Coding part

Remark: This is a ipynb containing both Q2.1 and Q2.2

Q2.1

we import the packages we need to use

In [ ]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

k-means

The below code will define a function to achieve the k-means algorithm

In [ ]:
```
def kmeans(X, k, max_iters=1000):
    # randomly initialize centers
    centers = X[np.random.choice(X.shape[0], k, replace=False)]

    for _ in range(0,max_iters):
        # divide each point into the nearest center
        labels = np.argmin(np.linalg.norm(X[:, np.newaxis] - centers, axis=2), a

        # update centers
        new_centers = np.array([X[labels == i].mean(axis=0) for i in range(0,k)]

        # if convergence, break
        if np.all(centers == new_centers):
            break
        centers = new_centers
    return labels, centers
```

GMM

The below code will define a function to achieve the GMM algorithm

In [ ]:
```
from scipy.stats import multivariate_normal

def initialize_parameters(X, k):
    # randomly initialize means and use the whole covariance as covariance
    indices = np.random.choice(X.shape[0], k, replace=False)
    ini_means = X[indices]
    ini_covariances = [np.cov(X.T,bias = True) for _ in range(0,k)]
    ini_weights = np.ones(k) / k
    return ini_means, ini_covariances, ini_weights

def expectation_step(X, k, means, covariances, weights):
    # calculate the probability of each point belonging to each distribution
    likelihoods = [multivariate_normal.pdf(X, mean=means[i], cov=covariances[i])
```

```
    likelihoods = np.array(likelihoods)
    weights = weights.flatten()
    # calculate the responsibility of each distribution for each point
    responsibilities = (likelihoods.T * weights) / np.sum(likelihoods.T * weight
    return responsibilities


def maximization_step(X, k, responsibilities):
    # update means, covariances, and weights using responsibilities
    N_k = np.sum(responsibilities, axis=0)[:, np.newaxis]
    means = (responsibilities.T @ X) / N_k
    covariances = []
    for i in range(0,k):
        temp = ((X - means[i]).T @ (responsibilities[:, i:i+1] * (X - means[i]))
        # deal with the covariance matrix so that it will not treat the small da
        temp += 1e-6 * np.eye(len(temp))
        # temp = np.diagonal((responsibilities[:, i:i+1] * (X - means[i])).T @ (
        covariances.append(temp)
    covariances = np.array(covariances)
    weights = N_k / len(X)
    return means, covariances, weights

def gmm(X, k, max_iters=100):
    means, covariances, weights = initialize_parameters(X, k)
    # keep repeating e-step and m-step
    for _ in range(0,max_iters):
        responsibilities = expectation_step(X, k, means, covariances, weights)
        means, covariances, weights = maximization_step(X, k, responsibilities)
    labels = np.argmax(responsibilities, axis=1)
    return labels, means, covariances, weights
```

Silhouette Coefficient

The below code will define a function to calculate the silhouette coefficient

In [ ]:

```
def silhouette_coefficient(labels, X):
    sc = []
    for i in range(0,len(labels)):
        # find out distances towards different clustters and store them in a lis
        norm = np.zeros((len(labels),2))
        for l in range(0,i):
            norm[labels[l]][0] += np.linalg.norm(X[i] - X[l])
            norm[labels[l]][1] += 1
        for l in range(i+1,len(labels)):
            norm[labels[l]][0] += np.linalg.norm(X[i] - X[l])
            norm[labels[l]][1] += 1
        # distance = all the distance / numbers of points in the other clustter
        norm = norm[:,0:1] / norm[:,1:2]
        a = norm[labels[i]]
        norm = np.delete(norm, labels[i])
        # find out the smallest distance
        b = min(norm)
        s = (b-a)/max(a,b)
        sc.append(s)
    return np.mean(np.array(sc))
```

Random Index

The below code will define a function to calculate the random index

```
In [ ]: def rand_index(labels, Y):
            a = 0
            b = 0
            c = 0
            d = 0
            for i in range(0,len(labels)):
                Y=Y.flatten()
                current_label = labels[i]
                current_Y = Y[i]
                # calculating a, b, c, d
                for j in range(i+1,len(labels)):
                    if labels[j] == current_label:
                        if Y[j] == current_Y:
                            a+=1
                        else:
                            c+=1
                    else:
                        if Y[j] == current_Y:
                            d+=1
                        else:
                            b+=1
            ri = (a+b)/(a+b+c+d)
            # check out if it is correct
            # ri2 = 2*(a+b)/(len(labels)*(len(labels)-1))
            return ri
```

Normalized Mutual Information

The below code will define a function to calculate the normalized mutual information

```
In [ ]: # def a function to find out H(x) and H(y)
        def calculate_entropy(labels):
            _, counts = np.unique(labels, return_counts=True)
            probabilities = counts / len(labels)
            entropy = -np.sum(probabilities * np.log2(probabilities))
            return entropy

        def calculate_mutual_information(Y, labels):
            Y = Y.flatten()
            # use histogram2d to find the number of each combination of x and y
            joint_prob = np.histogram2d(Y, labels, bins=(len(np.unique(Y)), len(np.uniqu
            joint_prob /= len(Y)
            Y_prob = np.sum(joint_prob, axis=1)
            labels_prob = np.sum(joint_prob, axis=0)

            # sum up mutual indormation
            mutual_information = 0
            for i in range(0,joint_prob.shape[0]):
                for j in range(0,joint_prob.shape[1]):
                    if joint_prob[i, j] > 0:
                        mutual_information += joint_prob[i, j] * np.log2(joint_prob[i, j
            return mutual_information

        # combine all the functions and calculate the final nmi
        def calculate_nmi(labels, Y):
```

```
    entropy_Y = calculate_entropy(Y)
    entropy_labels = calculate_entropy(labels)
    mutual_information = calculate_mutual_information(Y, labels)
    nmi = mutual_information / np.sqrt(entropy_Y * entropy_labels)
    return nmi
```

Result for Q2.1

Seeds

get the datas from seeds.csv

In [ ]:

```
x_Matrix = pd.read_csv('seeds.csv')
x_Matrix = np.array(x_Matrix)
Y = x_Matrix[:,-1:]
x_Matrix = x_Matrix[:,:-1]
```

using the algorithms and calculate the metrics

In [ ]:

```
# i means there are i centers
for i in range(1,4):

    # using k-means
    labels, centroids = kmeans(x_Matrix, k=i)
    sc1 = silhouette_coefficient(labels,x_Matrix)
    ri1 = rand_index(labels, Y)
    nmi1 = calculate_nmi(labels, Y)
    # using gmm
    labels, means, covariances, weights = gmm(x_Matrix, k=i)
    sc2 = silhouette_coefficient(labels,x_Matrix)
    ri2 = rand_index(labels, Y)
    nmi2 = calculate_nmi(labels, Y)

    # print out the results
    print('When k = '+str(i)+': ')
    print('  For k-means:')
    print('    Silhouette Coefficient: '+str(sc1)+'  Rand Index: '+str(ri1)+'  N
    print('  For GMM:')
    print('    Silhouette Coefficient: '+str(sc2)+'  Rand Index: '+str(ri2)+'  N
    print()
```

```
C:\Users\黄嘉赫\AppData\Roaming\Python\Python37\site-packages\ipykernel_launcher.
py:13: RuntimeWarning: invalid value encountered in true_divide
  del sys.path[0]
C:\Users\黄嘉赫\AppData\Roaming\Python\Python37\site-packages\ipykernel_launcher.
py:29: RuntimeWarning: invalid value encountered in double_scalars
```

```
When k = 1:
  For k-means:
    Silhouette Coefficient: nan  Rand Index: 0.33014354066985646  NMI: nan
  For GMM:
    Silhouette Coefficient: nan  Rand Index: 0.33014354066985646  NMI: nan

When k = 2:
  For k-means:
    Silhouette Coefficient: 0.5253981519704325  Rand Index: 0.7258601048074732  N
MI: 0.5514899572480163
  For GMM:
    Silhouette Coefficient: 0.4539292148003259  Rand Index: 0.73734335839599  NM
I: 0.5770062706599562

When k = 3:
  For k-means:
    Silhouette Coefficient: 0.47193373191268945  Rand Index: 0.8743677375256322
NMI: 0.694926576382053
  For GMM:
    Silhouette Coefficient: 0.42622852998165767  Rand Index: 0.7415812257917521
NMI: 0.555738014137945
```

Vowel

get the datas from vowel.csv Since y is not marked with numbers, we should deal with them and ramark them with numbers

In [ ]:
```python
x_Matrix = pd.read_csv('vowel.csv')
x_Matrix = np.array(x_Matrix)
Y = x_Matrix[:,-1:].flatten()
# deal with Y labels
y_dic = {}
count = 0
for i in range(0,len(Y)):
    if Y[i] not in y_dic:
        y_dic[Y[i]] = count
        Y[i] = count
        count+=1
    else:
        Y[i] = y_dic[Y[i]]
Y = np.array(Y)

# deal with x to avoid 0
x_Matrix = x_Matrix[:,:-1]+1e-7
x_Matrix = x_Matrix.astype('float')
```

using the algorithms and calculate the metrics

In [ ]:
```python
# i means there are i centers
for i in range(1,4):
    # using kmeans
    labels, centroids = kmeans(x_Matrix, k=i)
    sc1 = silhouette_coefficient(labels,x_Matrix)
    ri1 = rand_index(labels, Y)
    nmi1 = calculate_nmi(labels, Y)

    # using gmm
```

```
    labels, means, covariances, weights = gmm(x_Matrix, k=i)
    sc2 = silhouette_coefficient(labels,x_Matrix)
    ri2 = rand_index(labels, Y)
    nmi2 = calculate_nmi(labels, Y)

    # print out the results
    print('When k = '+str(i)+': ')
    print('  For k-means:')
    print('    Silhouette Coefficient: '+str(sc1)+'  Rand Index: '+str(ri1)+'  N
    print('  For GMM:')
    print('    Silhouette Coefficient: '+str(sc2)+'  Rand Index: '+str(ri2)+'  N
    print()
```

```
C:\Users\黄嘉赫\AppData\Roaming\Python\Python37\site-packages\ipykernel_launcher.
py:13: RuntimeWarning: invalid value encountered in true_divide
  del sys.path[0]
C:\Users\黄嘉赫\AppData\Roaming\Python\Python37\site-packages\ipykernel_launcher.
py:29: RuntimeWarning: invalid value encountered in double_scalars
When k = 1:
  For k-means:
    Silhouette Coefficient: nan  Rand Index: 0.08998988877654196  NMI: nan
  For GMM:
    Silhouette Coefficient: nan  Rand Index: 0.08998988877654196  NMI: nan

When k = 2:
  For k-means:
    Silhouette Coefficient: 0.49056277913153595  Rand Index: 0.49767441860465117
NMI: 9.20044694746647e-17
  For GMM:
    Silhouette Coefficient: 0.07248914838909598  Rand Index: 0.5168816578321128
NMI: 0.09227031896959355

When k = 3:
  For k-means:
    Silhouette Coefficient: 0.378094826049739  Rand Index: 0.6287158746208291  NM
I: 2.752976482225353e-17
  For GMM:
    Silhouette Coefficient: 0.018609583776160857  Rand Index: 0.6143906200529052
NMI: 0.1489176160328054
```

Q2.2

seeds

get the data

In [ ]:
```
x_Matrix = pd.read_csv('seeds.csv')
x_Matrix = np.array(x_Matrix)
Y = x_Matrix[:,-1:]
x_Matrix = x_Matrix[:,:-1] + 1e-7
```

find out metrics with clusttering center ranging from 2 to 9

In [ ]:
```
label_kmeans = []
label_gmm = []
```

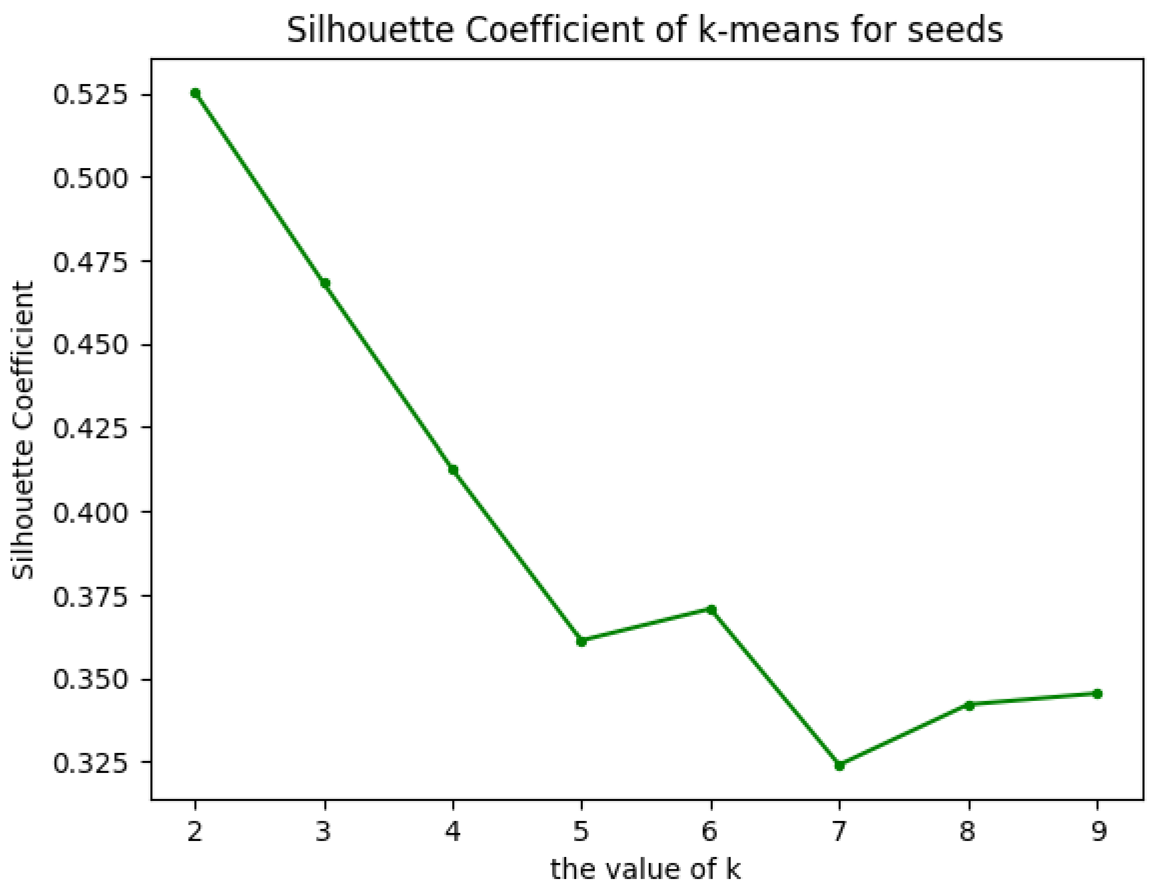
```
sc_kmeans = []
sc_gmm    = []
ri_kmeans = []
ri_gmm    = []
for z in range(2,10):
    labels, centroids = kmeans(x_Matrix, z)
    label_kmeans.append(labels)
    sc1 = silhouette_coefficient(labels,x_Matrix)
    ri1 = rand_index(labels, Y)
    sc_kmeans.append(sc1)
    ri_kmeans.append(ri1)
for z in range(2,10):
    labels, means, covariances, weights = gmm(x_Matrix, z)
    label_gmm.append(labels)
    sc2 = silhouette_coefficient(labels,x_Matrix)
    ri2 = rand_index(labels, Y)
    sc_gmm.append(sc2)
    ri_gmm.append(ri2)
```

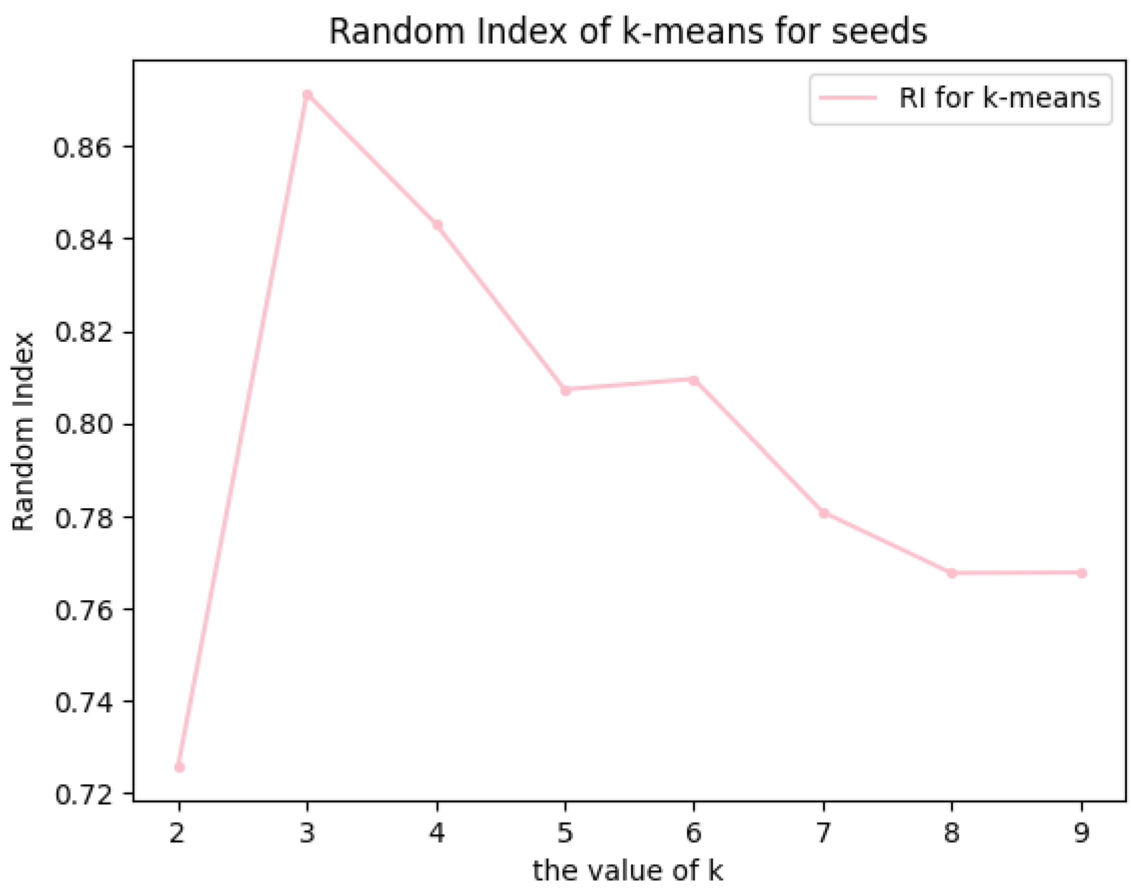
```
C:\Users\黄嘉赫\AppData\Roaming\Python\Python37\site-packages\ipykernel_launcher.
py:13: RuntimeWarning: invalid value encountered in true_divide
  del sys.path[0]
```

plotting metrics for k-means

In [ ]:

```
x = np.array(range(2,10))
figure1,ax1 = plt.subplots()
plt.title('Silhouette Coefficient of k-means for seeds')
figure2,ax2 = plt.subplots()
plt.title('Random Index of k-means for seeds')


# use green to plot the sc of kmeans
ax1.scatter(x,sc_kmeans,s=8,color = 'green')
ax1.plot(x,sc_kmeans,color="green", linestyle = 'solid', label='SC for k-means')

# use pink to plot the ri of kmeans
ax2.scatter(x,ri_kmeans,s=8,color='pink')
ax2.plot(x,ri_kmeans,color='pink',linestyle = 'solid', label='RI for k-means')

ax1.set_xlabel('the value of k')
ax1.set_ylabel('Silhouette Coefficient')
ax2.set_xlabel('the value of k')
ax2.set_ylabel('Random Index')
plt.legend()
plt.show()
```

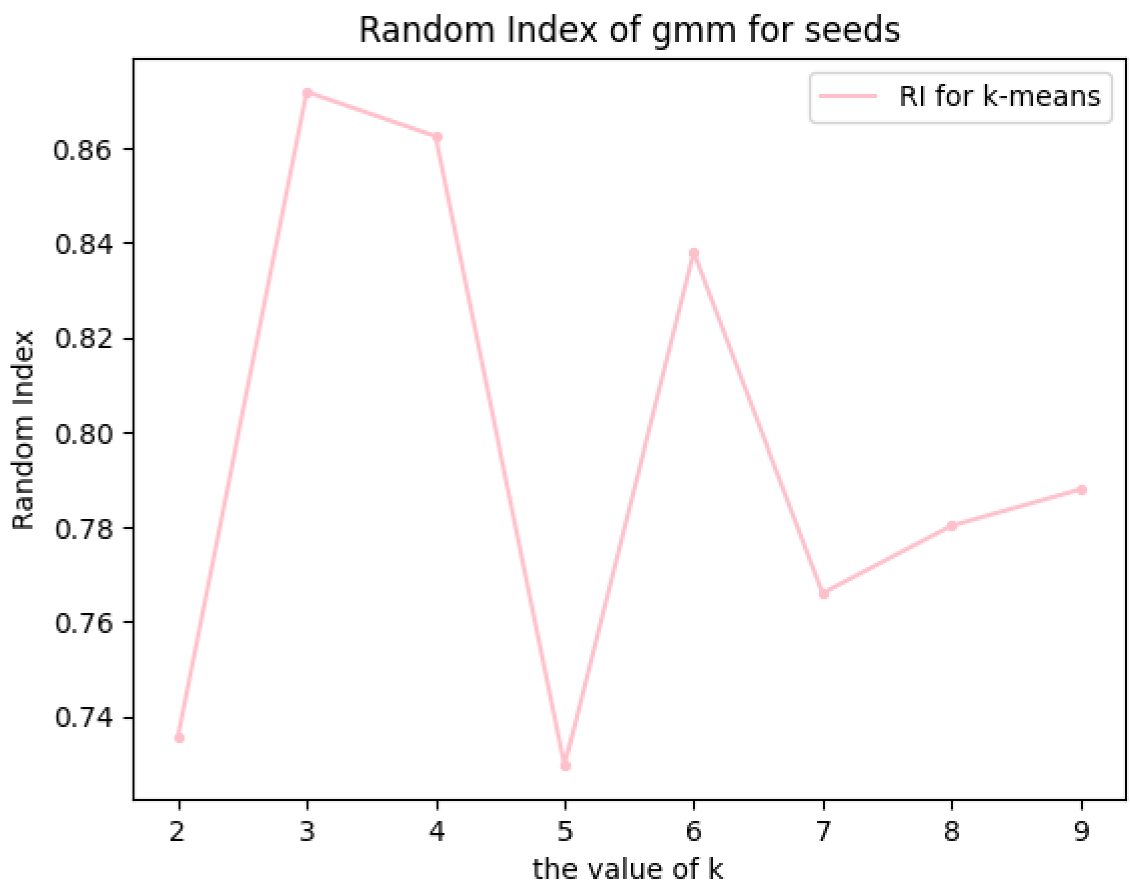




plotting metrics for GMM

In [ ]:
```
x = np.array(range(2,10))
figure1,ax1 = plt.subplots()
```

```
plt.title('Silhouette Coefficient of gmm for seeds')
figure2,ax2 = plt.subplots()
plt.title('Random Index of gmm for seeds')


# use pink to plot the sc of gmm
ax1.scatter(x,sc_gmm,s=8,color = 'green')
ax1.plot(x,sc_gmm,color="green", linestyle = 'solid', label='SC for k-means')

# use pink to plot the ri of gmm
ax2.scatter(x,ri_gmm,s=8,color='pink')
ax2.plot(x,ri_gmm,color='pink',linestyle = 'solid', label='RI for k-means')

ax1.set_xlabel('the value of k')
ax1.set_ylabel('Silhouette Coefficient')
ax2.set_xlabel('the value of k')
ax2.set_ylabel('Random Index')
plt.legend()
plt.show()
```



calculating best nmi

we can find that:

best k for Silhouette Coefficient of kmeans is 2

best k for Random Index of kmeans is 3

best k for Silhouette Coefficient of GMM is 2

best k for Random Index of GMM is 3

In [ ]:
```
nmi_sc_kmeans = calculate_nmi(label_kmeans[0],Y)
nmi_ri_kmeans = calculate_nmi(label_kmeans[1],Y)
nmi_sc_gmm = calculate_nmi(label_gmm[0],Y)
nmi_ri_gmm = calculate_nmi(label_gmm[1],Y)
print('nmi of best kmeans model found by sc: '+str(nmi_sc_kmeans))
print('nmi of best kmeans model found by ri: '+str(nmi_ri_kmeans))
print('nmi of best gmm model found by sc: '+str(nmi_sc_gmm))
print('nmi of best gmm model found by ri: '+str(nmi_ri_gmm))
```

```
nmi of best kmeans model found by sc: 0.5514899572480163
nmi of best kmeans model found by ri: 0.7100683008832275
nmi of best gmm model found by sc: 0.5717595817086311
nmi of best gmm model found by ri: 0.6685032617053913
```

Vowel

get the data

In [ ]:
```
x_Matrix = pd.read_csv('vowel.csv')
x_Matrix = np.array(x_Matrix)
Y = x_Matrix[:,-1:].flatten()
```

```
y_dic = {}
count = 0
for i in range(0,len(Y)):
    if Y[i] not in y_dic:
        y_dic[Y[i]] = count
        Y[i] = count
        count+=1
    else:
        Y[i] = y_dic[Y[i]]
Y = np.array(Y)
x_Matrix = x_Matrix[:,:-1] + 1e-7
x_Matrix = x_Matrix.astype('float')
```

find out metrics with clusttering center ranging from 10 to 19

In [ ]:

```
label_kmeans = []
label_gmm = []
sc_kmeans = []
sc_gmm    = []
ri_kmeans = []
ri_gmm    = []
for z in range(10,20):
    labels, centroids = kmeans(x_Matrix, k=z)
    label_kmeans.append(labels)
    sc1 = silhouette_coefficient(labels,x_Matrix)
    ri1 = rand_index(labels, Y)
    sc_kmeans.append(sc1)
    ri_kmeans.append(ri1)
```

```
C:\Users\黄嘉赫\AppData\Roaming\Python\Python37\site-packages\ipykernel_launcher.
py:13: RuntimeWarning: invalid value encountered in true_divide
  del sys.path[0]
```

In [ ]:

```
for z in range(10,20):
    labels, means, covariances, weights = gmm(x_Matrix, z)
    label_gmm.append(labels)
    sc2 = silhouette_coefficient(labels,x_Matrix)
    ri2 = rand_index(labels, Y)
    sc_gmm.append(sc2)
    ri_gmm.append(ri2)
```

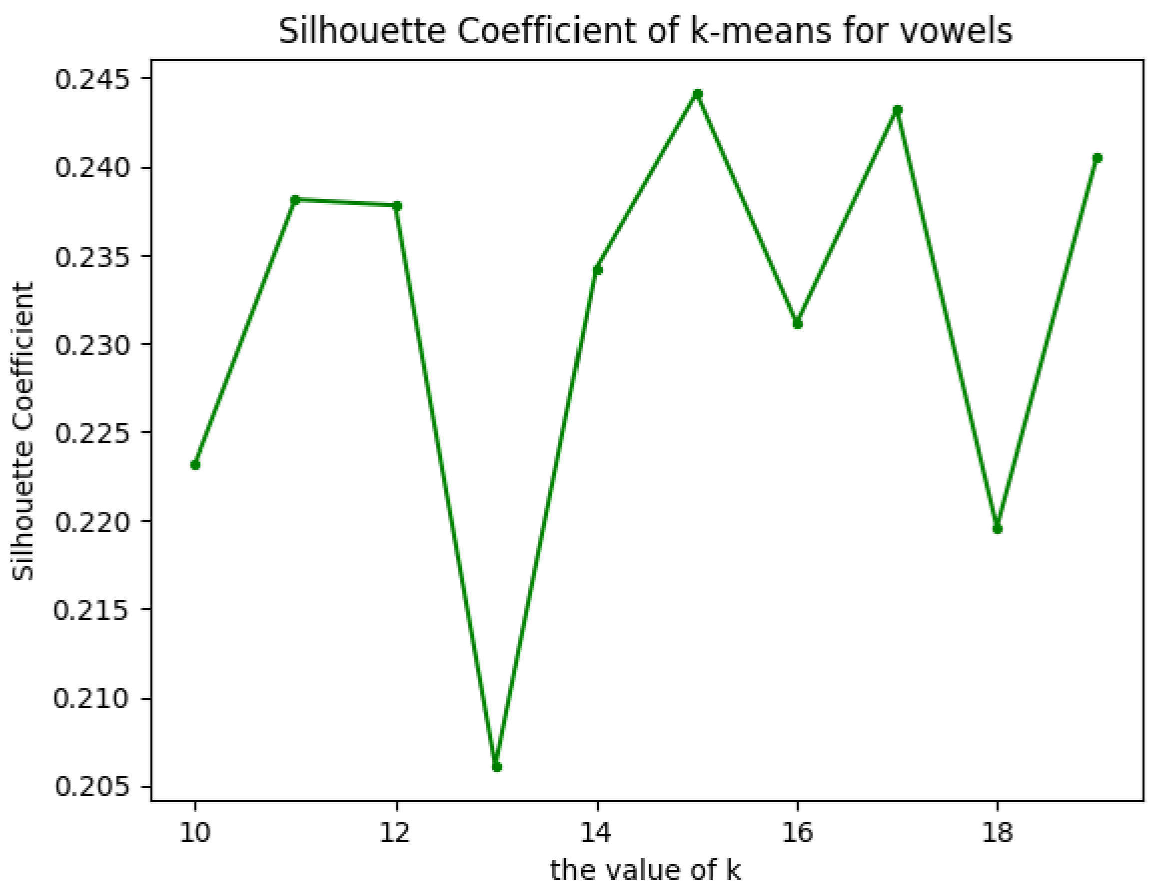
```
C:\Users\黄嘉赫\AppData\Roaming\Python\Python37\site-packages\ipykernel_launcher.
py:13: RuntimeWarning: invalid value encountered in true_divide
  del sys.path[0]
```

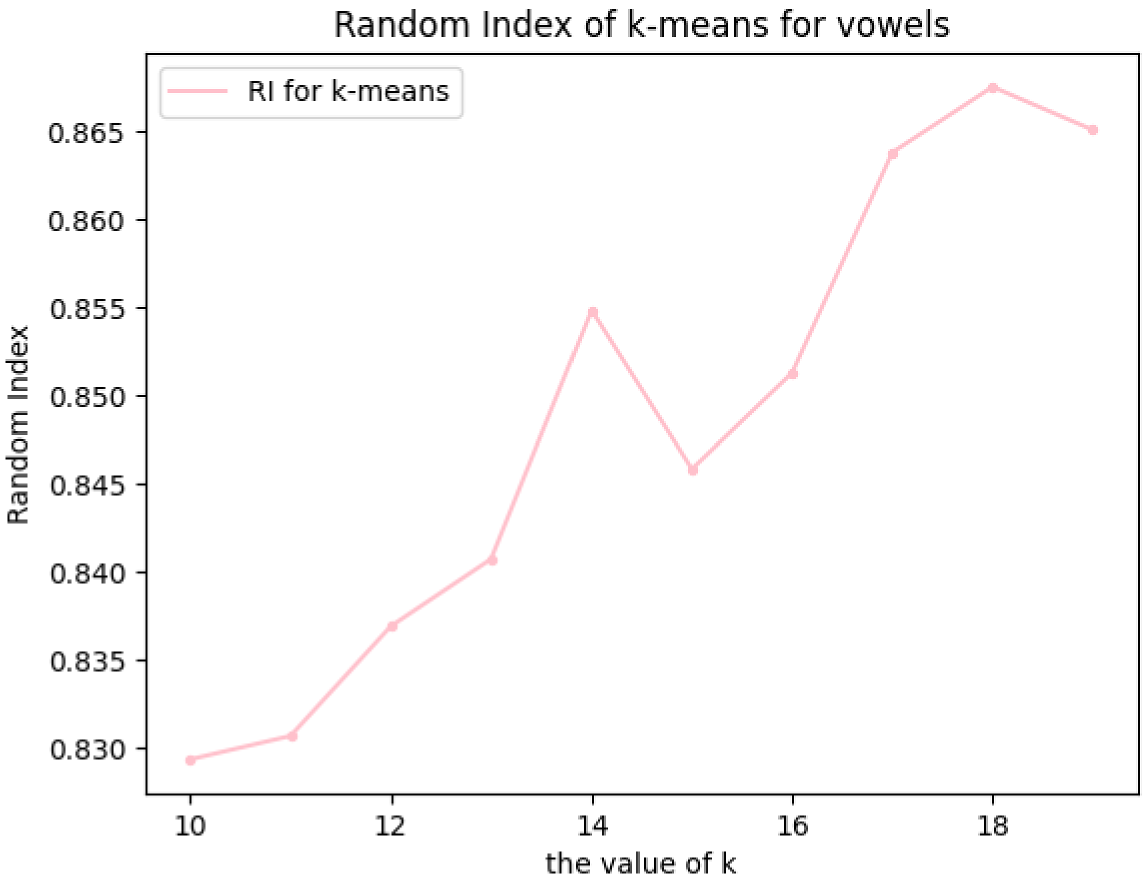
plotting metrics for k-means

In [ ]:

```
x = np.array(range(10,20))
figure1,ax1 = plt.subplots()
plt.title('Silhouette Coefficient of k-means for vowels')
figure2,ax2 = plt.subplots()
plt.title('Random Index of k-means for vowels')


# use green to plot the sc of kmeans
ax1.scatter(x,sc_kmeans,s=8,color = 'green')
ax1.plot(x,sc_kmeans,color="green", linestyle = 'solid', label='SC for k-means')

# use pink to plot the ri of kmeans
```

```
ax2.scatter(x,ri_kmeans,s=8,color='pink')
ax2.plot(x,ri_kmeans,color='pink',linestyle = 'solid', label='RI for k-means')

ax1.set_xlabel('the value of k')
ax1.set_ylabel('Silhouette Coefficient')
ax2.set_xlabel('the value of k')
ax2.set_ylabel('Random Index')
plt.legend()
plt.show()
```

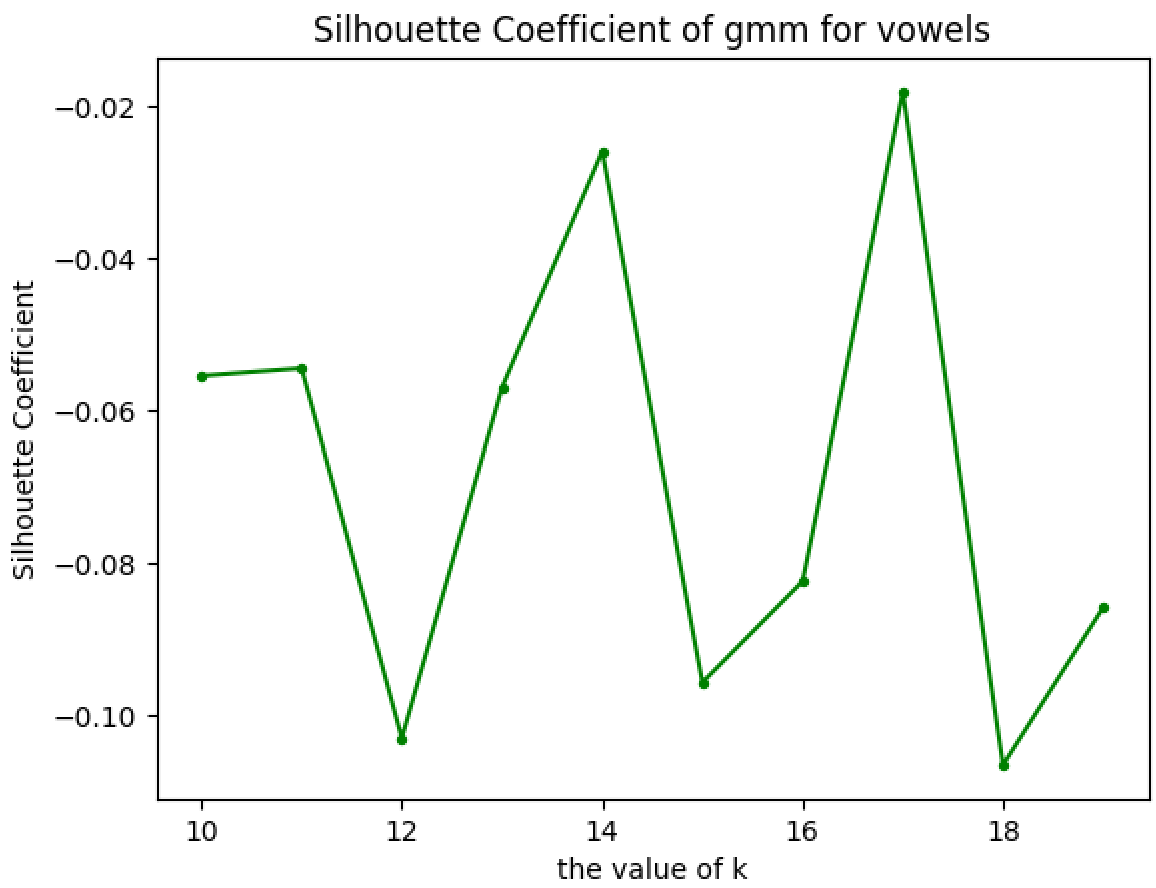


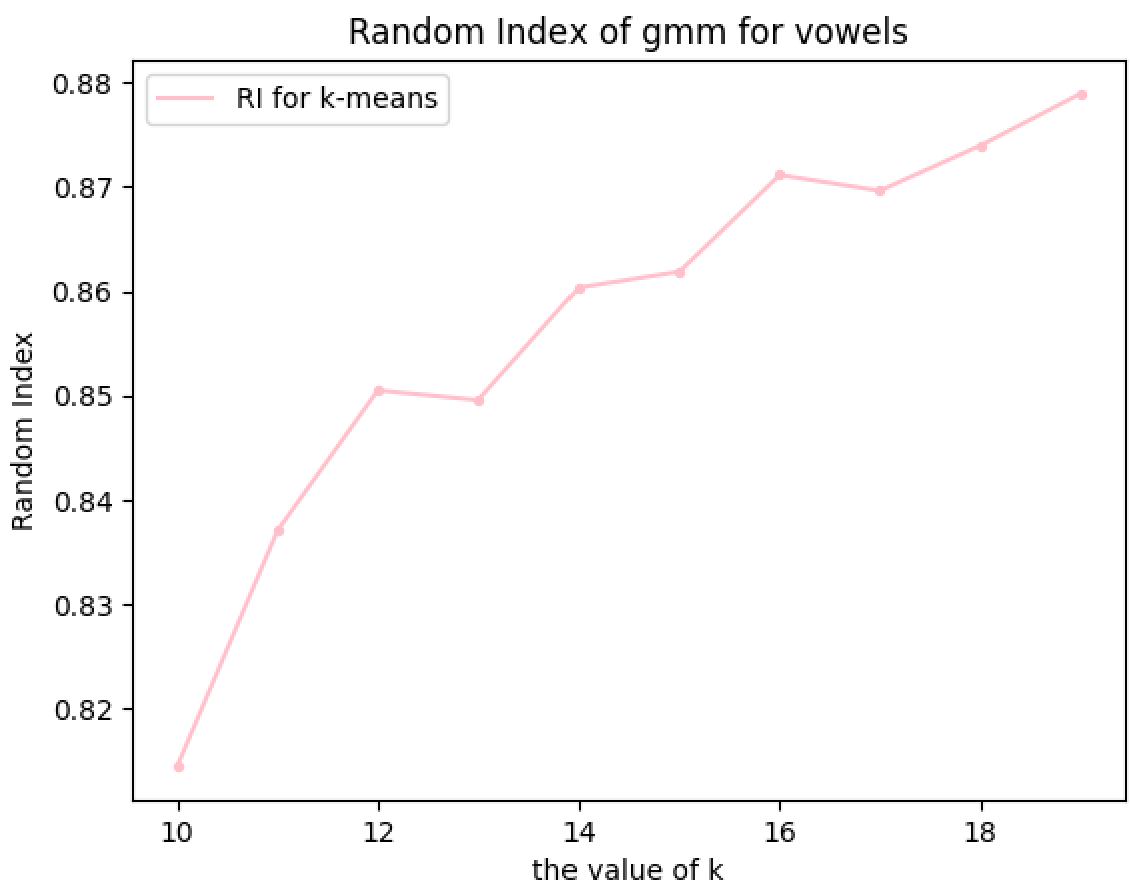


plotting metrics for GMM

In [ ]:

```
x = np.array(range(10,20))
figure1,ax1 = plt.subplots()
plt.title('Silhouette Coefficient of gmm for vowels')
figure2,ax2 = plt.subplots()
plt.title('Random Index of gmm for vowels')


# use green to plot the sc of gmm
ax1.scatter(x,sc_gmm,s=8,color = 'green')
ax1.plot(x,sc_gmm,color="green", linestyle = 'solid', label='SC for k-means')

# use pink to plot the ri of gmm
ax2.scatter(x,ri_gmm,s=8,color='pink')
ax2.plot(x,ri_gmm,color='pink',linestyle = 'solid', label='RI for k-means')

ax1.set_xlabel('the value of k')
ax1.set_ylabel('Silhouette Coefficient')
ax2.set_xlabel('the value of k')
ax2.set_ylabel('Random Index')
plt.legend()
plt.show()
```





calculating best nmi

we can find that:

best k for Silhouette Coefficient of kmeans is 15 best k for Random Index of kmeans is 18

best k for Silhouette Coefficient of GMM is 17

best k for Random Index of GMM is 19

In [ ]:
```
nmi_sc_kmeans = calculate_nmi(label_kmeans[5],Y)
nmi_ri_kmeans = calculate_nmi(label_kmeans[8],Y)
nmi_sc_gmm = calculate_nmi(label_gmm[7],Y)
nmi_ri_gmm = calculate_nmi(label_gmm[9],Y)
print('nmi of best kmeans model found by sc: '+str(nmi_sc_kmeans))
print('nmi of best kmeans model found by ri: '+str(nmi_ri_kmeans))
print('nmi of best gmm model found by sc: '+str(nmi_sc_gmm))
print('nmi of best gmm model found by ri: '+str(nmi_ri_gmm))
```

```
nmi of best kmeans model found by sc: 0.18484355110053674
nmi of best kmeans model found by ri: 0.26464876999701037
nmi of best gmm model found by sc: 0.3072633722444779
nmi of best gmm model found by ri: 0.3120806603249001
```