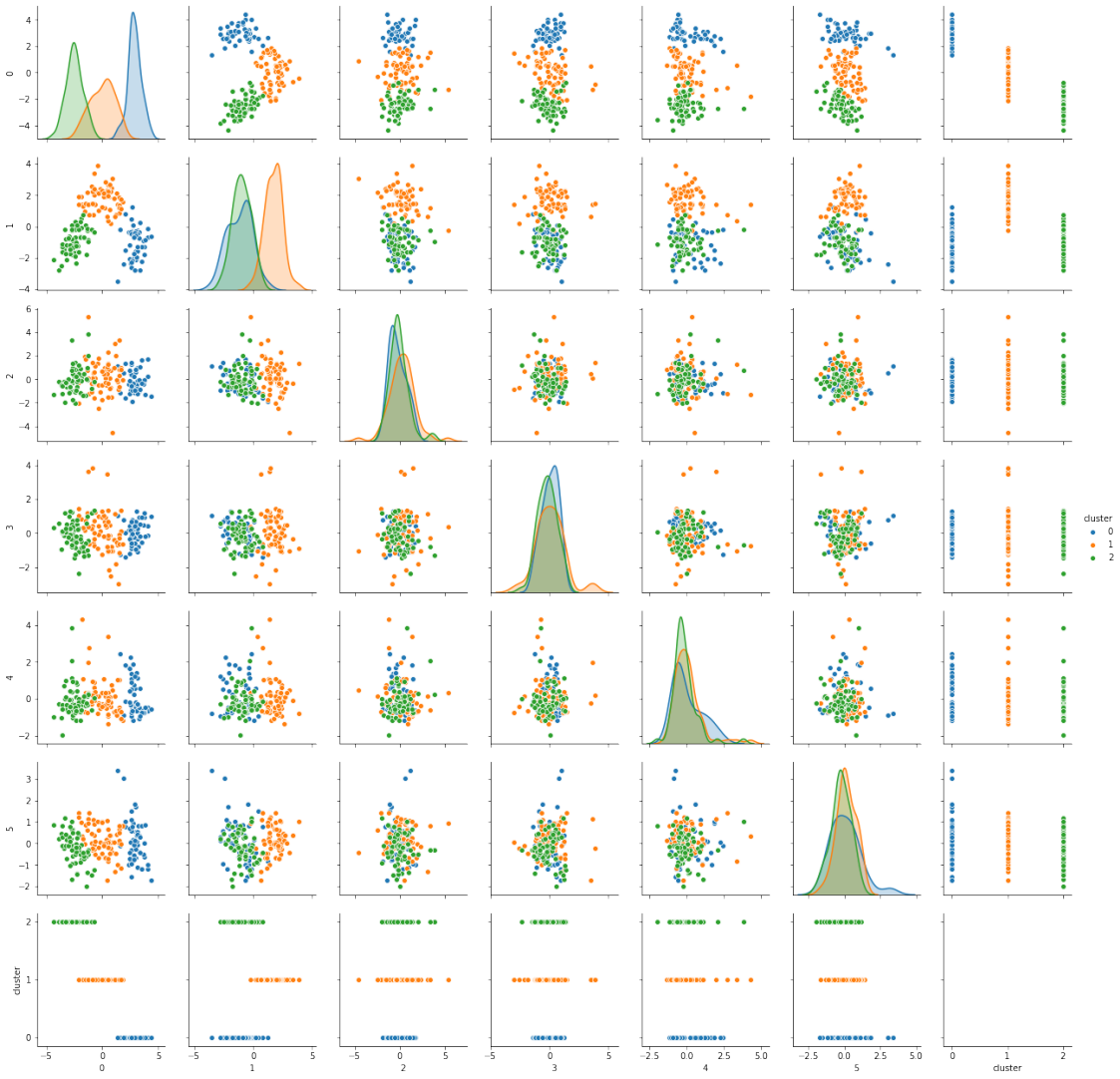
```
In [92]: # we slecte six components
         pca = PCA(n_components = 6, random_state=seed)
         pca.fit(winenorm)
         winenorm_pca_array = pca.transform(winenorm)
         winenorm_PCA = pd.DataFrame(winenorm_pca_array)
         var_ratio = pca.explained_variance_ratio_
         print("Sum of top 6 PCs:",sum(var_ratio[0:5]))

         # K-Means + PCA
         KM = KMeans(n_clusters = 3, random_state=seed)
```

```
        res = KM.fit(winenorm_PCA)
        label_pred_KM_PCA = KM.predict(winenorm_PCA)
        print("Labels predicted by KM+PCA:",label_pred_KM_PCA)

        # GMM + PCA
        GMM = GaussianMixture(n_components = 3, random_state=seed)
        res_GMM = GMM.fit(winenorm_PCA)
        label_pred_GMM_PCA = GMM.predict(winenorm_PCA)
        print("Labels predicted by GMM+PCA:",label_pred_KM_PCA)
```

```
Sum of top 6 PCs: 0.8046704240372956
Labels predicted by KM+PCA: [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 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 1 0 1 1 1 1 1 1 1 1 1 1 1 2
 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 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]
Labels predicted by GMM+PCA: [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 2 2
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 0 1 1 1 1 1 1 1 1 1 1 1 2
 1 1 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1 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]
```

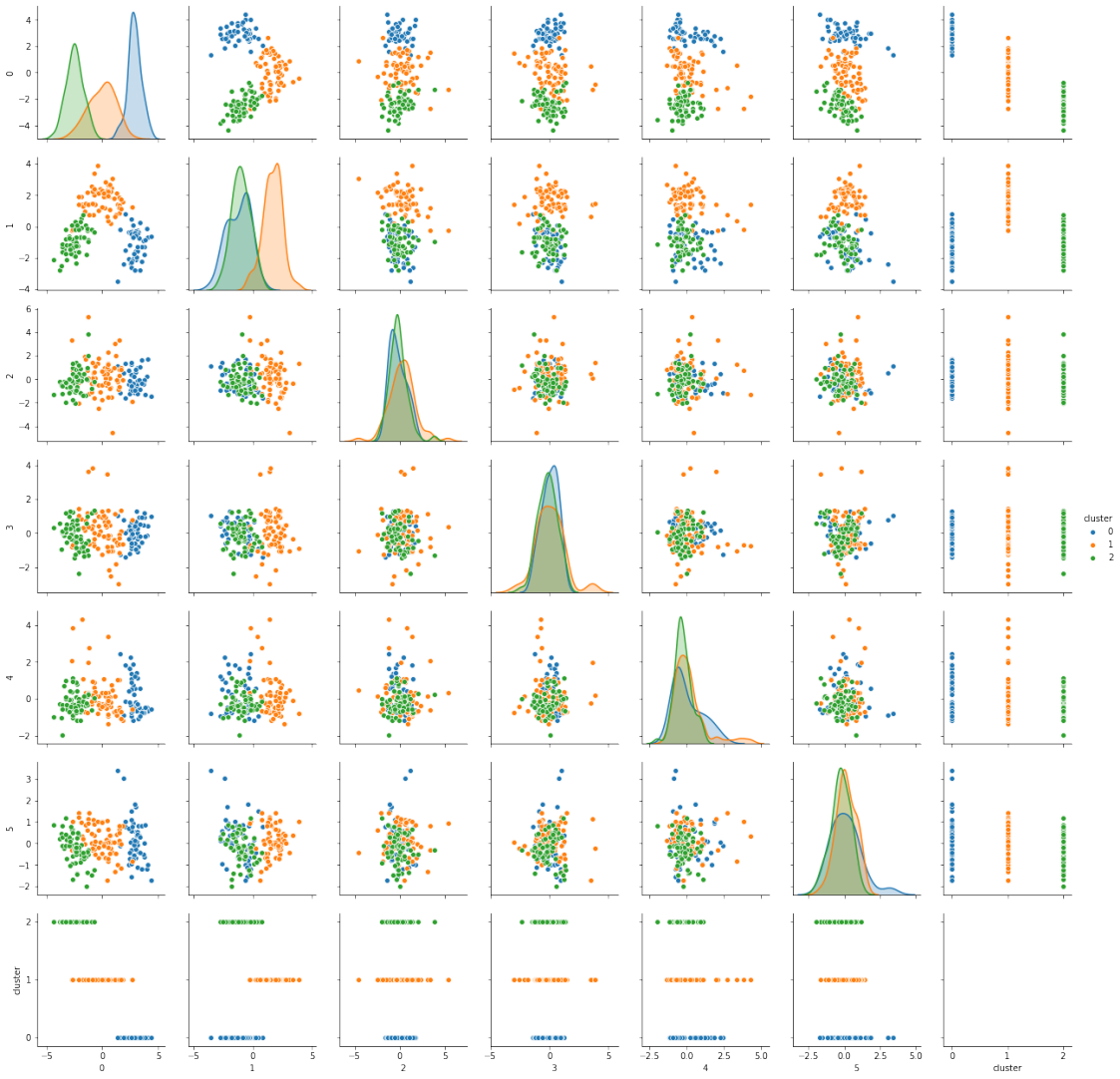
```
In [93]: # Pairplot of KM
        winenorm_PCA['cluster'] = label_pred_KM_PCA.astype(str)
        sns_plot = sns.pairplot(winenorm_PCA, hue = "cluster")
```

```
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWar
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kde.py:488
  binned = fast_linbin(X, a, b, gridsize) / (delta * nobs)
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kdetools.p
  FAC1 = 2*(np.pi*bw/RANGE)**2
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/numpy/core/fromnumeric.py:83: Runtim
  return ufunc.reduce(obj, axis, dtype, out, **passkwargs)
```




```
In [94]: # Pairplot of GMM
         winenorm_PCA['cluster'] = label_pred_GMM_PCA.astype(str)
         sns_plot = sns.pairplot(winenorm_PCA, hue = "cluster")
```

```
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWar
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kde.py:488
  binned = fast_linbin(X, a, b, gridsize) / (delta * nobs)
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/statsmodels/nonparametric/kdetools.p
  FAC1 = 2*(np.pi*bw/RANGE)**2
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/numpy/core/fromnumeric.py:83: Runtim
  return ufunc.reduce(obj, axis, dtype, out, **passkwargs)
```



7 Evaluation

7.1 Average Silhouette Score

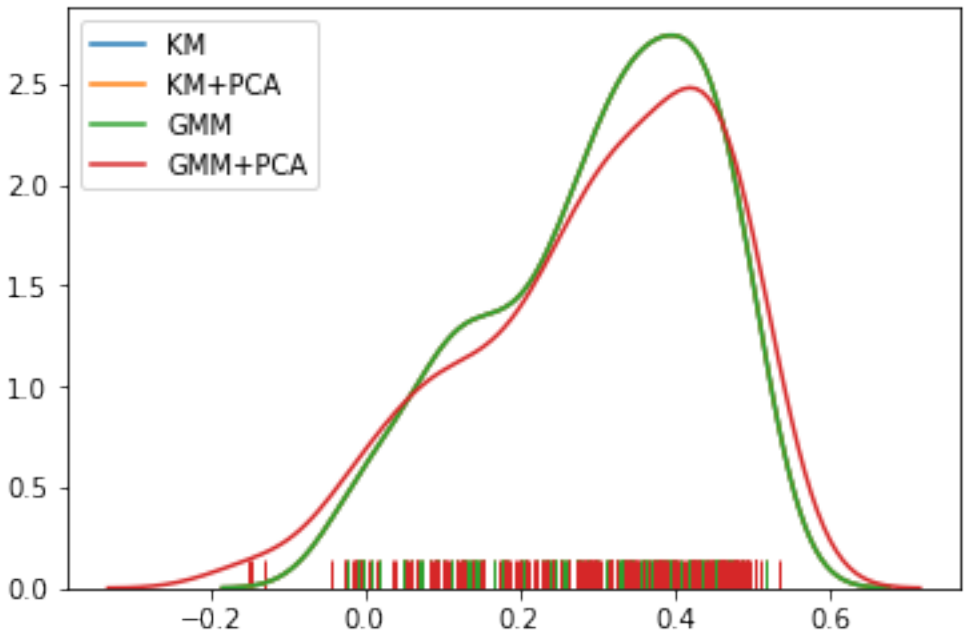
Firstly, we use Silihouette score to evaluate the K-Means (KM), Gaussian Mixture Model (GMM), KM+PCA, GMM+PCA methods.

```
In [95]: sh_score_KM = silhouette_score(winenorm, label_pred_KM)
         print("Silhouette score of cluster by KM:",sh_score_KM)
         sh_scores_KM = silhouette_samples(winenorm, label_pred_KM)
         p1=sns.distplot(sh_scores_KM, hist=False, rug=True,label = 'KM');

         sh_score_KM_PCA = silhouette_score(winenorm, label_pred_KM_PCA)
         print("Silhouette score of cluster by KM+PCA:",sh_score_KM_PCA)
```

```
sh_scores_KM_PCA = silhouette_samples(winenorm, label_pred_KM_PCA)
p2=sns.distplot(sh_scores_KM_PCA, hist=False, rug=True, label = 'KM+PCA');

sh_score_GMM = silhouette_score(winenorm, label_pred_GMM)
print("Silhouette score of cluster by GMM:",sh_score_GMM)
sh_scores_GMM = silhouette_samples(winenorm, label_pred_GMM)
p3=sns.distplot(sh_scores_GMM, hist=False, rug=True, label = 'GMM');

sh_score_GMM_PCA = silhouette_score(winenorm, label_pred_GMM_PCA)
print("Silhouette score of cluster by GMM+PCA:",sh_score_GMM_PCA)
sh_scores_GMM_PCA = silhouette_samples(winenorm, label_pred_GMM_PCA)
p4=sns.distplot(sh_scores_GMM_PCA, hist=False, rug=True, label = 'GMM+PCA');
```

```
Silhouette score of cluster by KM: 0.301135931311762
Silhouette score of cluster by KM+PCA: 0.301135931311762
Silhouette score of cluster by GMM: 0.301135931311762
Silhouette score of cluster by GMM+PCA: 0.29783451509126274
```

```
/Users/huwei/anaconda/envs/py36/lib/python3.6/site-packages/scipy/stats/stats.py:1713: FutureWar
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
```



According to the average Silhouette score, it is hard to decide which model is the best model with highest score value.

7.2 Rand index adjusted for chance

The Rand Index computes a similarity measure between two clusterings by considering all pairs of samples and counting pairs that are assigned in the same or different clusters in the predicted and true clusterings.

The raw RI score is then "adjusted for chance" into the ARI score using the following scheme:
`ARI = (RI - Expected_RI) / (max(RI) - Expected_RI)`

We compare the predicted label with true label provided. Thus the higher the Rand Index, the more precise the cluster is.

```
In [96]: ar_score_KM = adjusted_rand_score(label, label_pred_KM)
         print("Adjusted Rand Index of cluster by KM:",ar_score_KM)

         ar_score_KM_PCA = adjusted_rand_score(label, label_pred_KM_PCA)
         print("Adjusted Rand Index of cluster by KM+PCA:",ar_score_KM_PCA)

         ar_score_GMM = adjusted_rand_score(label, label_pred_GMM)
         print("Adjusted Rand Index of cluster by GMM:",ar_score_GMM)

         ar_score_GMM_PCA = adjusted_rand_score(label, label_pred_GMM_PCA)
         print("Adjusted Rand Index of cluster by GMM+PCA:",ar_score_GMM_PCA)
```

```
Adjusted Rand Index of cluster by KM: 0.9148795960669529
Adjusted Rand Index of cluster by KM+PCA: 0.9148795960669529
Adjusted Rand Index of cluster by GMM: 0.9148795960669529
Adjusted Rand Index of cluster by GMM+PCA: 0.9667411092064137
```

From the result above, we can conclude that the best model is GMM+PCA with the highest adjusted rand index value.