

# AML\_HW4\_Write up

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Submission: Late

## Programming Exercises

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### Question 1

#### 1.(a)

```
1 # import modules
2
3 import numpy as np
4 import pandas as pd
5 import matplotlib.pyplot as plt
6 %matplotlib inline
7 import math
```

```
1 # load .npy file
2
3 dw_matrix = np.load('data/science2k-doc-word.npy')
4
5 print (dw_matrix)
6 print (len(dw_matrix))
7 print (type(dw_matrix))
8 print (dw_matrix.shape)
```

```

1  [[-0.2521619 -0.2521619  9.36371    ... -0.2521619 -0.2521619
   -0.2521619]
2  [-0.2875293 -0.2875293  8.229864    ... -0.2875293 -0.2875293
   -0.2875293]
3  [-0.3634041 -0.3634041  9.252468    ... -0.3634041 -0.3634041
   -0.3634041]
4  ...
5  [10.04846    -0.7713402  9.132197    ... -0.7713402 -0.7713402
   -0.7713402]
6  [11.00702    -0.8423803 10.38288     ... -0.8423803 -0.8423803
   -0.8423803]
7  [ 9.710337   -0.7527946  9.556191    ... -0.7527946 -0.7527946
   -0.7527946]]
8  1373
9  <class 'numpy.ndarray'>
10 (1373, 5476)

```

```

1  # a-1: implement kmeans
2
3  from numpy import *
4  import matplotlib.pyplot as plt
5
6  # Compute Euclidean distance
7  def euclidean_distance(vec1, vec2):
8      eu_distance = sqrt(sum(power(vec2 - vec1, 2)))
9      return eu_distance
10
11 # init centroids with random samples
12 def init_centroids(data, k):
13     num_samples, dim = data.shape
14     centroids = zeros((k, dim))
15     for i in range(k):
16         idx = int(random.uniform(0, num_samples))
17         centroids[i, :] = data[idx, :]
18     return centroids
19
20 # kmeans
21 def kmeans(data, k):
22     num_samples = data.shape[0]
23

```

```

24 doc_cluster = mat(zeros((num_samples, 2)))
25 cls_changed = True
26
27 # init centroids
28 centroids = init_centroids(data, k)
29
30 while cls_changed:
31     cls_changed = False
32     for i in range(num_samples):
33         min_dist = 100000.0
34         min_idx = 0
35         # for each centroid, find the centroid who is closest
36         for j in range(k):
37             distance = euclidean_distance(centroids[j, :], data[i,
:]))
38             if distance < min_dist:
39                 min_dist = distance
40                 min_idx = j
41
42         # update its cluster
43         if doc_cluster[i, 0] != min_idx:
44             cls_changed = True
45             doc_cluster[i, :] = min_idx, min_dist**2
46
47         # update centroids
48         for j in range(k):
49             points_cls = data[nonzero(doc_cluster[:, 0].A == j)[0]]
50             centroids[j, :] = mean(points_cls, axis = 0)
51
52     return centroids, doc_cluster
53
54 # plot the cluster
55 def show_cluster(data, k, centroids, doc_cluster):
56     num_samples, dim = data.shape
57     if dim != 5476:
58         return 1
59
60     marks = ['or', 'ob', 'og', 'ok', '^r', '+r', 'sr', 'dr',
<r', 'pr', 'or', 'ob', 'og', 'ok', '^r', '+r', 'sr', 'dr',
<r', 'pr']
61     if k > len(marks):
62         return 1

```

```

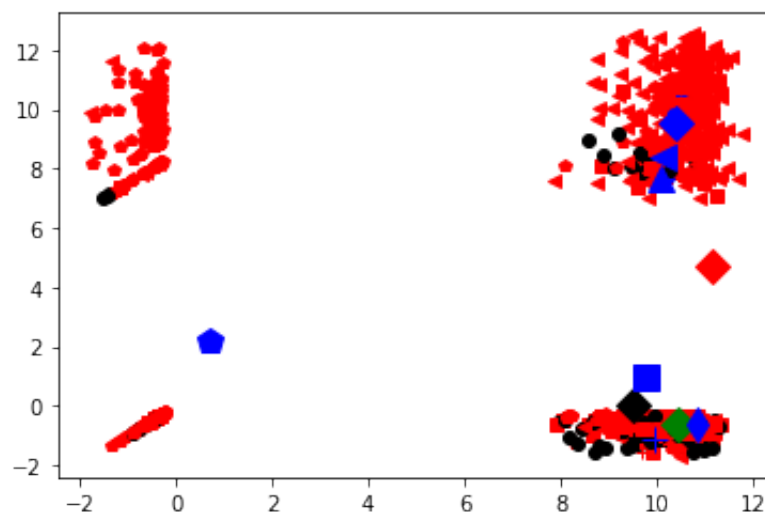
63
64     # plot all samples
65     for i in range(num_samples):
66         mark_idx = int(doc_cluster[i, 0])
67         plt.plot(data[i, 0], data[i, 1], marks[mark_idx])
68
69     marks = ['Dr', 'Db', 'Dg', 'Dk', '^b', '+b', 'sb', 'db',
70             '<b', 'pb', 'Dr', 'Db', 'Dg', 'Dk', '^b', '+b', 'sb', 'db',
71             '<b', 'pb']
72     # draw the centroids
73     for i in range(k):
74         plt.plot(centroids[i, 0], centroids[i, 1], marks[i],
75                 markersize = 12)
76
77     plt.show()

```

```

1  # Run the model
2  ## clustering, k=10
3  data = mat(dw_matrix)
4  k = 10
5  centroids, doc_cluster = kmeans(data, k)
6
7  ## plot
8  show_cluster(data, k, centroids, doc_cluster)

```



```

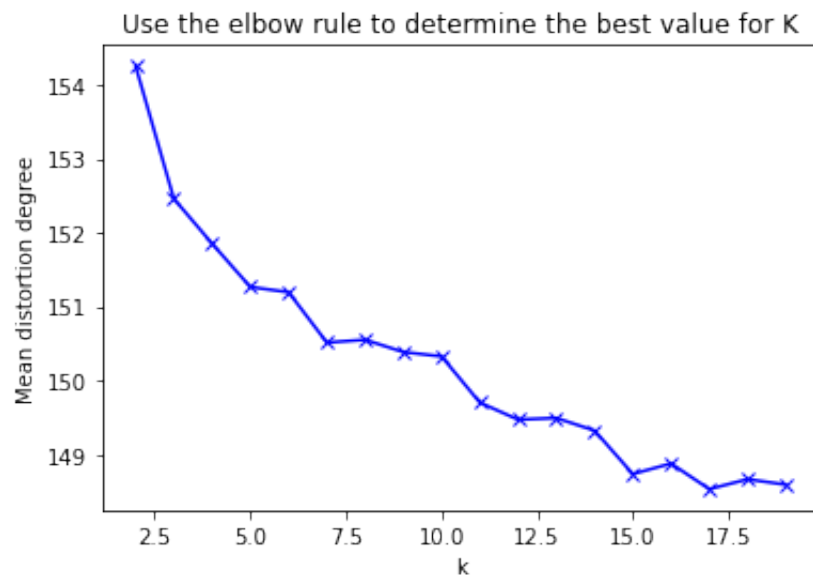
1  # a-2: Select the best value for k
2
3  from sklearn.cluster import KMeans

```

```

4  from sklearn import metrics
5  from scipy.spatial.distance import cdist
6  import matplotlib.pyplot as plt
7
8  K = range(2, 20)
9  meandistortions = []
10
11  X = mat(dw_matrix)
12
13  for k in K:
14      kmeans = KMeans(n_clusters=k)
15      kmeans.fit(X)
16      meandistortions.append(sum(np.min(cdist(X,
17      kmeans.cluster_centers_, 'euclidean'), axis=1)) / X.shape[0])
18
19  plt.plot(K, meandistortions, 'bx-')
20  plt.xlabel('k')
21  plt.ylabel(u'Mean distortion degree')
22  plt.title(u'Use the elbow rule to determine the best value for K');
23  plt.show()

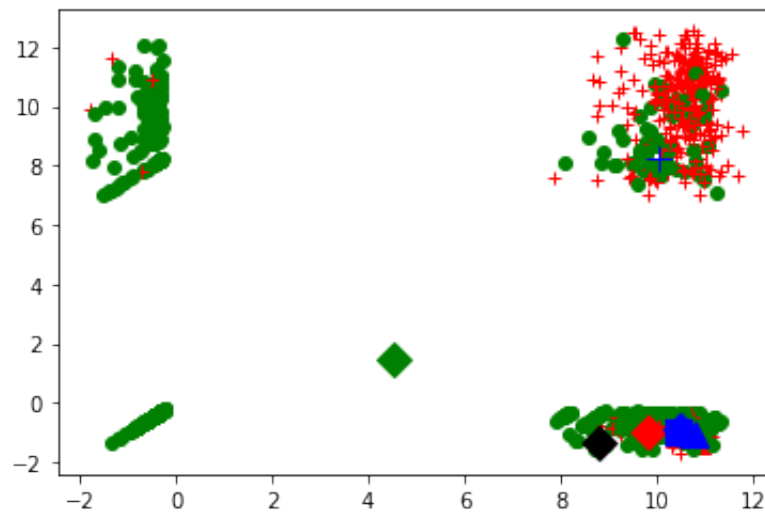
```



```

1 # a-3: Run the model
2
3 ## clustering
4 ## set k=7, because according to elbow rule, we can see that in
   the process of K value increasing, the K value corresponding to
   the position where the improvement effect of average distortion
   degree decreases the most is 7.
5
6 data = mat(dw_matrix)
7 k = 7
8 centroids, doc_cluster = kmeans(data, k)
9
10 ## plot
11 show_cluster(data, k, centroids, doc_cluster)

```



```

1 # central points
2 print (centroids)
3 print (len(centroids))
4 print (type(centroids))
5 print (centroids.shape)
6
7 # labels
8 print (doc_cluster)
9 print (len(doc_cluster))
10 print (type(doc_cluster))
11 print (doc_cluster.shape)
12
13 labels = doc_cluster[:,0]

```

```

14 labels = list(map(int, labels))
15 print (labels[:20])
16
17 cls = set(labels)
18 print ("clusters:", cls)

```

```

1  [[ 9.807132   -1.012666    9.114005   ... -1.012666   -1.012666
2     -1.012666   ]
3  [10.46259    -0.8878248    9.421161   ... -0.8878248
4     -0.8878248   ]
5  [ 4.53212466  1.47859304  8.96488063 ... -0.49527608
6     -0.56887007
7     -0.47825439]
8  ...
9  [10.77862    -1.08089     9.627346   ... -1.08089     -1.08089
10     -1.08089    ]
11 [10.02691817  8.2438794   9.13370419 ... -0.51721605
12     -0.6103251
13     -0.79039602]
14 [10.45232    -0.9552607    9.6414     ... -0.9552607
15     -0.9552607 ]]
16 7
17 <class 'numpy.ndarray'>
18 (7, 5476)
19 [[2.00000000e+00 2.11885050e+04]
20 [2.00000000e+00 2.22859889e+04]
21 [2.00000000e+00 2.44449395e+04]
22 ...
23 [5.00000000e+00 4.20898259e+04]
24 [2.00000000e+00 4.61358903e+04]
25 [2.00000000e+00 4.30799672e+04]]
26 1373
27 <class 'numpy.matrix'>
28 (1373, 2)
29 [2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 5]
30 clusters: {0, 1, 2, 3, 4, 5, 6}

```

```

1 # a-4: Report top 10 words in each cluster

```

```

2
3 import heapq
4
5 # calculate x_average
6 x_avg = np.mean(dw_matrix, axis=0)
7
8 vocab_df = pd.read_csv("data/science2k-vocab.txt", header=None)
9 vocab_array = np.array(vocab_df)
10 vocabs = vocab_array.tolist()
11 #print (vocabs[:20])
12 #print (len(vocabs))
13
14 def cal_cn_idx_list(n):
15     i = 0
16     cn = []
17     cn_idx_list = []
18     for p in labels:
19         if p == n:
20             doc = dw_matrix[i]
21             cn.append(doc)
22             cn_idx_list.append(i)
23
24             if i >= len(labels)-1:
25                 break
26             i = i + 1
27     #print (cn_idx_list)
28     return cn_idx_list,cn
29
30 print ("-----Top 10 words in each cluster-----")
31
32 for n in cls:
33     cn_idx_list,cn = cal_cn_idx_list(n)
34     cn_matrix = np.array(cn)
35     cn_mean_matrix = np.mean(cn_matrix, axis=0)
36
37     cn_sig_matrix = cn_mean_matrix - x_avg
38     cn_sig_list = cn_sig_matrix.tolist()
39
40     # top 10 largest numbers
41     max_idx = map(cn_sig_list.index, heapq.nlargest(10,
cn_sig_list))
42     max_idx_list = list(max_idx)

```



```

43     #print(list(max_idx_list))
44
45     # report top 10 words
46     top_word_list = []
47     for m in max_idx_list:
48         top_word = vocabs[m]
49         top_word_list.append(top_word)
50     print ("Cluster",n,":")
51     print (top_word_list)

```

```

1  -----Top 10 words in each cluster-----
2  Cluster 0 :
3  [['eros'], ['solar'], ['kev'], ['sun'], ['elemental'],
   ['ratios'], ['asteroid'], ['ray'], ['ordinary'], ['detector']]
4  Cluster 1 :
5  [['coherence'], ['extinction'], ['patch'], ['dispersal'],
   ['coherent'], ['probabilities'], ['patches'], ['oscillations'],
   ['criteria'], ['probability']]
6  Cluster 2 :
7  [['years'], ['year'], ['scientists'], ['world'],
   ['researchers'], ['says'], ['field'], ['mail'], ['million'],
   ['focus']]
8  Cluster 3 :
9  [['co2'], ['terrestrial'], ['carbon'], ['ocean'],
   ['ecosystems'], ['atmospheric'], ['nitrogen'], ['oceans'],
   ['sink'], ['interglacial']]
10 Cluster 4 :
11 [['spectral'], ['longitude'], ['wavelengths'], ['spectra'],
   ['band'], ['wavelength'], ['incident'], ['kilometers'],
   ['elongated'], ['images']]
12 Cluster 5 :
13 [['protein'], ['cell'], ['cells'], ['expression'],
   ['proteins'], ['fig'], ['gene'], ['specific'], ['binding'],
   ['expressed']]
14 Cluster 6 :
15 [['titans'], ['clouds'], ['methane'], ['spectra'], ['cloud'],
   ['altitude'], ['atmosphere'], ['albedo'], ['flux'],
   ['saturated']]

```

```

1  # a-5: Report the top ten documents that fall closest to each
   cluster center
2
3  title_df = pd.read_csv("data/science2k-titles.txt",
   header=None)
4  title_array = np.array(title_df)
5  titles = title_array.tolist()
6  #print (titles[:20])
7  #print (len(titles))
8
9  def get_distances(n):
10     cn_idx_list,cn = cal_cn_idx_list(n)
11     cn_matrix = np.array(cn)
12     cn_mean_matrix = np.mean(cn_matrix, axis=0)
13     distances = []
14     for j in range(len(cn)):
15         distances.append(euclidean_distance(cn[j],
   cn_mean_matrix))
16     return distances
17
18  print ("-----Top 10 documents that fall closest to each
   cluster center-----")
19
20  for n in cls:
21     cn_distances = get_distances(n)
22     #print (len(cn_distances))
23     #print (cn_distances)
24
25     # top 10 smallest distances in each cluster
26     min_idx = map(cn_distances.index, heapq.nsmallest(10,
   cn_distances))
27     min_idx_list = list(min_idx)
28     #print(list(min_idx_list))
29
30     # report top 10 documents in each cluster
31     top_doc_list = []
32     for m in min_idx_list:
33         top_doc = titles[m]
34         top_doc_list.append(top_doc)
35     print ("Cluster",n,":")
36     print (top_doc_list)

```

```

1  -----Top 10 documents that fall closest to each cluster
   center-----
2  Cluster 0 :
3  [['Archaeology in the Holy Land']]
4  Cluster 1 :
5  [['Archaeology in the Holy Land']]
6  Cluster 2 :
7  [['Similar Requirements of a Plant Symbiont and a Mammalian
   Pathogen for Prolonged Intracellular Survival'], ['A Deluge of
   Patents Creates Legal Hassles for Research'], ['Childhood
   Cancer'], ['Trojan Horses'], ['An Integrative Science Finds a
   Home'], ['An Integrative Science Finds a Home'], ['An
   Integrative Science Finds a Home'], ['Archaeology in the Holy
   Land'], ['Close Encounters: Details Veto Depth from Shadows'],
   ['Thermal, Catalytic, Regiospecific Functionalization of
   Alkanes']]
8  Cluster 3 :
9  [['Archaeology in the Holy Land']]
10 Cluster 4 :
11 [['Archaeology in the Holy Land'], ["Baedeker's Guide, or Just
   Plain 'Trouble'?"]]
12 Cluster 5 :
13 [['Reforming the Patent System'], ["On the Hunt for a Wolf in
   Sheep's Clothing"], ['Is Bigger Better in Cricket?'], ['Was
   Lamarck Just a Little Bit Right?'], ['Hydrogen Storage in
   Nanotubes'], ['When Pharma Merges, R&D Is the Dowry'],
   ['Superplastic Extensibility of Nanocrystalline Copper at Room
   Temperature'], ['Coupling of Stress in the ER to Activation of
   JNK Protein Kinases by Transmembrane Protein Kinase IRE1'],
   ['Mice Are Not Furry Petri Dishes'], ['<latex>$H_3^{+}$</latex>-
   an Ion with Many Talents']]
14 Cluster 6 :
15 [['Archaeology in the Holy Land']]

```

## a-6

Comment on these results.

1.What has the algorithm captured?

- This algorithm mainly captures the topic information. It clusters documents, helps to get the relevant documents for each cluster center. From this, we can know which documents belong to the same topic.

## 2.How might such an algorithm be useful?

- This algorithm can be applied to document classification/topic clustering. By using it, we can know what topic a document belongs to and which documents belong to the same topic.
- Through the Top 10 words, we can know the key words in certain topics. Through the top 10 documents, we can find the documents that are most relevant to a certain topic.

## 1.(b)

```
1 # import modules
2
3 import numpy as np
4 import pandas as pd
5 import matplotlib.pyplot as plt
6 %matplotlib inline
7 import math
```

```
1 # load .npy file
2
3 dw_matrix = np.load('data/science2k-word-doc.npy')
4
5 print (dw_matrix)
6 print (len(dw_matrix))
7 print (type(dw_matrix))
8 print (dw_matrix.shape)
```

```
1 [[-6.755691  -6.755691  -6.755691  ...  4.064107   5.093713
2      3.707441  ]
3  [-4.028205  -4.028205  -4.028205  ... -4.028205  -4.028205
4      -4.028205  ]
5  [-0.03370464 -1.132184  -0.03370464 ...  0.2539608   1.57568
6      0.6594092  ]
7  ...
8  [-0.1301101  -0.1301101  -0.1301101  ... -0.1301101
   -0.1301101
9      -0.1301101  ]
10 [-0.05128021 -0.05128021 -0.05128021 ... -0.05128021
   -0.05128021
```

```
11     -0.05128021]
12     [-0.06441435 -0.06441435 -0.06441435 ... -0.06441435
    -0.06441435
13     -0.06441435]]
14 5476
15 <class 'numpy.ndarray'>
16 (5476, 1373)
```

```
1  # b-1: implement kmeans
2
3  from numpy import *
4  import matplotlib.pyplot as plt
5
6  # Compute Euclidean distance
7  def euclidean_distance(vec1, vec2):
8      eu_distance = sqrt(sum(power(vec2 - vec1, 2)))
9      return eu_distance
10
11  # init centroids with random samples
12  def init_centroids(data, k):
13      num_samples, dim = data.shape
14      centroids = zeros((k, dim))
15      for i in range(k):
16          idx = int(random.uniform(0, num_samples))
17          centroids[i, :] = data[idx, :]
18      return centroids
19
20  # kmeans
21  def kmeans(data, k):
22      num_samples = data.shape[0]
23
24      doc_cluster = mat(zeros((num_samples, 2)))
25      cls_changed = True
26
27      # init centroids
28      centroids = init_centroids(data, k)
29
30      while cls_changed:
31          cls_changed = False
32          for i in range(num_samples):
```

```

33     min_dist = 100000.0
34     min_idx = 0
35     # for each centroid, find the centroid who is closest
36     for j in range(k):
37         distance = euclidean_distance(centroids[j, :], data[i,
:]))
38         if distance < min_dist:
39             min_dist = distance
40             min_idx = j
41
42     # update its cluster
43     if doc_cluster[i, 0] != min_idx:
44         cls_changed = True
45         doc_cluster[i, :] = min_idx, min_dist**2
46
47     # update centroids
48     for j in range(k):
49         points_cls = data[nonzero(doc_cluster[:, 0].A == j)[0]]
50         centroids[j, :] = mean(points_cls, axis = 0)
51
52     return centroids, doc_cluster
53
54 # plot the cluster
55 def show_cluster(data, k, centroids, doc_cluster):
56     num_samples, dim = data.shape
57     if dim != 5476:
58         return 1
59
60     marks = ['or', 'ob', 'og', 'ok', '^r', '+r', 'sr', 'dr',
<r', 'pr', 'or', 'ob', 'og', 'ok', '^r', '+r', 'sr', 'dr',
<r', 'pr']
61     if k > len(marks):
62         return 1
63
64     # plot all samples
65     for i in range(num_samples):
66         mark_idx = int(doc_cluster[i, 0])
67         plt.plot(data[i, 0], data[i, 1], marks[mark_idx])
68
69     marks = ['Dr', 'Db', 'Dg', 'Dk', '^b', '+b', 'sb', 'db',
<b', 'pb', 'Dr', 'Db', 'Dg', 'Dk', '^b', '+b', 'sb', 'db',
<b', 'pb']

```

```

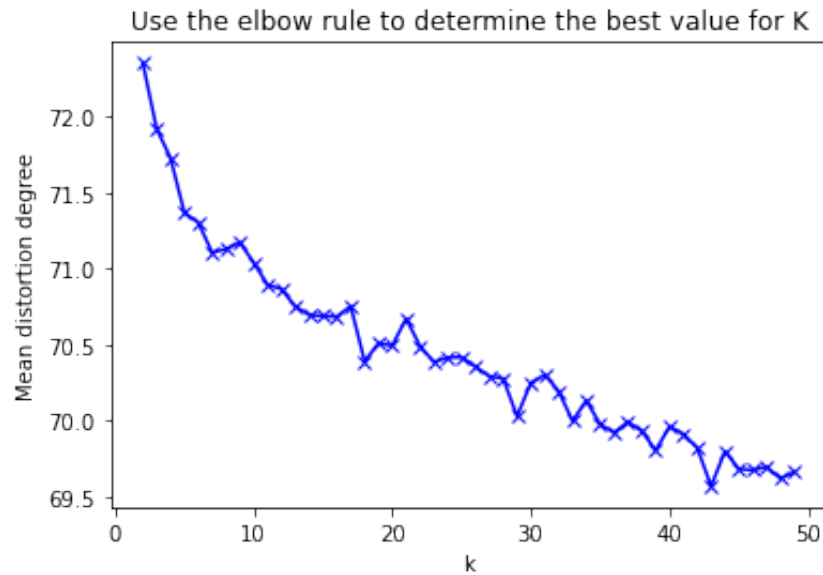
70     # draw the centroids
71     for i in range(k):
72         plt.plot(centroids[i, 0], centroids[i, 1], marks[i],
73                 markersize = 12)
74     plt.show()

```

```

1  # b-2: Select the best value for k
2
3  from sklearn.cluster import KMeans
4  from sklearn import metrics
5  from scipy.spatial.distance import cdist
6  import matplotlib.pyplot as plt
7
8  K = range(2, 50)
9  meandistortions = []
10
11 X = mat(dw_matrix)
12
13 for k in K:
14     kmeans = KMeans(n_clusters=k)
15     kmeans.fit(X)
16     meandistortions.append(sum(np.min(cdist(X,
17     kmeans.cluster_centers_, 'euclidean'), axis=1)) / X.shape[0])
17
18 plt.plot(K, meandistortions, 'bx-')
19 plt.xlabel('k')
20 plt.ylabel(u'Mean distortion degree')
21 plt.title(u'Use the elbow rule to determine the best value for
22 K');
23 plt.show()

```



```
1 # b-3: Run the model
2 ## clustering
3 ## set k=29, because according to elbow rule, we can see that
  in the process of K value increasing, the K value corresponding
  to the position where the improvement effect of average
  distortion degree decreases the most is 29.
4
5 data = mat(dw_matrix)
6 k = 29
7 centroids, doc_cluster = kmeans(data, k)
8
9 ## plot
10 show_cluster(data, k, centroids, doc_cluster)
```

```
1 # central points
2 print (centroids)
3 print (len(centroids))
4 print (type(centroids))
5 print (centroids.shape)
6
7 # labels
8 print (doc_cluster)
9 print (len(doc_cluster))
10 print (type(doc_cluster))
11 print (doc_cluster.shape)
```



```

12
13 labels = doc_cluster[:,0]
14 labels = list(map(int,labels))
15 print (labels[:20])
16
17 cls = set(labels)
18 print ("clusters:", cls)

```

```

1  [[-0.18002037 -0.1617278  -0.11142196 ...  0.09050765
    0.19292803
2     0.18388448]
3  [-2.836106  -2.836106  -2.836106  ... -2.836106  -2.836106
4     5.681287  ]
5  [-0.62982567 -0.61657324 -0.46394096 ...  0.11452273
    -0.34449929
6     -0.38625112]
7  ...
8  [-3.18032  -3.18032  -0.96434087 ... -2.11564588
    -1.05097175
9     -2.029015  ]
10 [-1.32743722 -1.60219184 -1.32743722 ... -1.30508087
    -0.98561187
11    -0.75557164]
12 [-0.4221642  -0.4221642  -0.4221642  ... -0.4221642
    -0.4221642
13    -0.4221642  ]]
14 29
15 <class 'numpy.ndarray'>
16 (29, 1373)
17 [[2.40000000e+01 2.82920211e+04]
18  [2.60000000e+01 2.36386680e+04]
19  [0.00000000e+00 0.00000000e+00]
20  ...
21  [0.00000000e+00 0.00000000e+00]
22  [0.00000000e+00 0.00000000e+00]
23  [0.00000000e+00 0.00000000e+00]]
24 5476
25 <class 'numpy.matrix'>
26 (5476, 2)
27 [24, 26, 0, 20, 0, 26, 24, 26, 11, 0, 2, 0, 0, 24, 27, 24, 24,
    26, 4, 4]

```

```
28 clusters: {0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14,
15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28}
```

```
1  # b-4: Report top 10 documents in each cluster
2
3  import heapq
4
5  # calculate x_average
6  x_avg = np.mean(dw_matrix, axis=0)
7
8  title_df = pd.read_csv("data/science2k-titles.txt",
9                          header=None)
10 title_array = np.array(title_df)
11 titles = title_array.tolist()
12 #print (titles[:20])
13 #print (len(titles))
14
15 def cal_cn_idx_list(n):
16     i = 0
17     cn = []
18     cn_idx_list = []
19     for p in labels:
20         if p == n:
21             doc = dw_matrix[i]
22             cn.append(doc)
23             cn_idx_list.append(i)
24
25             if i >= len(labels)-1:
26                 break
27             i = i + 1
28     #print (cn_idx_list)
29     return cn_idx_list,cn
30
31 print ("-----Top 10 documents-----")
32
33 for n in cls:
34     cn_idx_list,cn = cal_cn_idx_list(n)
35     cn_matrix = np.array(cn)
36     cn_mean_matrix = np.mean(cn_matrix, axis=0)
```

```

37     cn_sig_matrix = cn_mean_matrix - x_avg
38     cn_sig_list = cn_sig_matrix.tolist()
39
40     # top 10 largest numbers
41     max_idx = map(cn_sig_list.index, heapq.nlargest(10,
cn_sig_list))
42     max_idx_list = list(max_idx)
43     #print(list(max_idx_list))
44
45     # report top 10 documents
46     top_word_list = []
47     for m in max_idx_list:
48         top_word = titles[m]
49         top_word_list.append(top_word)
50     print ("Cluster",n,":")
51     print (top_word_list)

```

```

1  -----Top 10 documents-----
2  Cluster 0 :
3  [['National Academy of Sciences Elects New Members'],
['Biological Control of Invading Species'], ['Scientists at
Brookhaven'], ['Corrections and Clarifications: Timing the
Ancestor of the HIV-1 Pandemic Strains'], ['Corrections and
Clarifications: Timing the Ancestor of the HIV-1 Pandemic
Strains'], ['Corrections and Clarifications: Marking Time for a
Kingdom'], ['Corrections and Clarifications: Marking Time for a
Kingdom'], ['Corrections and Clarifications: Marking Time for a
Kingdom'], ['Corrections and Clarifications: One Hundred Years
of Quantum Physics'], ['Corrections and Clarifications: One
Hundred Years of Quantum Physics']]
4  Cluster 1 :

```

5 [[ 'Global Biodiversity Scenarios for the Year 2100' ],  
[ 'Proximity of Chromosomal Loci That Participate in Radiation-  
Induced Rearrangements in Human Cells' ], [ 'Mate Selection and  
the Evolution of Highly Polymorphic Self/Nonself Recognition  
Genes' ], [ 'Population Dynamical Consequences of Climate Change  
for a Small Temperate Songbird' ], [ 'Intersubband  
Electroluminescence from Silicon-Based Quantum Cascade  
Structures' ], [ 'On the Origin of Internal Structure of Word  
Forms' ], [ 'Evidence for Superfluidity in Para-Hydrogen Clusters  
inside Helium-4 Droplets at 0.15 Kelvin' ], [ 'Real-Space Imaging  
of Two-Dimensional Antiferromagnetism on the Atomic Scale' ],  
[ 'Scanometric DNA Array Detection with Nanoparticle Probes' ],  
[ 'The Evolutionary Fate and Consequences of Duplicate Genes' ]]

6 Cluster 2 :

7 [[ 'Central Role for G Protein-Coupled Phosphoinositide 3-Kinase  
g in Inflammation' ], [ 'Function of PI3Kg in Thymocyte  
Development, T Cell Activation, and Neutrophil Migration' ],  
[ 'Noxa, a BH3-Only Member of the Bcl-2 Family and Candidate  
Mediator of p53-Induced Apoptosis' ], [ 'Kinesin Superfamily  
Motor Protein KIF17 and mLin-10 in NMDA Receptor-Containing  
Vesicle Transport' ], [ 'Requirement of JNK for Stress-Induced  
Activation of the Cytochrome c-Mediated Death Pathway' ],  
[ 'Requirement for RORg in Thymocyte Survival and Lymphoid Organ  
Development' ], [ 'Immune Inhibitory Receptors' ], [ 'Role of the  
Mouse ank Gene in Control of Tissue Calcification and  
Arthritis' ], [ 'An Oral Vaccine against NMDAR1 with Efficacy in  
Experimental Stroke and Epilepsy' ], [ 'Ubiquitin Protein Ligase  
Activity of IAPs and Their Degradation in Proteasomes in  
Response to Apoptotic Stimuli' ]]

8 Cluster 3 :

9 [[ 'DNA Damage-Induced Activation of p53 by the Checkpoint  
Kinase Chk2' ], [ 'Timing the Radiations of Leaf Beetles:  
Hispiines on Gingers from Latest Cretaceous to Recent' ], [ 'Rapid  
Destruction of Human Cdc25A in Response to DNA Damage' ],  
[ 'Resonant Formation of DNA Strand Breaks by Low-Energy (3 to  
20 eV) Electrons' ], [ 'Northridge Earthquake Damage Caused by  
Geologic Focusing of Seismic Waves' ], [ 'Radiation Tolerance of  
Complex Oxides' ], [ 'Heightened Odds of Large Earthquakes near  
Istanbul: An Interaction-Based Probability Calculation' ], [ 'A  
Sense of the End' ], [ 'Stem Cells in Epithelial Tissues' ],  
[ 'Response to RAG-Mediated V(D)J Cleavage by NBS1 and g-H2AX' ]]

10 Cluster 4 :

11 [['A Mouse Chronology'], ['Meltdown on Long Island'], ['Atom-Scale Research Gets Real'], ['Presidential Forum: Gore and Bush Offer Their Views on Science'], ['Help Needed to Rebuild Science in Yugoslavia'], ["I'd like to See America Used as a Global Lab"], ["Silent No Longer: 'Model Minority' Mobilizes"], ["Soft Money's Hard Realities"], ['Ecologists on a Mission to Save the World'], ['Clones: A Hard Act to Follow']]

12 Cluster 5 :

13 [['Retinal Stem Cells in the Adult Mammalian Eye'], ['Mammalian Neural Stem Cells'], ['From Marrow to Brain: Expression of Neuronal Phenotypes in Adult Mice'], ['Out of Eden: Stem Cells and Their Niches'], ['Turning Blood into Brain: Cells Bearing Neuronal Antigens Generated in Vivo from Bone Marrow'], ['The Genetic Program of Hematopoietic Stem Cells'], ['Genomic Analysis of Gene Expression in *C. elegans*'], ['The Initial Domestication of Goats (*Capra hircus*) in the Zagros Mountains 10,000 Years Ago'], ['The Osteoblast: A Sophisticated Fibroblast under Central Surveillance'], ['Allosteric Effects of Pit-1 DNA Sites on Long-Term Repression in Cell Type Specification']]

14 Cluster 6 :

15 [['Principles for Human Gene Therapy Studies'], ['Oxidative Damage Linked to Neurodegeneration by Selective  $\alpha$ -Synuclein Nitration in Synucleinopathy Lesions'], ['Synapses Call the Shots'], ['Of Chimps and Men'], ['Quantized Phonon Spectrum of Single-Wall Carbon Nanotubes'], ['Information Technology Takes a Different Tack'], ['Mothers Setting Boundaries'], ['L1 Retrotransposons Shape the Mammalian Genome'], ['Fossils Come to Life in Mexico'], ['Requirement of the RNA Editing Deaminase ADAR1 Gene for Embryonic Erythropoiesis']]

16 Cluster 7 :

17 [[ 'An Orientational Transition of Bent-Core Molecules in an Anisotropic Matrix'], ['Molecular Identification of a Taste Receptor Gene for Trehalose in Drosophila'], ['Multidecadal Changes in the Vertical Temperature Structure of the Tropical Troposphere'], ['Coherent High- and Low-Latitude Climate Variability during the Holocene Warm Period'], ['Quantum Criticality: Competing Ground States in Low Dimensions'], ['Rapid Changes in the Hydrologic Cycle of the Tropical Atlantic during the Last Glacial'], ['Quantum Dots as Tunable Kondo Impurities'], ['The Mouse House as a Recruiting Tool'], ['Epitopes Involved in Antibody-Mediated Protection from Ebola Virus'], ['Tracing the Origins of Salmonella Outbreaks']]

18 Cluster 8 :

19 [[ 'Rapid Extragranular Plasticity in the Absence of Thalamocortical Plasticity in the Developing Primary Visual Cortex'], ['Proximity of Chromosomal Loci That Participate in Radiation-Induced Rearrangements in Human Cells'], ['The Internet of Tomorrow'], ["Detection of SO in Io's Exosphere"], ['The Structural Basis of Ribosome Activity in Peptide Bond Synthesis'], ['How Snapping Shrimp Snap: Through Cavitating Bubbles'], ['Learning-Induced LTP in Neocortex'], ['Heretical Idea Faces Its Sternest Test'], ['Cantilever Tales'], ['Single Photons on Demand']]

20 Cluster 9 :

21 [[ 'How Cells Handle Cholesterol'], ['Ethanol-Induced Apoptotic Neurodegeneration and Fetal Alcohol Syndrome'], ['Molecular Evidence for the Early Evolution of Photosynthesis'], ['Direct Targeting of Light Signals to a Promoter Element-Bound Transcription Factor'], ['Architecture of RNA Polymerase II and Implications for the Transcription Mechanism'], ['Structural Evidence for Evolution of the b/a Barrel Scaffold by Gene Duplication and Fusion'], ['Timing the Ancestor of the HIV-1 Pandemic Strains'], ['The Structural Basis of Ribosome Activity in Peptide Bond Synthesis'], ['Noxa, a BH3-Only Member of the Bcl-2 Family and Candidate Mediator of p53-Induced Apoptosis'], ['Calcium Sensitivity of Glutamate Release in a Calyx-Type Terminal']]

22 Cluster 10 :

23 [['Diversity and Dynamics of Dendritic Signaling'], ['Actin-Based Plasticity in Dendritic Spines'], ['Dopaminergic Loss and Inclusion Body Formation in a-Synuclein Mice: Implications for Neurodegenerative Disorders'], ['Untangling Dendrites with Quantitative Models'], ['Functional Requirement for Class I MHC in CNS Development and Plasticity'], ['Turning Blood into Brain: Cells Bearing Neuronal Antigens Generated in Vivo from Bone Marrow'], ['Breaking down Scientific Barriers to the Study of Brain and Mind'], ['Neuronal Plasticity: Increasing the Gain in Pain'], ['Response of Schwann Cells to Action Potentials in Development'], ['Kinesin Superfamily Motor Protein KIF17 and mLin-10 in NMDA Receptor-Containing Vesicle Transport']]

24 Cluster 11 :

25 [['Status and Improvements of Coupled General Circulation Models'], ['Sedimentary Rocks of Early Mars'], ['Climate Extremes: Observations, Modeling, and Impacts'], ["A 22,000-Year Record of Monsoonal Precipitation from Northern Chile's Atacama Desert"], ['Causes of Climate Change over the past 1000 Years'], ['Rapid Changes in the Hydrologic Cycle of the Tropical Atlantic during the Last Glacial'], ['Internal Structure and Early Thermal Evolution of Mars from Mars Global Surveyor Topography and Gravity'], ['Climate Impact of Late Quaternary Equatorial Pacific Sea Surface Temperature Variations'], ['Coherent High- and Low-Latitude Climate Variability during the Holocene Warm Period'], ['Is El Nino Changing?']]

26 Cluster 12 :

27 [['Patients' Voices: The Powerful Sound in the Stem Cell Debate'], ['Warming of the World Ocean'], ['A Lifelong Fascination with the Chick Embryo'], ['Rapid Evolution of Reproductive Isolation in the Wild: Evidence from Introduced Salmon'], ['National Academy of Sciences Elects New Members'], ['Trans-Pacific Air Pollution'], ['Scientists at Brookhaven'], ['Does Science Drive the Productivity Train?'], ['Clinical Research'], ['Corrections and Clarifications: Luzia Is Not Alone']]

28 Cluster 13 :

29 [[ 'Mechanism of ATP-Dependent Promoter Melting by Transcription  
Factor IIH'], ['b-Arrestin 2: A Receptor-Regulated MAPK  
Scaffold for the Activation of JNK3'], ['Role for Rapid  
Dendritic Protein Synthesis in Hippocampal mGluR-Dependent  
Long-Term Depression'], ['Interacting Molecular Loops in the  
Mammalian Circadian Clock'], ["Packard Heir Signs up for  
National 'Math Wars'"], ['Virus-Induced Neuronal Apoptosis  
Blocked by the Herpes Simplex Virus Latency-Associated  
Transcript'], ['Transgenic Mouse Model of Stunned Myocardium'],  
['Interconnected Feedback Loops in the Neurospora Circadian  
System'], ['Inhibition of Adipogenesis by Wnt Signaling'], ['An  
Inherited Functional Circadian Clock in Zebrafish Embryos']]

30 Cluster 14 :

31 [[ 'N-Cadherin, a Cell Adhesion Molecule Involved in  
Establishment of Embryonic Left-Right Asymmetry'], ['Transgenic  
Mouse Model of Stunned Myocardium'], ['Nota Bene: Contortions  
of the Heart'], ['Cardiovascular Evidence for an Intermediate  
or Higher Metabolic Rate in an Ornithischian Dinosaur'],  
['Resetting of Circadian Time in Peripheral Tissues by  
Glucocorticoid Signaling'], ['NIH, under Pressure, Boosts  
Minority Health Research'], ['Generalized Potential of Adult  
Neural Stem Cells'], ['New Age Semiconductors Pick up the  
Pace'], ["Stress: The Invisible Hand in Eastern Europe's Death  
Rates"], ['Role of Adenine Nucleotide Translocator 1 in mtDNA  
Maintenance']]

32 Cluster 15 :

33 [[ 'Emerging Infectious Diseases of Wildlife-Threats to  
Biodiversity and Human Health'], ['A Tale of Two Futures: HIV  
and Antiretroviral Therapy in San Francisco'], ['Predictions of  
Biodiversity Response to Genetically Modified Herbicide-  
Tolerant Crops'], ['A Tale of Two Selves'], ['Origins of HIV'],  
['Fairness versus Reason in the Ultimatum Game'], ['One  
Sequence, Two Ribozymes: Implications for the Emergence of New  
Ribozyme Folds'], ['Reversal of Antipsychotic-Induced Working  
Memory Deficits by Short-Term Dopamine D1 Receptor  
Stimulation'], ['Potent Analgesic Effects of GDNF in  
Neuropathic Pain States'], ['AIDS in a New Millennium']]

34 Cluster 16 :



35 [[ "Evidence for Crystalline Water and Ammonia Ices on Pluto's  
Satellite Charon"], ['Mount St. Helens, Master Teacher'],  
['Atomic Layer Deposition of Oxide Thin Films with Metal  
Alkoxides as Oxygen Sources'], ['Dynamics of the Pacific-North  
American Plate Boundary in the Western United States'],  
['Discovery of a Transient Absorption Edge in the X-ray  
Spectrum of GRB 990705'], ['Differential Clustering of CD4 and  
CD3z during T Cell Recognition'], ['Memory-A Century of  
Consolidation'], ['Motility Powered by Supramolecular Springs  
and Ratchets'], ['Response of Schwann Cells to Action  
Potentials in Development'], ['Piecing Together the Biggest  
Puzzle of All']]

36 Cluster 17 :

37 [['An Arresting Start for MAPK'], ["CERN's Gamble Shows Perils,  
Rewards of Playing the Odds"], ["Outrageous Events: Don't Count  
Them out"], ['Mechanism of ATP-Dependent Promoter Melting by  
Transcription Factor IIH'], ['A Wetter, Younger Mars  
Emerging'], ['Rapid Extragranular Plasticity in the Absence of  
Thalamocortical Plasticity in the Developing Primary Visual  
Cortex'], ['Rounding out Solutions to Three Conjectures'], ['On  
the Origin of Internal Structure of Word Forms'], ['Alternative  
Views on Alternative Medicine'], ["Candida's Arranged  
Marriage"]]

38 Cluster 18 :

39 [['Mode-Specific Energy Disposal in the Four-Atom Reaction  
 $\text{OH} + \text{D}_2 \rightarrow \text{HOD} + \text{D}$ '], ['A Short Fe-  
Fe Distance in Peroxodiferric Ferritin: Control of Fe Substrate  
versus Cofactor Decay?'], ['The Evolutionary Fate and  
Consequences of Duplicate Genes'], ["Fermat's Last Theorem's  
First Cousin"], ['Social Mentalizing Abilities in Mental  
Patients'], ['Nonavian Feathers in a Late Triassic Archosaur'],  
['Nonbiological Fractionation of Iron Isotopes'], ['A Cyclic  
Carbanionic Valence Isomer of a Carbocation: Diphosphino  
Analogues of Diaminocarboxocations'], ['Mechanisms of Ordering in  
Striped Patterns'], ['Bioinformatics in the Information Age']]

40 Cluster 19 :

41 [['Uptake of Glutamate into Synaptic Vesicles by an Inorganic  
Phosphate Transporter'], ['Gatekeepers of the Nucleus'],  
['VirB/D4-Dependent Protein Translocation from Agrobacterium  
into Plant Cells'], ['Structure of the Light-Driven Chloride  
Pump Halorhodopsin at 1.8  $\text{\AA}$  Resolution'],  
['Rab1 Recruitment of p115 into a cis-SNARE Complex:  
Programming Budding COPII Vesicles for Fusion'], ['Connectivity  
of Marine Populations: Open or Closed?'], ['How Cells Handle  
Cholesterol'], ['Trans-Pacific Air Pollution'], ['Transmembrane  
Molecular Pump Activity of Niemann-Pick C1 Protein'], ['The  
Influence of Canadian Forest Fires on Pollutant Concentrations  
in the United States']]

42 Cluster 20 :

43 [['Crystal Structure of the Ribonucleoprotein Core of the  
Signal Recognition Particle'], ['The Complete Atomic Structure  
of the Large Ribosomal Subunit at 2.4  $\text{\AA}$  Resolution'], ['Three-Dimensional Structure of the Tn5 Synaptic  
Complex Transposition Intermediate'], ['The Structural Basis of  
Ribosome Activity in Peptide Bond Synthesis'], ['Architecture  
of RNA Polymerase II and Implications for the Transcription  
Mechanism'], ['Comparative Genomics of the Eukaryotes'],  
['Positional Syntenic Cloning and Functional Characterization  
of the Mammalian Circadian Mutation tau'], ['The Way Things  
Move: Looking under the Hood of Molecular Motor Proteins'],  
['The Genome Sequence of Drosophila melanogaster'], ['Structure  
of the RNA Polymerase Domain of E. coli Primase']]

44 Cluster 21 :

45 [['ORCA3, a Jasmonate-Responsive Transcriptional Regulator of  
Plant Primary and Secondary Metabolism'], ['Psychological and  
Neural Mechanisms of the Affective Dimension of Pain'], ['The  
Complete Atomic Structure of the Large Ribosomal Subunit at 2.4  
 $\text{\AA}$  Resolution'], ['Green, Catalytic  
Oxidation of Alcohols in Water'], ['One Sequence, Two  
Ribozymes: Implications for the Emergence of New Ribozyme  
Folds'], ['A Structural Model of Transcription Elongation'],  
['Template Boundary in a Yeast Telomerase Specified by RNA  
Structure'], ['Impacts of Climatic Change and Fishing on  
Pacific Salmon Abundance over the past 300 Years'], ['Evidence  
for Recent Groundwater Seepage and Surface Runoff on Mars'],  
['Calcium-Aluminum-Rich Inclusions from Enstatite Chondrites:  
Indigenous or Foreign?']]

46 Cluster 22 :

47 [[ "Packard Heir Signs up for National 'Math Wars'", ['Islamic Women in Science'], ['Not (Just) in Kansas Anymore'], ['Graduate Educators Struggle to Grade Themselves'], ['The Spirit of Discovery'], ['Support Grows for British Exercise to Allocate University Funds'], ['Sharp Jump in Teaching Fellows Draws Fire from Educators'], ['Presidential Forum: Gore and Bush Offer Their Views on Science'], ["Iran's Scientists Cautiously Reach out to the World"], ['Scaling up HIV/AIDS Programs to National Coverage'] ]]

48 Cluster 23 :

49 [[ 'Advances in the Physics of High-Temperature Superconductivity', ['Quantum Criticality: Competing Ground States in Low Dimensions'], ['Orbital Physics in Transition-Metal Oxides'], ['The Atom-Cavity Microscope: Single Atoms Bound in Orbit by Single Photons'], ["Negative Poisson's Ratios for Extreme States of Matter"], ['Self-Mode-Locking of Quantum Cascade Lasers with Giant Ultrafast Optical Nonlinearities'], ['Generating Solitons by Phase Engineering of a Bose-Einstein Condensate'], ['Imaging Precessional Motion of the Magnetization Vector'], ['Subatomic Features on the Silicon (111)-(7 x 7) Surface Observed by Atomic Force Microscopy'], ['Blue-Fluorescent Antibodies'] ]]

50 Cluster 24 :

51 [[ 'NEAR at Eros: Imaging and Spectral Results', ['Climate Extremes: Observations, Modeling, and Impacts'], ['Reduction of Tropical Cloudiness by Soot'], ['Causes of Climate Change over the past 1000 Years'], ['The Atom-Cavity Microscope: Single Atoms Bound in Orbit by Single Photons'], ['High Magma Storage Rates before the 1983 Eruption of Kilauea, Hawaii'], ['Hematopoietic Stem Cell Quiescence Maintained by  $\text{p21}^{\text{cip1/waf1}}$ '], ['Climate Impact of Late Quaternary Equatorial Pacific Sea Surface Temperature Variations'], ['Internal Structure and Early Thermal Evolution of Mars from Mars Global Surveyor Topography and Gravity'], ['Isotope Fractionation and Atmospheric Oxygen: Implications for Phanerozoic  $\text{O}_2$  Evolution'] ]]

52 Cluster 25 :

53 [['Can Protected Areas Be Expanded in Africa?'], ['Status and Improvements of Coupled General Circulation Models'], ['Surveying the SBIR Program'], ['Tissue Engineers Build New Bone'], ['Interfering with Gene Expression'], ['Corrections and Clarifications: Commercialization of Genetic Research and Public Policy'], ['Corrections and Clarifications: Commercialization of Genetic Research and Public Policy'], ['Thyroid Tumor Banks'], ['Corrections and Clarifications: The Global Spread of Malaria in a Future, Warmer World'], ["Corrections and Clarifications: Fermat's Last Theorem's First Cousin"]]

54 Cluster 26 :

55 [['Global Analysis of the Genetic Network Controlling a Bacterial Cell Cycle'], ['Mitotic Misregulation and Human Aging'], ['Genes Expressed in Human Tumor Endothelium'], ['Inhibition of Adipogenesis by Wnt Signaling'], ['Interacting Molecular Loops in the Mammalian Circadian Clock'], ['From Marrow to Brain: Expression of Neuronal Phenotypes in Adult Mice'], ['Noxa, a BH3-Only Member of the Bcl-2 Family and Candidate Mediator of p53-Induced Apoptosis'], ['Translocation of C. elegans CED-4 to Nuclear Membranes during Programmed Cell Death'], ['Stat3-Mediated Transformation of NIH-3T3 Cells by the Constitutively Active Q205L  $\alpha$ -O<sub>2</sub> Protein'], ['A Subset of Viral Transcripts Packaged within Human Cytomegalovirus Particles']]

56 Cluster 27 :

57 [['Positional Syntenic Cloning and Functional Characterization of the Mammalian Circadian Mutation tau'], ['The Genome Sequence of Drosophila melanogaster'], ['Gridlock, an HLH Gene Required for Assembly of the Aorta in Zebrafish'], ['Piflp Helicase, a Catalytic Inhibitor of Telomerase in Yeast'], ['Conservation and Novelty in the Evolution of Cell Adhesion and Extracellular Matrix Genes'], ['Requirement of Mis6 Centromere Connector for Localizing a CENP-A-Like Protein in Fission Yeast'], ['Role of the Mouse ank Gene in Control of Tissue Calcification and Arthritis'], ['Comparative Genomics of the Eukaryotes'], ['Resetting of Circadian Time in Peripheral Tissues by Glucocorticoid Signaling'], ['Accumulation of Dietary Cholesterol in Sitosterolemia Caused by Mutations in Adjacent ABC Transporters']]

58 Cluster 28 :

```
59 [['New Observational Constraints for Atmospheric Hydroxyl on  
Global and Hemispheric Scales'], ['Dimensionality Effects in  
the Lifetime of Surface States'], ['Forster Energy Transfer in  
an Optical Microcavity'], ['Quantitative Imaging of Lateral  
ErbB1 Receptor Signal Propagation in the Plasma Membrane'], ['A  
Potent Greenhouse Gas Identified in the Atmosphere:  
$SF_5CF_3$'], ['Why Stem Cells?'], ['Intersubband  
Electroluminescence from Silicon-Based Quantum Cascade  
Structures'], ['Blue-Fluorescent Antibodies'], ['Molecules in a  
Bose-Einstein Condensate'], ['Quantifying Denitrification and  
Its Effect on Ozone Recovery']]
```

```
1  # b-5: Report the top ten words
2
3  vocab_df = pd.read_csv("data/science2k-vocab.txt", header=None)
4  vocab_array = np.array(vocab_df)
5  vocabs = vocab_array.tolist()
6  #print (vocabs[:20])
7  #print (len(vocabs))
8
9  def get_distances(n):
10     cn_idx_list,cn = cal_cn_idx_list(n)
11     cn_matrix = np.array(cn)
12     cn_mean_matrix = np.mean(cn_matrix, axis=0)
13     distances = []
14     for j in range(len(cn)):
15         distances.append(euclidean_distance(cn[j],
16 cn_mean_matrix))
17     return distances
18
19
20 print ("-----Top 10 words-----")
21
22 for n in cls:
23     cn_distances = get_distances(n)
24     #print (len(cn_distances))
25     #print (cn_distances)
26
27     # top 10 smallest distances in each cluster
28     min_idx = map(cn_distances.index, heapq.nsmallest(10,
29 cn_distances))
```

```

27     min_idx_list = list(min_idx)
28     #print(list(min_idx_list))
29
30     # report top 10 words
31     top_doc_list = []
32     for m in min_idx_list:
33         top_doc = vocabs[m]
34         top_doc_list.append(top_doc)
35     print ("Cluster",n,":")
36     print (top_doc_list)

```

```

1  -----Top 10 words-----
2  Cluster 0 :
3  [['graduate'], ['cyclin'], ['historical'], ['magnification'],
4  ['switching'], ['radial'], ['apart'], ['digital'],
5  ['stronger'], ['tuning']]
6  Cluster 1 :
7  [['fig']]
8  Cluster 2 :
9  [['amount'], ['identical'], ['patterns'], ['cortex'],
10 ['origin'], ['correspondence'], ['estimates'], ['working'],
11 ['thin'], ['voltage']]
12 Cluster 3 :
13 [['fig']]
14 Cluster 4 :
15 [['medium'], ['june'], ['spin'], ['united'], ['cellular'],
16 ['century'], ['method'], ['step'], ['helix'], ['increasing']]
17 Cluster 5 :
18 [['fig'], ['fig']]
19 Cluster 6 :
20 [['fig'], ['fig']]
21 Cluster 7 :
22 [['fig']]
23 Cluster 8 :
24 [['fig']]
25 Cluster 9 :
26 [['start'], ['vol'], ['www'], ['end'], ['cells'], ['time'],
27 ['data'], ['cell'], ['two'], ['science']]
28 Cluster 10 :
29 [['cell'], ['data'], ['time'], ['science'], ['two'],
30 ['protein'], ['end'], ['fig'], ['cells']]
31 Cluster 11 :

```

```
25  [['view'], ['band'], ['developed'], ['atoms'], ['chemical'],
    ['crystal'], ['correspondence'], ['expressed'], ['isolated'],
    ['oxygen']]
26  Cluster 12 :
27  [['fig']]
28  Cluster 13 :
29  [['fig']]
30  Cluster 14 :
31  [['fig']]
32  Cluster 15 :
33  [['fig']]
34  Cluster 16 :
35  [['fig']]
36  Cluster 17 :
37  [['fig']]
38  Cluster 18 :
39  [['fig']]
40  Cluster 19 :
41  [['fig']]
42  Cluster 20 :
43  [['information'], ['sequences'], ['neurons'], ['point'],
    ['determined'], ['age'], ['current'], ['addition'],
    ['activation'], ['expressed']]
44  Cluster 21 :
45  [['fig']]
46  Cluster 22 :
47  [['fig']]
48  Cluster 23 :
49  [['metal'], ['black'], ['chemical'], ['atoms'], ['involved'],
    ['open'], ['transition'], ['class'], ['components'],
    ['measurements']]
50  Cluster 24 :
51  [['science'], ['nature'], ['change'], ['site'], ['specific'],
    ['studies'], ['molecular'], ['changes'], ['says'], ['long']]
52  Cluster 25 :
53  [['fig']]
54  Cluster 26 :
55  [['science'], ['end'], ['cell'], ['cells'], ['fig'],
    ['protein'], ['data'], ['two']]
56  Cluster 27 :
```

```
57 [['results'], ['university'], ['shown'], ['genes'],  
    ['observed'], ['different'], ['type'], ['expression'],  
    ['high'], ['dna']]  
58 Cluster 28 :  
59 [['fig']]
```

## b-6

Comment on these results.

1.How might such an algorithm be useful?

- This algorithm can be applied to subject retrieval/document retrieval, which is to retrieve documents based on keywords. For example, if I want to search for science fiction documents, I can find the relevant documents by searching for the keyword "science fiction".

2.What is different about clustering terms from clustering documents?

- The difference is that clustering terms can retrieve documents by keywords, but clustering documents cannot retrieve documents by keywords.

## Question 2

```
1 import numpy as np  
2 import matplotlib.pyplot as plt  
3 import math  
4 import random
```

**2.(a) Download the Old Faithful Geyser Dataset. The data file contains 272 observations of (eruption time, waiting time). Treat each entry as a 2 dimensional feature vector. Parse and plot all data points on 2-D plane.**

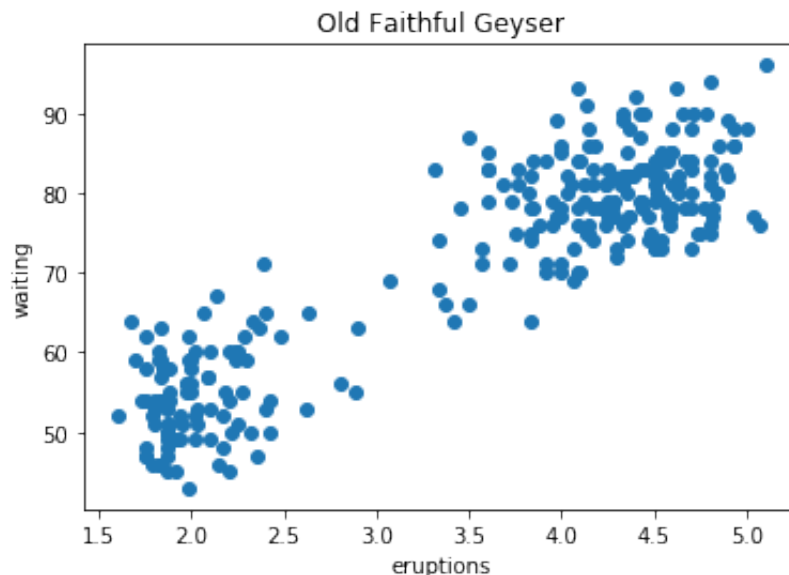
```
1 Data_list = []  
2 with open("old.txt", 'r') as in_file:  
3     for line in in_file.readlines():  
4         point = []  
5         point.append(float(line.split()[1]))
```



```

6         point.append(float(line.split()[2]))
7         Data_list.append(point)
8     Data = np.array(Data_list)
9     eruptions=[]
10    waiting=[]
11    for i in range(len(Data)):
12        eruptions.append(Data[i][0])
13        waiting.append(Data[i][1])
14
15    #plot scatter
16    plt.title('Old Faithful Geyser')
17    plt.scatter(eruptions, waiting)
18    plt.xlabel('eruptions')
19    plt.ylabel('waiting')
20    plt.show()

```



As can be seen from the scatter plot, the data set has two categories.

**2.(b) Implement a bimodal GMM model to fit all data points using EM algorithm. Explain the reasoning behind your termination criteria. For this problem, we assume the covariance matrix is spherical (i.e., it has the form of  $\sigma^2 I$  for scalar  $\sigma$ ) and you can randomly initialize Gaussian parameters. For evaluation purposes, please submit the following figures:**

Since the initial guess of mu and sigma are whole numbers, I set the termination criteria=0.01. When the difference between the two iterations is less than 0.01, it is considered that the parameters no longer change.

```
1 parameter_dict = {}
2 parameter_dict["mu1"] = np.array([0, 0])
3 parameter_dict["sigma1"] = np.array([[1, 0], [0, 1]])
4 parameter_dict["mu2"] = np.array([0, 0])
5 parameter_dict["sigma2"] = np.array([[1, 0], [0, 1]])
6 parameter_dict["piweight"] = 0.5
7 parameter_dict["gama_list"] = []
8
9
10 def set_parameter(mu_1, sigma_1, mu_2, sigma_2, pi_weight):
11     parameter_dict["mu1"] = mu_1
12     parameter_dict["mu1"].shape = (2, 1)
13     parameter_dict["sigma1"] = sigma_1
14     parameter_dict["mu2"] = mu_2
15     parameter_dict["mu2"].shape = (2, 1)
16     parameter_dict["sigma2"] = sigma_2
17     parameter_dict["piweight"] = pi_weight
18
19
20 def PDF(data, mu, sigma):
21
22     sigma_sqrt = math.sqrt(np.linalg.det(sigma))
23     sigma_inv = np.linalg.inv(sigma)
24     data.shape = (2, 1)
25     mu.shape = (2, 1)
26     minus_mu = data - mu
27     minus_mu_trans = np.transpose(minus_mu)
28     res = (1.0 / (2.0 * math.pi * sigma_sqrt)) * math.exp(
29         (-0.5) * (np.dot(np.dot(minus_mu_trans, sigma_inv),
30             minus_mu)))
31     return res
32
33 def E_step(Data):
34     sigma_1 = parameter_dict["sigma1"]
35     sigma_2 = parameter_dict["sigma2"]
36     pw = parameter_dict["piweight"]
37     mu_1 = parameter_dict["mu1"]
38     mu_2 = parameter_dict["mu2"]
```

```

38
39     parameter_dict["gama_list"] = []
40     for point in Data:
41         gama_i = (pw * PDF(point, mu_2, sigma_2)) / (
42             (1.0 - pw) * PDF(point, mu_1, sigma_1) + pw *
PDF(point, mu_2, sigma_2))
43         parameter_dict["gama_list"].append(gama_i)
44
45
46 def M_step(Data):
47     N1 = 0
48     N2 = 0
49     for i in range(len(parameter_dict["gama_list"])):
50         N1 += 1.0 - parameter_dict["gama_list"][i]
51         N2 += parameter_dict["gama_list"][i]
52
53     new_mu_1 = np.array([0, 0])
54     new_mu_2 = np.array([0, 0])
55     for i in range(len(parameter_dict["gama_list"])):
56         new_mu_1 = new_mu_1 + Data[i] * (1 -
parameter_dict["gama_list"][i]) / N1
57         new_mu_2 = new_mu_2 + Data[i] *
parameter_dict["gama_list"][i] / N2
58
59
60     new_mu_1.shape = (2, 1)
61     new_mu_2.shape = (2, 1)
62
63     new_sigma_1 = np.array([[0, 0], [0, 0]])
64     new_sigma_2 = np.array([[0, 0], [0, 0]])
65     for i in range(len(parameter_dict["gama_list"])):
66         data_tmp = [0, 0]
67         data_tmp[0] = Data[i][0]
68         data_tmp[1] = Data[i][1]
69         vec_tmp = np.array(data_tmp)
70         vec_tmp.shape = (2, 1)
71         new_sigma_1 = new_sigma_1 + np.dot((vec_tmp -
new_mu_1), (vec_tmp - new_mu_1).transpose()) * (1.0 -
parameter_dict["gama_list"][i]) / N1
72         new_sigma_2 = new_sigma_2 + np.dot((vec_tmp -
new_mu_2), (vec_tmp - new_mu_2).transpose()) *
parameter_dict["gama_list"][i] / N2

```

```

73         # print np.dot((vec_tmp-new_mu_1), (vec_tmp-
new_mu_1).transpose())
74     new_pi = N2 / len(parameter_dict["gama_list"])
75
76     parameter_dict["mu1"] = new_mu_1
77     parameter_dict["mu2"] = new_mu_2
78     parameter_dict["sigma1"] = new_sigma_1
79     parameter_dict["sigma2"] = new_sigma_2
80     parameter_dict["piweight"] = new_pi
81

```

i). Plot the trajectories of two mean vectors in 2 dimensions (i.e., coordinates vs. iteration).

```

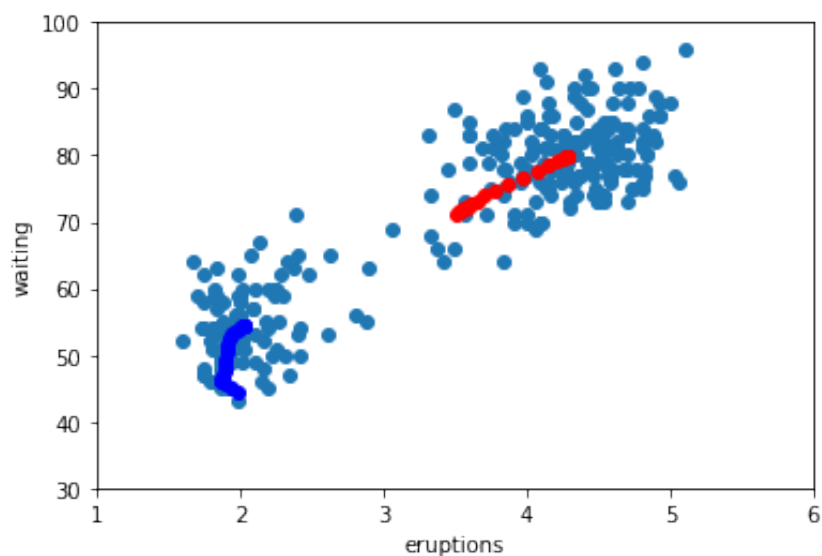
1  #Plot the trajectories
2  def EM_iterate_trajectories(iter_time, Data, mu_1, sigma_1,
mu_2, sigma_2, pi_weight, esp=0.01):
3
4      mean_trace_1 = [[], []]
5      mean_trace_2 = [[], []]
6
7      set_parameter(mu_1, sigma_1, mu_2, sigma_2, pi_weight)
8      if iter_time == None:
9          while (True):
10             old_mu_1 = parameter_dict["mu1"].copy()
11             old_mu_2 = parameter_dict["mu2"].copy()
12             E_step(Data)
13             M_step(Data)
14             delta_1 = parameter_dict["mu1"] - old_mu_1
15             delta_2 = parameter_dict["mu2"] - old_mu_2
16
17             mean_trace_1[0].append(parameter_dict["mu1"][0][0])
18             mean_trace_1[1].append(parameter_dict["mu1"][1][0])
19             mean_trace_2[0].append(parameter_dict["mu2"][0][0])
20             mean_trace_2[1].append(parameter_dict["mu2"][1][0])
21             if math.fabs(delta_1[0]) < esp and
math.fabs(delta_1[1]) < esp and math.fabs(
22                 delta_2[0]) < esp and math.fabs(delta_2[1])
< esp:
23                 break
24             else:

```

```

25         for i in range(iter_time):
26             pass
27
28         plt.xlim(xmax=6, xmin=1)
29         plt.ylim(ymax=100, ymin=30)
30         plt.xlabel("eruptions")
31         plt.ylabel("waiting")
32         plt.scatter(eruptions, waiting)
33         plt.plot(mean_trace_1[0], mean_trace_1[1], 'ro')
34         plt.plot(mean_trace_2[0], mean_trace_2[1], 'bo')
35         plt.show()
36
37     def task_1():
38         Mu_1 = np.array([3, 60])
39         Sigma_1 = np.array([[10, 0], [0, 10]])
40         Mu_2 = np.array([1, 30])
41         Sigma_2 = np.array([[10, 0], [0, 10]])
42         Pi_weight = 0.5
43         EM_iterate_trajectories(None, Data, Mu_1, Sigma_1, Mu_2,
44                                Sigma_2, Pi_weight)
45     task_1()

```



Choose  $\mu_1 = [3, 60]$ ,  $\mu_2 = [1, 30]$ ,  $\sigma_1 = [[10, 0], [0, 10]]$ ,  $\sigma_2 = [[10, 0], [0, 10]]$  as the initial input since after observing the scatter plot of the dataset we can see the two  $\mu$  we guess is on the left side of the bottom of two categories. Thus, we could see the trajectories clearly and as complete as possible.

ii). Run your program for 50 times with different initial parameter guesses. Show the distribution of the total number of iterations needed for algorithm to converge.

```
1  #Run the program for 50 times with different initial parameter
   guesses.
2  def EM_iterate_times(Data, mu_1, sigma_1, mu_2, sigma_2,
   pi_weight, esp=0.01):
3
4      set_parameter(mu_1, sigma_1, mu_2, sigma_2, pi_weight)
5      iter_times = 0
6      while (True):
7          iter_times += 1
8          old_mu_1 = parameter_dict["mu1"].copy()
9          old_mu_2 = parameter_dict["mu2"].copy()
10         E_step(Data)
11         M_step(Data)
12         delta_1 = parameter_dict["mu1"] - old_mu_1
13         delta_2 = parameter_dict["mu2"] - old_mu_2
14         if math.fabs(delta_1[0]) < esp and
math.fabs(delta_1[1]) < esp and math.fabs(
15             delta_2[0]) < esp and math.fabs(delta_2[1]) <
esp:
16             break
17         return iter_times
18
19 def task_2():
20     iter_times=0
21     try:
22         x_11 = random.uniform(0, 4)
23         x_12 = random.uniform(30, 70)
24         x_21 = random.uniform(2, 6)
25         x_22 = random.uniform(50, 100)
26         Mu_1 = np.array([x_11, x_12])
27         x_31 = random.uniform(1, 20)
28         Sigma_1 = np.array([[x_31, 0], [0, x_31]])
29         Mu_2 = np.array([x_21, x_22])
30         Sigma_2 = np.array([[x_31, 0], [0, x_31]])
31         Pi_weight = 0.5
```

```

32     iter_times = EM_iterate_times(Data, Mu_1, Sigma_1,
Mu_2, Sigma_2, Pi_weight)
33     print ('mu1=[',x_11,',',x_12,'],mu2=
['',x_21,',',x_22,'],'total number of iterations=',iter_times)
34     except Exception:
35         print (Exception)
36     return iter_times
37
38 iteration=[]
39 for i in range(50):
40     iteration.append(task_2())
41 plt.hist(iteration)
42 plt.title('GMM')
43 plt.show
44
45
46
47 def M_step_1(Data):
48     N1 = 0
49     N2 = 0
50     for i in range(len(parameter_dict["gama_list"])):
51         N1 += 1.0 - parameter_dict["gama_list"][i]
52         N2 += parameter_dict["gama_list"][i]
53
54     new_mu_1 = np.array([0, 0])
55     new_mu_2 = np.array([0, 0])
56     for i in range(len(parameter_dict["gama_list"])):
57         new_mu_1 = new_mu_1 + Data[i] * (1 -
parameter_dict["gama_list"][i]) / N1
58         new_mu_2 = new_mu_2 + Data[i] *
parameter_dict["gama_list"][i] / N2
59
60
61     new_mu_1.shape = (2, 1)
62     new_mu_2.shape = (2, 1)
63
64     new_sigma_1 = np.array([[0, 0], [0, 0]])
65     new_sigma_2 = np.array([[0, 0], [0, 0]])
66     for i in range(len(parameter_dict["gama_list"])):
67         data_tmp = [0, 0]
68         data_tmp[0] = Data[i][0]
69         data_tmp[1] = Data[i][1]

```

```

70     vec_tmp = np.array(data_tmp)
71     vec_tmp.shape = (2, 1)
72     new_sigma_1 = new_sigma_1 + np.dot((vec_tmp -
new_mu_1), (vec_tmp - new_mu_1).transpose()) * (1.0 -
parameter_dict["gama_list"][i]) / N1
73     new_sigma_2 = new_sigma_2 + np.dot((vec_tmp -
new_mu_2), (vec_tmp - new_mu_2).transpose()) *
parameter_dict["gama_list"][i] / N2
74     # print np.dot((vec_tmp-new_mu_1), (vec_tmp-
new_mu_1).transpose())
75     new_pi = N2 / len(parameter_dict["gama_list"])
76
77     parameter_dict["mu1"] = new_mu_1
78     parameter_dict["mu2"] = new_mu_2
79     parameter_dict["sigma1"] = new_sigma_1
80     parameter_dict["sigma2"] = new_sigma_2
81     parameter_dict["piweight"] = new_pi
82     covm1=[ ]
83     covm2=[ ]
84     print(new_mu_1)
85     print(new_mu_2)
86     covm1.append(new_sigma_1[0][0])
87     covm1.append(new_sigma_1[1][1])
88     covm2.append(new_sigma_2[0][0])
89     covm2.append(new_sigma_2[1][1])
90     print(covm1)
91     print(covm2)
92     #EM result:center and covariance matrix
93     E_step(Data)
94     M_step_1(Data)

```

```

1  mu1=[ 0.1893135405201245 , 35.369020344606255 ],mu2=[
4.345307785548732 , 64.63663783179955 ] total number of
iterations= 15
2  mu1=[ 2.221758431528942 , 45.47747359129394 ],mu2=[
4.0934557777931495 , 53.714273021455675 ] total number of
iterations= 15
3  mu1=[ 2.8432992305101483 , 31.42269914464936 ],mu2=[
4.31931126754017 , 83.83778519912337 ] total number of
iterations= 10

```



4 mul=[ 3.094910237592582 , 53.37228667775115 ],mu2=[  
4.619537418786634 , 64.63983267902262 ] total number of  
iterations= 9

5 mul=[ 0.8719747538166236 , 46.76388076310295 ],mu2=[  
2.005938861877005 , 91.38603886689017 ] total number of  
iterations= 6

6 mul=[ 0.0845258727660041 , 59.246730062985264 ],mu2=[  
2.49894764043518 , 60.130329127166405 ] total number of  
iterations= 13

7 mul=[ 2.9629717440087098 , 53.06543041297001 ],mu2=[  
4.555527171270407 , 86.03855911794619 ] total number of  
iterations= 6

8 mul=[ 1.9769560409458733 , 44.13450566893186 ],mu2=[  
3.041613249704096 , 77.49528397696082 ] total number of  
iterations= 8

9 mul=[ 1.9968414447742209 , 31.062437605032972 ],mu2=[  
5.274612911990247 , 55.565061254341444 ] total number of  
iterations= 9

10 mul=[ 2.2803772969098466 , 33.976268025059234 ],mu2=[  
3.8430136950093567 , 76.18116984311325 ] total number of  
iterations= 11

11 mul=[ 1.1376652390642539 , 45.43551455238631 ],mu2=[  
4.36609105083032 , 84.43625665492587 ] total number of  
iterations= 3

12 mul=[ 3.6629922126674384 , 46.86452042143449 ],mu2=[  
2.2748867821848564 , 52.294834501504766 ] total number of  
iterations= 16

13 mul=[ 0.3915060586649006 , 69.2662185623231 ],mu2=[  
3.268545013895078 , 88.83529026087001 ] total number of  
iterations= 13

14 mul=[ 2.630806312503527 , 39.35272269523833 ],mu2=[  
5.220488801727269 , 52.28495969819305 ] total number of  
iterations= 17

15 mul=[ 1.7861812550507268 , 35.90250627140895 ],mu2=[  
3.9633365219410694 , 94.03209006667464 ] total number of  
iterations= 4

16 mul=[ 0.3691169903609919 , 48.44419814390284 ],mu2=[  
5.229180814491622 , 70.2663021636601 ] total number of  
iterations= 8

17 mul=[ 0.8603210513259905 , 46.90288032657365 ],mu2=[  
4.233308171087751 , 51.212466118429504 ] total number of  
iterations= 16

18 mul=[ 0.4911690066962877 , 66.02275700646787 ],mu2=[  
2.944335115977025 , 97.9389785646695 ] total number of  
iterations= 16

19 mul=[ 0.8051782769011528 , 48.5732584441359 ],mu2=[  
2.546086943527769 , 93.16077946406496 ] total number of  
iterations= 7

20 mul=[ 3.4854843931704442 , 47.73486188316144 ],mu2=[  
5.979177585377549 , 61.28617570938973 ] total number of  
iterations= 11

21 mul=[ 2.852386438452337 , 36.637774289861255 ],mu2=[  
4.383406686700793 , 71.54195119524215 ] total number of  
iterations= 12

22 mul=[ 2.0043255070479726 , 36.400725821714545 ],mu2=[  
5.739160437971196 , 73.44246797647395 ] total number of  
iterations= 11

23 mul=[ 2.6957374475102016 , 31.539154708990512 ],mu2=[  
5.232567282361543 , 84.33006323297006 ] total number of  
iterations= 10

24 mul=[ 3.3878592670906844 , 38.89144997455178 ],mu2=[  
4.7804473273958 , 63.991090254053475 ] total number of  
iterations= 14

25 mul=[ 3.513569268511476 , 31.790252280542767 ],mu2=[  
5.613092774672461 , 68.48760949542064 ] total number of  
iterations= 15

26 mul=[ 0.9846761978958227 , 45.85074014878293 ],mu2=[  
5.893955561355381 , 88.01744812757072 ] total number of  
iterations= 5

27 mul=[ 1.6084893867380616 , 69.44175084065354 ],mu2=[  
2.099294439324174 , 82.90147379022544 ] total number of  
iterations= 10

28 mul=[ 2.572486164344156 , 41.12062253180023 ],mu2=[  
2.226112724849305 , 93.70290690390274 ] total number of  
iterations= 5

29 mul=[ 0.9535833498412507 , 57.176492968114694 ],mu2=[  
5.568121493274575 , 54.1627517305873 ] total number of  
iterations= 11

30 mul=[ 3.318145031187072 , 42.376800664958765 ],mu2=[  
4.378244151290286 , 74.93711588049547 ] total number of  
iterations= 9

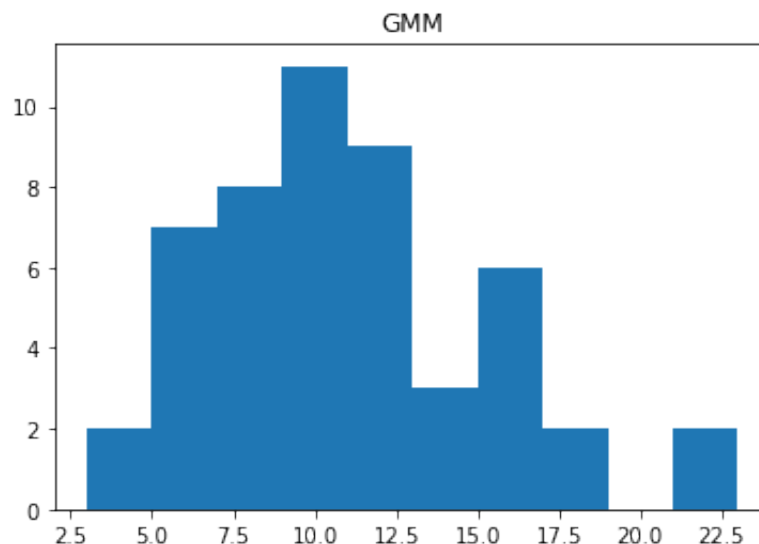
31 mul=[ 3.049698162970447 , 35.677793710549864 ],mu2=[  
2.777281161152568 , 58.39125094218829 ] total number of  
iterations= 18

```
32 mul=[ 0.04830041564780041 , 43.20119999087454 ],mu2=[  
4.820290852579051 , 99.37770639034278 ] total number of  
iterations= 7  
33 mul=[ 2.683818372497481 , 52.69776536228356 ],mu2=[  
5.579858632363873 , 92.0928442357467 ] total number of  
iterations= 7  
34 mul=[ 2.103102347922838 , 39.74264015852395 ],mu2=[  
4.683514312055834 , 72.10140166404754 ] total number of  
iterations= 10  
35 mul=[ 1.9050722120931396 , 45.28556168427721 ],mu2=[  
3.888850058106143 , 95.51868786005926 ] total number of  
iterations= 7  
36 mul=[ 1.217966932603813 , 43.386403151642625 ],mu2=[  
3.9644910623022818 , 69.28408547870853 ] total number of  
iterations= 10  
37 mul=[ 1.4699657079480386 , 45.206730753849 ],mu2=[  
3.4684049139009185 , 64.83729537736575 ] total number of  
iterations= 11  
38 mul=[ 3.772247987679945 , 53.971735638719466 ],mu2=[  
2.6725264456168514 , 61.172305234158266 ] total number of  
iterations= 10  
39 mul=[ 3.484023151232147 , 34.245693344673505 ],mu2=[  
2.2162015261379664 , 56.46513266029492 ] total number of  
iterations= 23  
40 mul=[ 1.6654685051621012 , 55.8290731210131 ],mu2=[  
5.984902395692766 , 78.96466958464332 ] total number of  
iterations= 5  
41 mul=[ 2.116223197482958 , 64.82651145356806 ],mu2=[  
3.329457762612093 , 63.36197863011105 ] total number of  
iterations= 9  
42 mul=[ 3.1358889079370194 , 54.768000392499616 ],mu2=[  
3.849384314442742 , 65.12947860169258 ] total number of  
iterations= 8  
43 mul=[ 0.581119062404257 , 61.63814314559249 ],mu2=[  
3.3661240839425646 , 58.260926370224766 ] total number of  
iterations= 7  
44 mul=[ 1.0382006112690023 , 66.03695087230457 ],mu2=[  
3.208217531208292 , 87.56361837596404 ] total number of  
iterations= 11  
45 mul=[ 3.8022212377216573 , 42.506701341004586 ],mu2=[  
2.760074054725767 , 90.82317636218744 ] total number of  
iterations= 5
```

```

46 mu1=[ 0.39827078755873657 , 62.396269838122656 ],mu2=[
    4.956109112338703 , 93.86805504834047 ] total number of
    iterations= 12
47 mu1=[ 1.135347070198784 , 59.74306249721188 ],mu2=[
    2.871591896482854 , 55.82066991182267 ] total number of
    iterations= 9
48 mu1=[ 1.45475524405298 , 60.66978871723049 ],mu2=[
    2.400002795883992 , 94.22238571061874 ] total number of
    iterations= 12
49 mu1=[ 1.4575503927461755 , 44.062498563433834 ],mu2=[
    3.324706803550839 , 88.27731477686163 ] total number of
    iterations= 5
50 mu1=[ 1.1775053987034951 , 34.99770923313082 ],mu2=[
    3.678004414331871 , 54.29914446593736 ] total number of
    iterations= 21
51 [[ 2.03637021]
52  [54.47833297]]
53 [[ 4.28964582]
54  [79.96791981]]
55 [0.06915319086909583, 33.69625389445514]
56 [0.16998893740998494, 36.049148881677446]

```



After observing the scatter plot on dataset, randomly choose  $\mu_1, \mu_2$  in uniform distribution  $[U(0, 4), U(30, 70)]$  and  $[U(2, 6), U(50, 100)]$ , randomly choose  $\sigma_1, \sigma_2$  in  $[[U(1, 20), 0], [0, U(1, 20)]]$  as the initial guess. The distribution of the total number of iterations needed for algorithm to converge is nearly a normal distribution.

## 2.(c) Repeat the task in (b) but with the initial guesses of the parameters generated from the following process:

i). Run a k-means algorithm over all the data points with  $K = 2$  and label each point with one of the two clusters.

```
1  import numpy as np
2  import math
3  import matplotlib.pyplot as plt
4
5  #load data
6  Data_list = []
7  with open("old.txt", 'r') as in_file:
8      for line in in_file.readlines():
9          point = []
10         point.append(float(line.split()[1]))
11         point.append(float(line.split()[2]))
12         Data_list.append(point)
13  Data = np.array(Data_list)
14  eruptions=[]
15  waiting=[]
16  for i in range(len(Data)):
17      eruptions.append(Data[i][0])
18      waiting.append(Data[i][1])
19
20  #k-means and label each point
21  def distEclud(vecA, vecB):
22      return np.sqrt(np.sum(np.power(vecA - vecB, 2)))
23
24  def randCent(dataSet, k):
25      n = np.shape(dataSet)[1]
26      centroids = np.mat(np.zeros([k, n]))
27      for j in range(n):
28          minj = np.min(dataSet[:,j])
29          rangej = float(np.max(dataSet[:,j]) - minj)
30          centroids[:,j] = np.mat(minj + rangej *
np.random.rand(k, 1))
31      print('initial kmeans guess:',centroids)
32      return centroids
33
```

```

34
35 def KMeans(dataSet, k, distMeans= distEclud, createCent=
randCent):
36     m = np.shape(dataSet)[0]
37     clusterAssement = np.mat(np.zeros([m,2]))
38     centroids = createCent(dataSet, k)
39     clusterChanged = True
40     while clusterChanged:
41         clusterChanged = False
42         for i in range(m):
43             minDist = np.inf
44             minIndex = -1
45             for j in range(k):
46                 distJ = distMeans(centroids[j,:], dataSet[i,:])
47                 if distJ < minDist:
48                     minDist = distJ
49                     minIndex = j
50             if clusterAssement[i,0] != minIndex:
51                 clusterChanged = True
52                 clusterAssement[i,:] = minIndex, minDist**2
53
54
55         cls0 = dataSet[np.nonzero(clusterAssement[:,0].A == 0)
[0]]
56         centroids[0,:] = np.mean(cls0, axis = 0)
57         cls1 = dataSet[np.nonzero(clusterAssement[:,0].A == 1)
[0]]
58         centroids[1,:] = np.mean(cls1, axis = 0)
59         return centroids, cls0,cls1
60
61 center, cls0,cls1 = KMeans(Data, 2)
62 print(center)

```

```

1 initial kmeans guess: [[ 2.69965796 78.79270623]
2 [ 1.91038355 54.62693443]]
3 [[ 4.29793023 80.28488372]
4 [ 2.09433      54.75      ]]

```

The initial guess is  $\mu_1=[2.69965796, 78.79270623]$ ,  $\mu_2=[1.91038355, 54.62693443]$  and the centre is  $[4.29793023, 80.28488372]$  and  $[2.09433, 54.75]$ .

ii). Estimate the first guess of the mean and covariance matrices using maximum likelihood over the labeled data points.

```
1  #maximum likelihood over the labeled data points
2  covm0=[ ]
3  covm1=[ ]

4  mu0 = cls0.mean(axis=0)

5  sigma0 = (cls0-mu0).T @ (cls0-mu0) / cls0.shape[0]
6  mu1 = cls1.mean(axis=0)

7  sigma1 = (cls1-mu1).T @ (cls1-mu1) / cls1.shape[0]

8  print(mu0)
9  print(mu1)
10 covm0.append(sigma0[0][0])
11 covm0.append(sigma0[1][1])
12 covm1.append(sigma1[0][0])
13 covm1.append(sigma1[1][1])
14 print(covm0)
15 print(covm1)
```

```
1  [ 4.29793023 80.28488372]
2  [ 2.09433 54.75 ]
3  [0.17761716955110854, 31.48279475392103]
4  [0.15427870109999997, 34.4075]
```

mean: [ 4.29793023, 80.28488372],[ 2.09433, 54.75 ] covariance matrix:  
[[0.17761716955110854, 31.48279475392103][0.15427870109999997, 34.4075]]

iii). Plot the trajectories of two mean vectors in 2 dimensions (i.e., coordinates vs. iteration).

---

```

1 parameter_dict = {}
2 parameter_dict["mu1"] = mu0
3 parameter_dict["sigma1"] = sigma0
4 parameter_dict["mu2"] = mu1
5 parameter_dict["sigma2"] = sigma1
6 parameter_dict["piweight"] = 0.5
7 parameter_dict["gama_list"] = []
8
9
10 def set_parameter(mu_1, sigma_1, mu_2, sigma_2, pi_weight):
11     parameter_dict["mu1"] = mu_1
12     parameter_dict["mu1"].shape = (2, 1)
13     parameter_dict["sigma1"] = sigma_1
14     parameter_dict["mu2"] = mu_2
15     parameter_dict["mu2"].shape = (2, 1)
16     parameter_dict["sigma2"] = sigma_2
17     parameter_dict["piweight"] = pi_weight
18
19
20 def PDF(data, mu, sigma):
21
22     sigma_sqrt = math.sqrt(np.linalg.det(sigma))
23     sigma_inv = np.linalg.inv(sigma)
24     data.shape = (2, 1)
25     mu.shape = (2, 1)
26     minus_mu = data - mu
27     minus_mu_trans = np.transpose(minus_mu)
28     res = (1.0 / (2.0 * math.pi * sigma_sqrt)) * math.exp(
29         (-0.5) * (np.dot(np.dot(minus_mu_trans, sigma_inv),
30 minus_mu)))
31     return res
32
33 def E_step(Data):
34     sigma_1 = parameter_dict["sigma1"]
35     sigma_2 = parameter_dict["sigma2"]
36     pw = parameter_dict["piweight"]
37     mu_1 = parameter_dict["mu1"]
38     mu_2 = parameter_dict["mu2"]
39
40     parameter_dict["gama_list"] = []
41     for point in Data:
42         gama_i = (pw * PDF(point, mu_2, sigma_2)) / (

```



```

42         (1.0 - pw) * PDF(point, mu_1, sigma_1) + pw *
PDF(point, mu_2, sigma_2))
43         parameter_dict["gama_list"].append(gama_i)
44
45
46 def M_step(Data):
47     N1 = 0
48     N2 = 0
49     for i in range(len(parameter_dict["gama_list"])):
50         N1 += 1.0 - parameter_dict["gama_list"][i]
51         N2 += parameter_dict["gama_list"][i]
52
53     new_mu_1 = np.array([0, 0])
54     new_mu_2 = np.array([0, 0])
55     for i in range(len(parameter_dict["gama_list"])):
56         new_mu_1 = new_mu_1 + Data[i] * (1 -
parameter_dict["gama_list"][i]) / N1
57         new_mu_2 = new_mu_2 + Data[i] *
parameter_dict["gama_list"][i] / N2
58
59
60     new_mu_1.shape = (2, 1)
61     new_mu_2.shape = (2, 1)
62
63     new_sigma_1 = np.array([[0, 0], [0, 0]])
64     new_sigma_2 = np.array([[0, 0], [0, 0]])
65     for i in range(len(parameter_dict["gama_list"])):
66         data_tmp = [0, 0]
67         data_tmp[0] = Data[i][0]
68         data_tmp[1] = Data[i][1]
69         vec_tmp = np.array(data_tmp)
70         vec_tmp.shape = (2, 1)
71         new_sigma_1 = new_sigma_1 + np.dot((vec_tmp -
new_mu_1), (vec_tmp - new_mu_1).transpose()) * (1.0 -
parameter_dict["gama_list"][i]) / N1
72         new_sigma_2 = new_sigma_2 + np.dot((vec_tmp -
new_mu_2), (vec_tmp - new_mu_2).transpose()) *
parameter_dict["gama_list"][i] / N2
73         # print np.dot((vec_tmp-new_mu_1), (vec_tmp-
new_mu_1).transpose())
74         new_pi = N2 / len(parameter_dict["gama_list"])
75

```

```

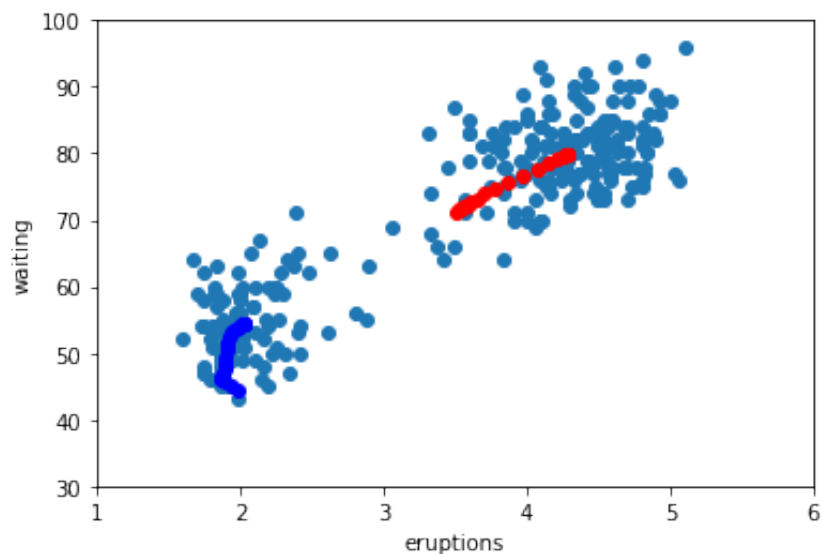
76     parameter_dict["mu1"] = new_mu_1
77     parameter_dict["mu2"] = new_mu_2
78     parameter_dict["sigma1"] = new_sigma_1
79     parameter_dict["sigma2"] = new_sigma_2
80     parameter_dict["piweight"] = new_pi
81
82     #Plot the trajectories
83     def EM_iterate_trajectories(iter_time, Data, mu_1, sigma_1,
84                                mu_2, sigma_2, pi_weight, esp=0.01):
85
86         mean_trace_1 = [[], []]
87         mean_trace_2 = [[], []]
88
89         set_parameter(mu_1, sigma_1, mu_2, sigma_2, pi_weight)
90         if iter_time == None:
91             while (True):
92                 old_mu_1 = parameter_dict["mu1"].copy()
93                 old_mu_2 = parameter_dict["mu2"].copy()
94                 E_step(Data)
95                 M_step(Data)
96                 delta_1 = parameter_dict["mu1"] - old_mu_1
97                 delta_2 = parameter_dict["mu2"] - old_mu_2
98
99                 mean_trace_1[0].append(parameter_dict["mu1"][0]
100 [0])
101                 mean_trace_1[1].append(parameter_dict["mu1"][1]
102 [0])
103                 mean_trace_2[0].append(parameter_dict["mu2"][0]
104 [0])
105                 mean_trace_2[1].append(parameter_dict["mu2"][1]
106 [0])
107
108                 if math.fabs(delta_1[0]) < esp and
109 math.fabs(delta_1[1]) < esp and math.fabs(
110 delta_2[0]) < esp and
111 math.fabs(delta_2[1]) < esp:
112                     break
113             else:
114                 for i in range(iter_time):
115                     pass
116
117     plt.xlim(xmax=6, xmin=1)
118     plt.ylim(ymax=100, ymin=30)

```

```

111 plt.xlabel("eruptions")
112 plt.ylabel("waiting")
113 plt.scatter(eruptions, waiting)
114 plt.plot(mean_trace_1[0], mean_trace_1[1], 'ro')
115 plt.plot(mean_trace_2[0], mean_trace_2[1], 'bo')
116 plt.show()
117
118 def task_1():
119     Mu_1 = np.array([3, 60])
120     Sigma_1 = np.array([[10, 0], [0, 10]])
121     Mu_2 = np.array([1, 30])
122     Sigma_2 = np.array([[10, 0], [0, 10]])
123     Pi_weight = 0.5
124
125     EM_iterate_trajectories(None, Data, Mu_1, Sigma_1, Mu_2,
126                             Sigma_2, Pi_weight)
127 task_1()

```



The choice of input is the same as (b)

**iv). Run your program for 50 times with different initial parameter guesses. Show the distribution of the total number of iterations needed for algorithm to converge.**

```

1 def EM_iterate_times(Data, mu_1, sigma_1, mu_2, sigma_2,
2   pi_weight, esp=0.01):

```

```

3     set_parameter(mu_1, sigma_1, mu_2, sigma_2, pi_weight)
4     iter_times = 0
5     while (True):
6         iter_times += 1
7         old_mu_1 = parameter_dict["mu1"].copy()
8         old_mu_2 = parameter_dict["mu2"].copy()
9         E_step(Data)
10        M_step(Data)
11        delta_1 = parameter_dict["mu1"] - old_mu_1
12        delta_2 = parameter_dict["mu2"] - old_mu_2
13        if math.fabs(delta_1[0]) < esp and
math.fabs(delta_1[1]) < esp and math.fabs(
14            delta_2[0]) < esp and math.fabs(delta_2[1]) <
esp:
15            break
16        return iter_times
17
18    def task_2():
19        center, cls0, cls1 = KMeans(Data, 2)
20
21        mu0 = cls0.mean(axis=0)
22
23        sigma0 = (cls0-mu0).T @ (cls0-mu0) / cls0.shape[0]
24        mu1 = cls1.mean(axis=0)
25
26        sigma1 = (cls1-mu1).T @ (cls1-mu1) / cls1.shape[0]
27
28        try:
29            Mu_1 = mu0
30            Sigma_1 = sigma0
31            Mu_2 = mu1
32            Sigma_2 = sigma1
33            Pi_weight = 0.5

```

```

30     iter_times = EM_iterate_times(Data, Mu_1, Sigma_1,
    Mu_2, Sigma_2, Pi_weight)
31     print ('input of EM:mu1=[',mu0,'],mu2=[',mu1,']','total
    number of iterations=',iter_times)
32     except Exception:
33         print (Exception)
34     return iter_times
35
36 iteration=[]
37 for i in range(50):
38     iteration.append(task_2())
39 plt.hist(iteration)
40 plt.title('K-means+ML')
41 plt.show
42

```

```

1  initial kmeans guess: [[ 2.68930826 93.75045882]
2  [ 3.65814928 54.44413587]]
3  input of EM:mu1=[ [ 4.29793023]
4  [80.28488372]] ],mu2=[ [ 2.09433]
5  [54.75    ]] ] total number of iterations= 4
6  initial kmeans guess: [[ 3.95760765 47.48360481]
7  [ 4.55666981 76.8755731 ]]
8  input of EM:mu1=[ [ 2.09433]
9  [54.75    ]] ],mu2=[ [ 4.29793023]
10 [80.28488372]] ] total number of iterations= 4
11 initial kmeans guess: [[ 4.07559629 51.21773633]
12 [ 3.48531779 66.4135674 ]]
13 input of EM:mu1=[ [ 2.09433]
14 [54.75    ]] ],mu2=[ [ 4.29793023]
15 [80.28488372]] ] total number of iterations= 4
16 initial kmeans guess: [[ 1.85806105 80.8013877 ]
17 [ 2.34142912 74.71229712]]
18 input of EM:mu1=[ [ 4.29793023]
19 [80.28488372]] ],mu2=[ [ 2.09433]
20 [54.75    ]] ] total number of iterations= 4
21 initial kmeans guess: [[ 3.81930558 93.10057294]
22 [ 2.68298853 85.2048207 ]]
23 input of EM:mu1=[ [ 4.29793023]
24 [80.28488372]] ],mu2=[ [ 2.09433]
25 [54.75    ]] ] total number of iterations= 4
26 initial kmeans guess: [[ 1.80286387 73.53321619]

```

```
27 [ 3.35986242 74.52127337]]
28 input of EM:mu1=[ [[ 2.09433]
29 [54.75 ] ] ],mu2=[ [[ 4.29793023]
30 [80.28488372]] ] total number of iterations= 4
31 initial kmeans guess: [[ 1.71396954 85.04776507]
32 [ 2.47802169 63.06664963]]
33 input of EM:mu1=[ [[ 4.29793023]
34 [80.28488372]] ],mu2=[ [[ 2.09433]
35 [54.75 ] ] ] total number of iterations= 4
36 initial kmeans guess: [[ 3.35683763 48.35045179]
37 [ 4.08482155 78.73504159]]
38 input of EM:mu1=[ [[ 2.09433]
39 [54.75 ] ] ],mu2=[ [[ 4.29793023]
40 [80.28488372]] ] total number of iterations= 4
41 initial kmeans guess: [[ 2.17308827 61.18730929]
42 [ 1.84641703 74.96256695]]
43 input of EM:mu1=[ [[ 2.09433]
44 [54.75 ] ] ],mu2=[ [[ 4.29793023]
45 [80.28488372]] ] total number of iterations= 4
46 initial kmeans guess: [[ 4.97404181 50.19363041]
47 [ 4.29541262 56.94099265]]
48 input of EM:mu1=[ [[ 2.09433]
49 [54.75 ] ] ],mu2=[ [[ 4.29793023]
50 [80.28488372]] ] total number of iterations= 4
51 initial kmeans guess: [[ 2.60041207 47.89032733]
52 [ 4.46614127 50.04936223]]
53 input of EM:mu1=[ [[ 2.09433]
54 [54.75 ] ] ],mu2=[ [[ 4.29793023]
55 [80.28488372]] ] total number of iterations= 4
56 initial kmeans guess: [[ 1.97204481 90.70224316]
57 [ 1.82401924 49.55252837]]
58 input of EM:mu1=[ [[ 4.29793023]
59 [80.28488372]] ],mu2=[ [[ 2.09433]
60 [54.75 ] ] ] total number of iterations= 4
61 initial kmeans guess: [[ 3.46424947 47.69736584]
62 [ 4.96898795 76.70892793]]
63 input of EM:mu1=[ [[ 2.09433]
64 [54.75 ] ] ],mu2=[ [[ 4.29793023]
65 [80.28488372]] ] total number of iterations= 4
66 initial kmeans guess: [[ 4.59551223 49.73542565]
67 [ 3.42556647 43.87720278]]
68 input of EM:mu1=[ [[ 4.29793023]
```

```

69 [80.28488372]] ],mu2=[ [[ 2.09433]
70 [54.75    ]] ] total number of iterations= 4
71 initial kmeans guess: [[ 1.86153908 52.30945672]
72 [ 2.1401814 91.44658995]]
73 input of EM:mu1=[ [[ 2.09433]
74 [54.75    ]] ],mu2=[ [[ 4.29793023]
75 [80.28488372]] ] total number of iterations= 4
76 initial kmeans guess: [[ 4.52906079 57.36557084]
77 [ 4.51072442 43.14278939]]
78 input of EM:mu1=[ [[ 4.29793023]
79 [80.28488372]] ],mu2=[ [[ 2.09433]
80 [54.75    ]] ] total number of iterations= 4
81 initial kmeans guess: [[ 2.51638293 51.89330513]
82 [ 4.10711885 77.54743741]]
83 input of EM:mu1=[ [[ 2.09433]
84 [54.75    ]] ],mu2=[ [[ 4.29793023]
85 [80.28488372]] ] total number of iterations= 4
86 initial kmeans guess: [[ 4.73400128 59.77954756]
87 [ 2.86143014 56.08758583]]
88 input of EM:mu1=[ [[ 4.29793023]
89 [80.28488372]] ],mu2=[ [[ 2.09433]
90 [54.75    ]] ] total number of iterations= 4
91 initial kmeans guess: [[ 4.79696047 51.73054456]
92 [ 4.47531679 69.03859155]]
93 input of EM:mu1=[ [[ 2.09433]
94 [54.75    ]] ],mu2=[ [[ 4.29793023]
95 [80.28488372]] ] total number of iterations= 4
96 initial kmeans guess: [[ 1.8144436 87.38689893]
97 [ 3.21827268 45.39302273]]
98 input of EM:mu1=[ [[ 4.29793023]
99 [80.28488372]] ],mu2=[ [[ 2.09433]
100 [54.75    ]] ] total number of iterations= 4
101 initial kmeans guess: [[ 2.49421492 91.71039159]
102 [ 4.83218578 70.43047377]]
103 input of EM:mu1=[ [[ 4.29793023]
104 [80.28488372]] ],mu2=[ [[ 2.09433]
105 [54.75    ]] ] total number of iterations= 4
106 initial kmeans guess: [[ 4.86453894 83.58398761]
107 [ 3.44933376 54.0810047 ]]
108 input of EM:mu1=[ [[ 4.29793023]
109 [80.28488372]] ],mu2=[ [[ 2.09433]
110 [54.75    ]] ] total number of iterations= 4

```

```
111 initial kmeans guess: [[ 3.72161422 55.6245174 ]
112 [ 4.1645047 94.33519971]]
113 input of EM:mu1=[ [[ 2.09433]
114 [54.75 ] ] ],mu2=[ [[ 4.29793023]
115 [80.28488372]] ] total number of iterations= 4
116 initial kmeans guess: [[ 4.72685566 55.22143181]
117 [ 3.70937265 57.19244001]]
118 input of EM:mu1=[ [[ 2.09433]
119 [54.75 ] ] ],mu2=[ [[ 4.29793023]
120 [80.28488372]] ] total number of iterations= 4
121 initial kmeans guess: [[ 3.96442249 72.11940614]
122 [ 4.29090986 91.98123798]]
123 input of EM:mu1=[ [[ 2.09433]
124 [54.75 ] ] ],mu2=[ [[ 4.29793023]
125 [80.28488372]] ] total number of iterations= 4
126 initial kmeans guess: [[ 3.41583864 74.9976597 ]
127 [ 3.67762104 82.04739125]]
128 input of EM:mu1=[ [[ 2.09433]
129 [54.75 ] ] ],mu2=[ [[ 4.29793023]
130 [80.28488372]] ] total number of iterations= 4
131 initial kmeans guess: [[ 2.55211655 50.5522158 ]
132 [ 4.09313488 58.99528298]]
133 input of EM:mu1=[ [[ 2.09433]
134 [54.75 ] ] ],mu2=[ [[ 4.29793023]
135 [80.28488372]] ] total number of iterations= 4
136 initial kmeans guess: [[ 4.61301796 90.35910438]
137 [ 4.25853596 93.48037608]]
138 input of EM:mu1=[ [[ 2.09433]
139 [54.75 ] ] ],mu2=[ [[ 4.29793023]
140 [80.28488372]] ] total number of iterations= 4
141 initial kmeans guess: [[ 2.64488169 43.96690331]
142 [ 2.93621295 87.03996643]]
143 input of EM:mu1=[ [[ 2.09433]
144 [54.75 ] ] ],mu2=[ [[ 4.29793023]
145 [80.28488372]] ] total number of iterations= 4
146 initial kmeans guess: [[ 3.85799134 87.83164891]
147 [ 3.82696073 76.04726566]]
148 input of EM:mu1=[ [[ 4.29793023]
149 [80.28488372]] ],mu2=[ [[ 2.09433]
150 [54.75 ] ] ] total number of iterations= 4
151 initial kmeans guess: [[ 2.83159657 87.65701463]
152 [ 4.21424683 77.71753788]]
```



```
153 input of EM:mu1=[ [[ 4.29793023]
154 [80.28488372]] ],mu2=[ [[ 2.09433]
155 [54.75 ] ] ] total number of iterations= 4
156 initial kmeans guess: [[ 1.69719895 95.90672076]
157 [ 3.85157929 66.11071965]]
158 input of EM:mu1=[ [[ 4.29793023]
159 [80.28488372]] ],mu2=[ [[ 2.09433]
160 [54.75 ] ] ] total number of iterations= 4
161 initial kmeans guess: [[ 2.21972208 49.80678854]
162 [ 2.5141585 69.92274499]]
163 input of EM:mu1=[ [[ 2.09433]
164 [54.75 ] ] ],mu2=[ [[ 4.29793023]
165 [80.28488372]] ] total number of iterations= 4
166 initial kmeans guess: [[ 1.73056185 80.60914335]
167 [ 3.15266925 77.45429361]]
168 input of EM:mu1=[ [[ 4.29793023]
169 [80.28488372]] ],mu2=[ [[ 2.09433]
170 [54.75 ] ] ] total number of iterations= 4
171 initial kmeans guess: [[ 3.5227987 71.64158428]
172 [ 4.87262107 63.782147 ] ]
173 input of EM:mu1=[ [[ 4.29793023]
174 [80.28488372]] ],mu2=[ [[ 2.09433]
175 [54.75 ] ] ] total number of iterations= 4
176 initial kmeans guess: [[ 3.10986969 63.49797944]
177 [ 2.13335105 83.37930532]]
178 input of EM:mu1=[ [[ 2.09433]
179 [54.75 ] ] ],mu2=[ [[ 4.29793023]
180 [80.28488372]] ] total number of iterations= 4
181 initial kmeans guess: [[ 4.46790643 45.05398005]
182 [ 2.12275439 54.85599037]]
183 input of EM:mu1=[ [[ 2.09433]
184 [54.75 ] ] ],mu2=[ [[ 4.29793023]
185 [80.28488372]] ] total number of iterations= 4
186 initial kmeans guess: [[ 3.63381039 52.25239261]
187 [ 2.14496275 94.66645222]]
188 input of EM:mu1=[ [[ 2.09433]
189 [54.75 ] ] ],mu2=[ [[ 4.29793023]
190 [80.28488372]] ] total number of iterations= 4
191 initial kmeans guess: [[ 1.61853871 77.69969726]
192 [ 3.98872359 61.66934164]]
193 input of EM:mu1=[ [[ 4.29793023]
194 [80.28488372]] ],mu2=[ [[ 2.09433]
```

```
195 [54.75 ] ] total number of iterations= 4
196 initial kmeans guess: [[ 3.71994071 63.39599433]
197 [ 3.46833509 84.39146801]]
198 input of EM:mu1=[ [[ 2.09433]
199 [54.75 ] ] ],mu2=[ [[ 4.29793023]
200 [80.28488372]] ] total number of iterations= 4
201 initial kmeans guess: [[ 4.16108689 53.33885575]
202 [ 2.28946327 45.27875717]]
203 input of EM:mu1=[ [[ 4.29793023]
204 [80.28488372]] ],mu2=[ [[ 2.09433]
205 [54.75 ] ] ] total number of iterations= 4
206 initial kmeans guess: [[ 2.90135358 67.89446122]
207 [ 2.13383438 74.67634701]]
208 input of EM:mu1=[ [[ 2.09433]
209 [54.75 ] ] ],mu2=[ [[ 4.29793023]
210 [80.28488372]] ] total number of iterations= 4
211 initial kmeans guess: [[ 1.90640453 53.61443618]
212 [ 3.13891829 77.77733164]]
213 input of EM:mu1=[ [[ 2.09433]
214 [54.75 ] ] ],mu2=[ [[ 4.29793023]
215 [80.28488372]] ] total number of iterations= 4
216 initial kmeans guess: [[ 3.43560554 86.47344161]
217 [ 2.18061814 79.21997948]]
218 input of EM:mu1=[ [[ 4.29793023]
219 [80.28488372]] ],mu2=[ [[ 2.09433]
220 [54.75 ] ] ] total number of iterations= 4
221 initial kmeans guess: [[ 4.1751348 70.45770346]
222 [ 4.89781251 92.16961094]]
223 input of EM:mu1=[ [[ 2.09433]
224 [54.75 ] ] ],mu2=[ [[ 4.29793023]
225 [80.28488372]] ] total number of iterations= 4
226 initial kmeans guess: [[ 1.81474318 61.91395859]
227 [ 4.09298786 56.24930173]]
228 input of EM:mu1=[ [[ 4.29793023]
229 [80.28488372]] ],mu2=[ [[ 2.09433]
230 [54.75 ] ] ] total number of iterations= 4
231 initial kmeans guess: [[ 4.6568279 81.10030167]
232 [ 4.29498886 46.66900458]]
233 input of EM:mu1=[ [[ 4.29793023]
234 [80.28488372]] ],mu2=[ [[ 2.09433]
235 [54.75 ] ] ] total number of iterations= 4
236 initial kmeans guess: [[ 4.27652784 66.5551966 ]
```

```

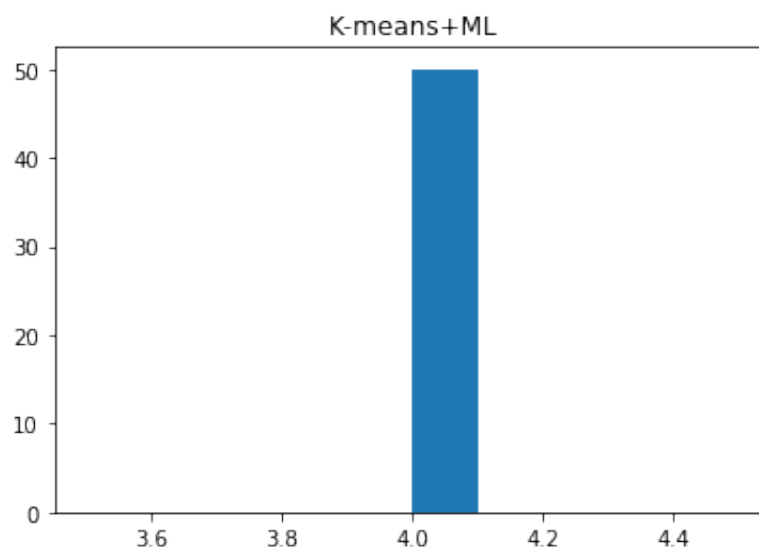
237 [ 3.70103244 63.07421508]]
238 input of EM:mu1=[ [[ 4.29793023]
239 [80.28488372]] ],mu2=[ [[ 2.09433]
240 [54.75 ] ] ] total number of iterations= 4
241 initial kmeans guess: [[ 2.77564956 70.93614324]
242 [ 5.00486974 81.14260518]]
243 input of EM:mu1=[ [[ 2.09433]
244 [54.75 ] ] ],mu2=[ [[ 4.29793023]
245 [80.28488372]] ] total number of iterations= 4
246 initial kmeans guess: [[ 3.36363973 52.05441611]
247 [ 4.57430121 70.03710333]]
248 input of EM:mu1=[ [[ 2.09433]
249 [54.75 ] ] ],mu2=[ [[ 4.29793023]
250 [80.28488372]] ] total number of iterations= 4

```

```

1 <function matplotlib.pyplot.show(*args, **kw)>

```

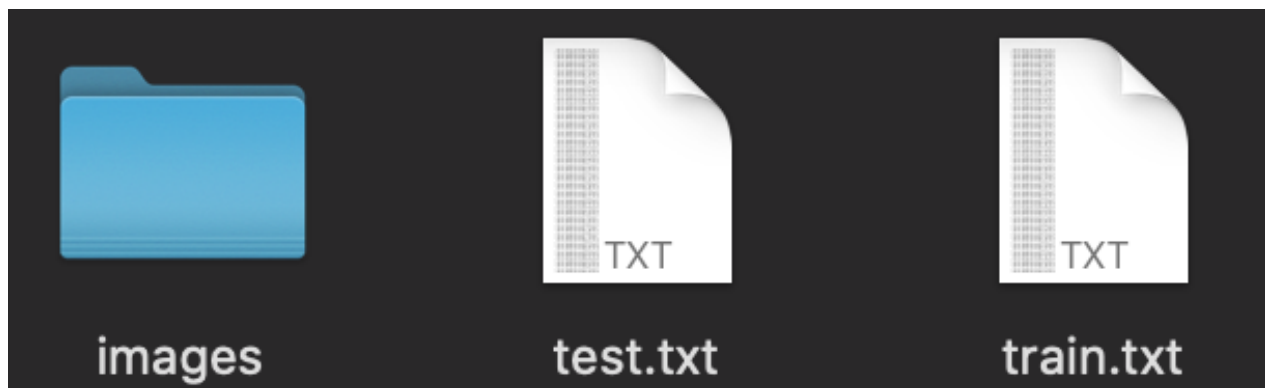


### Compare the algorithm performances of (b) and (c).

GMM+EM with random initial guess performed depending on its initial guess and the guess' distribution. K-means+GMM+EM performed stable since the centre after k-means calculation is a same result no matter how different the initial input of the k-means. The input of EM is the same, so the iteration times of EM is the same. However, the result of k-means is not perfect, the iteration times is always 4. In (b), with a more randomly initial guess, we have the chance to get a better initial input, so EM could be down within 2 iterations.

## Question 3

### 3.(a) Download and unzip The Face Dataset



3.(b) Load the training set into a matrix  $X$ : there are 540 training images in total, each has  $50 \times 50$  pixels that need to be concatenated into a 2500-dimensional vector. So the size of  $X$  should be  $540 \times 2500$ , where each row is a flattened face image. Pick a face image from  $X$  and display that image in grayscale. Do the same thing for the test set. The size of matrix  $X$  test for the test set should be  $100 \times 2500$ .

```
1 import imageio
2 import numpy as np
3 from matplotlib import pylab as plt
4 import matplotlib.cm as cm
5 #load data
6 train_labels, train_data = [], []
7 for line in open('train.txt'):
8     im = imageio.imread(line.strip().split()[0])
9     train_data.append(im.reshape(2500,))
10    train_labels.append(line.strip().split()[1])
11 train_data, train_labels = np.array(train_data, dtype=float),
12    np.array(train_labels, dtype=int)
13 #plot a train image
14 print(train_data.shape, train_labels.shape)
15 plt.imshow(train_data[10, :].reshape(50,50), cmap = cm.Greys_r)
16 plt.show()
```

```

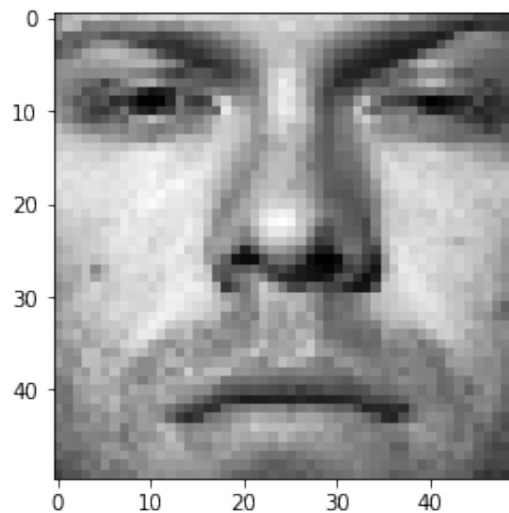
17 test_labels, test_data = [], []
18 for line in open('test.txt'):
19     im = imageio.imread(line.strip().split()[0])
20     test_data.append(im.reshape(2500,))
21     test_labels.append(line.strip().split()[1])
22 test_data, test_labels = np.array(test_data, dtype=float),
    np.array(test_labels, dtype=int)
23 #plot a test image
24 print(test_data.shape, test_labels.shape)
25 plt.imshow(test_data[10, :].reshape(50,50), cmap = cm.Greys_r)
26 plt.show()

```

```

1 | (540, 2500) (540,)

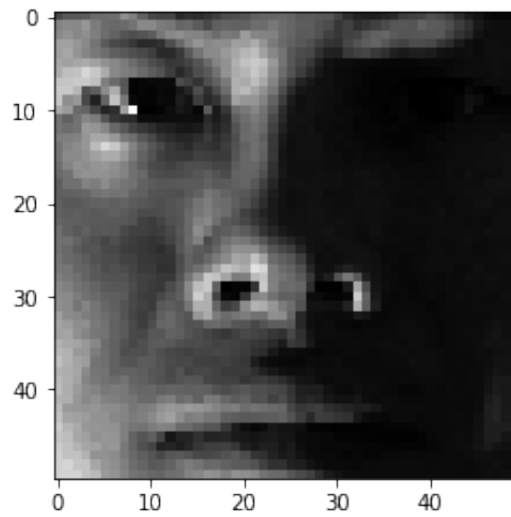
```



```

1 | (100, 2500) (100,)

```

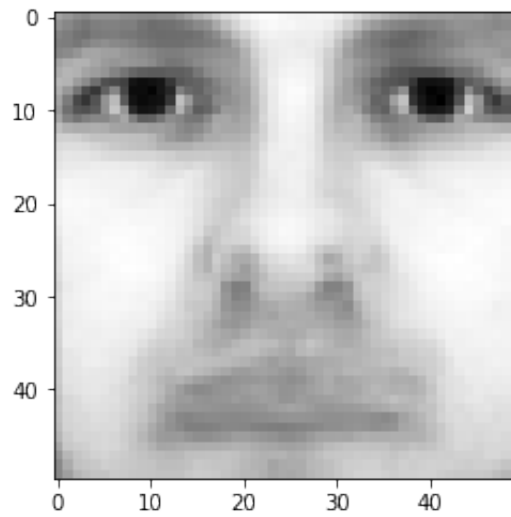


### 3.(c) Average Face.

```
1 mu = np.mean(train_data, axis= 0)
2 print(mu)
3 plt.imshow(mu.reshape(50,50),cmap = cm.Greys_r)
```

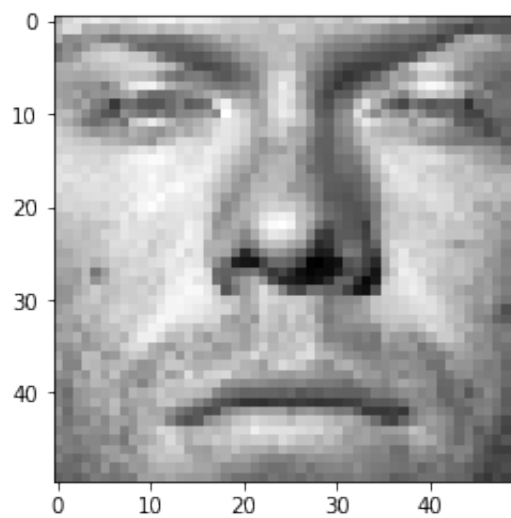
```
1 [59.25185185 56.10185185 52.42222222 ... 67.22222222 64.61851852
2  59.27592593]
```

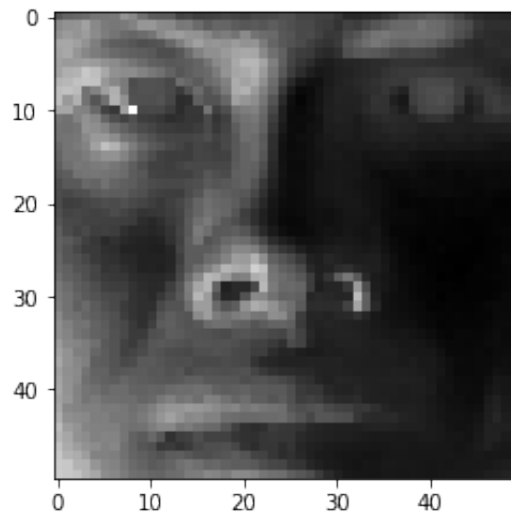
```
1 <matplotlib.image.AxesImage at 0x7faefa248b38>
```



### 3.(d) Mean Subtraction.

```
1 train_sub=train_data-mu
2 test_sub=test_data-mu
3 plt.imshow(train_sub[10, :].reshape(50,50), cmap = cm.Greys_r)
4 plt.show()
5 plt.imshow(test_sub[10, :].reshape(50,50), cmap = cm.Greys_r)
6 plt.show()
```



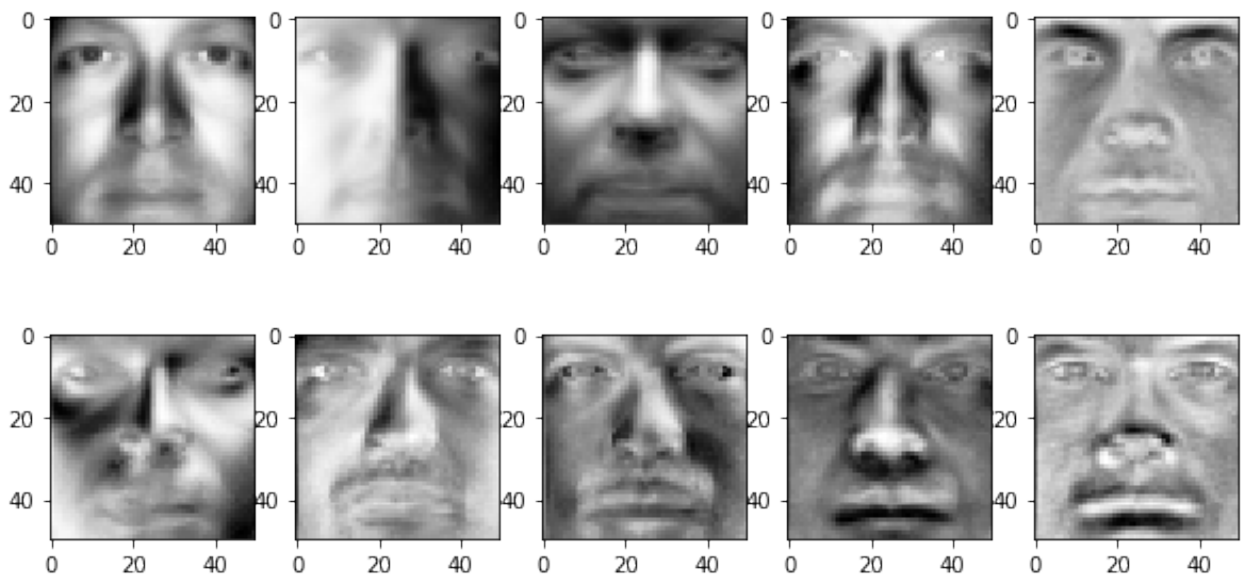


### 3.(e) Eigenface

```

1 X=train_sub
2 u,s,v = np.linalg.svd(X)
3 plt.figure(figsize=(10,5))
4 for i in range(10):
5     plt.subplot(2,5,i+1)
6     plt.imshow(v[i, :].reshape(50,50), cmap = cm.Greys_r)
7 plt.show()

```



### 3.(f) Eigenface Feature.



```

1 X_test=test_sub
2 def Eigenface_Feature(r):
3     V=v[:,r,:]
4     F=np.dot(X,V.T)
5
6     V_test=V
7     F_test=np.dot(X_test,V_test.T)
8     return F, F_test

```

### 3.(g) Face Recognition.

```

1 from sklearn.linear_model.logistic import LogisticRegression
2 from sklearn.multiclass import OneVsRestClassifier
3
4 #r=10
5 F,F_test=Eigenface_Feature(10)
6 F_label=train_labels
7 F_test_label=test_labels
8 lr=LogisticRegression(solver='lbfgs',max_iter=10000)
9 ovr=OneVsRestClassifier(lr)
10 ovr.fit(F,F_label)
11 print(ovr.score(F_test,F_test_label))

```

```

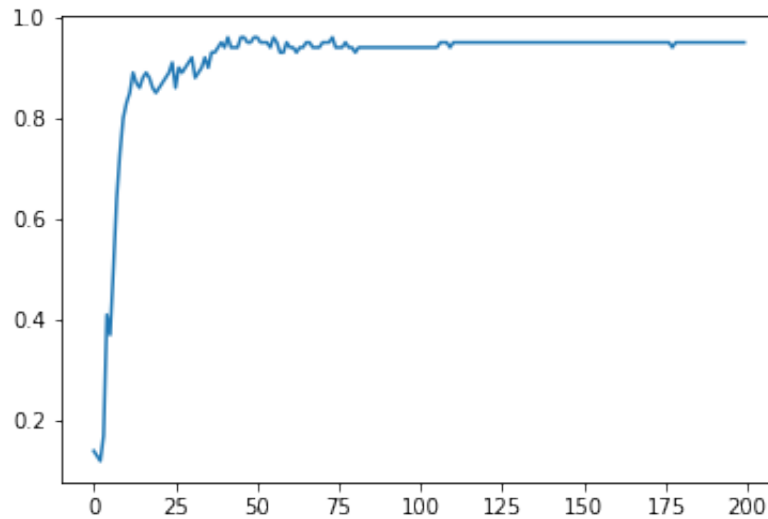
1 0.8

```

```

1 #r=1-200
2
3 acc=[]
4 R=[]
5 for i in range(200):
6     F,F_test=Eigenface_Feature(i+1)
7     ovr.fit(F,F_label)
8     acc.append(ovr.score(F_test,F_test_label))
9     R.append(i)
10 plt.plot(R,acc)
11 plt.show()

```



## Written Exercises

---

### Written 1

Question: Show that from the Singular Value Decomposition(SVD) of a matrix  $X$ , we can obtain the eigendecomposition of  $X^T X$ . This tells us that we can do an SVD of  $X$  and get same result as the eigendecomposition of  $X^T X$  but the SVD is faster and easier.

Answer:

The eigenvalue decomposition of a real symmetric matrix can be written as follows:

$$X = Q\Lambda Q^T \quad (1)$$

Assuming that matrix  $X$  is an  $m * n$  matrix, we can define the SVD of matrix  $X$  as follows:

$$X = U\Sigma V^T \quad (2)$$

The columns of  $V$  are composed of the eigenvectors of  $X^T X$ , and the eigenvectors are unit column vectors.

Here's the proof:

$$X = U\Sigma V^T \quad (3)$$

$$\Rightarrow X^T = V\Sigma^T U^T \quad (4)$$

$$\Rightarrow X^T X = V \Sigma^T U^T U \Sigma V = V \Sigma \Sigma^T V^T \quad (5)$$

Note:  $\Sigma$  is a  $m * n$  matrix, except for the elements on the main diagonal, the value of other elements are all zero. Every element on the main diagonal is a singular value. So we have:

$$\Sigma^T \Sigma = \Sigma^2 \quad (6)$$

Therefore, we can get:

$$\Rightarrow X^T X = V \Sigma^2 V^T \quad (7)$$

Here,  $\Sigma$  is a diagonal matrix with singular values as its elements, and  $\Sigma \Sigma^T$  is a diagonal matrix consisting of the square of singular values.

Thus, we can see that as a symmetric matrix, the form of the equation (7) of  $X^T X$  above is the same as the eigenvalue decomposition of a symmetric matrix.

Therefore, we can know that:

- The nonzero singular values of matrix  $X$  is the positive square root of the nonzero eigenvalues of  $X^T X$ .
- The orthogonal matrix  $V$  is the eigenvector of  $X^T X$ .

In conclusion, we can obtain the eigendecomposition of  $X^T X$  from the Singular Value Decomposition(SVD) of a matrix  $X$  very fast and easily.

## Written 2

$$z_{il} = x_{il} \left( \frac{w_l}{\sum_{l=1}^p w_l} \right)^{\frac{1}{2}} \Rightarrow z_{i'l} = x_{i'l} \left( \frac{w_l}{\sum_{l=1}^p w_l} \right)^{\frac{1}{2}} \quad (8)$$

$$d_e^{(w)}(x_i, x_{i'}) = \sum_{l=1}^p (z_{il} - z_{i'l})^2 \quad (9)$$

$$= \sum_{l=1}^p \left[ x_{il} \left( \frac{w_l}{\sum_{l=1}^p w_l} \right)^{\frac{1}{2}} - x_{i'l} \left( \frac{w_l}{\sum_{l=1}^p w_l} \right)^{\frac{1}{2}} \right]^2 \quad (10)$$

$$= \sum_{l=1}^p \left[ (x_{il} - x_{i'l}) \left( \frac{w_l}{\sum_{l=1}^p w_l} \right)^{\frac{1}{2}} \right]^2 \quad (11)$$

$$= \sum_{l=1}^p (x_{il} - x_{i'l})^2 \left( \frac{w_l}{\sum_{l=1}^p w_l} \right) \quad (12)$$

$$= \frac{\sum_{l=1}^p w_l (x_{il} - x_{i'l})^2}{\sum_{l=1}^p w_l} \quad (13)$$

## Written 3

```
1 # import modules
2
3 import numpy as np
4 import math
```

```
1 # create the matrix
2
3 M = np.array([[1,0,3],[3,7,2],[2,-2,8],[0,-1,1],[5,8,7]])
4 M = np.mat(M)
5 print (M)
6 print (M.shape)
7 print (type(M))
```

```
1 [[ 1  0  3]
2  [ 3  7  2]
3  [ 2 -2  8]
4  [ 0 -1  1]
5  [ 5  8  7]]
6 (5, 3)
7 <class 'numpy.matrix'>
```

```
1 # (a) Compute the matrices M^T*M and M*M^T
2
3 MT = M.T
4 print (MT)
5 print (MT.shape)
```

```
1 [[ 1  3  2  0  5]
2   [ 0  7 -2 -1  8]
3   [ 3  2  8  1  7]]
4 (3, 5)
```

```
1 # a-1: Compute the matrix  $M^T M$ 
2
3 MTM = MT*M
4 print (MTM)
5 print (MTM.shape)
```

```
1 [[ 39  57  60]
2   [ 57 118  53]
3   [ 60  53 127]]
4 (3, 3)
```

```
1 # a-2: Compute the matrix  $M M^T$ 
2
3 MMT = M*MT
4 print (MMT)
5 print (MMT.shape)
```

```
1 [[ 10   9  26   3  26]
2   [  9  62   8  -5  85]
3   [ 26   8  72  10  50]
4   [  3  -5  10   2  -1]
5   [ 26  85  50  -1 138]]
6 (5, 5)
```

```

1  # (b)&(c)
2
3  # 1.Find the eigenvalues and eigenvectors for  $M^T M$ 
4
5  MTM_E, MTM_V = np.linalg.eig(MTM)
6
7  print ("eigenvalues=", MTM_E)
8  print (type(MTM_E))
9  print ("eigenvector=", MTM_V)
10 print (type(MTM_V))

```

```

1  eigenvalues= [2.14670489e+02  9.32587341e-15  6.93295108e+01]
2  <class 'numpy.ndarray'>
3  eigenvector= [[ 0.42615127  0.90453403 -0.01460404]
4  [ 0.61500884 -0.30151134 -0.72859799]
5  [ 0.66344497 -0.30151134  0.68478587]]
6  <class 'numpy.matrix'>

```

```

1  # 1.Find the eigenvalues and eigenvectors for  $M M^T$ 
2
3  MMT_E, MMT_V = np.linalg.eig(MMT)
4
5  print ("eigenvalues=", MMT_E)
6  print (type(MMT_E))
7  print ("eigenvector=", MMT_V)
8  print (type(MMT_V))

```

```

1  eigenvalues= [ 2.14670489e+02 -8.88178420e-16  6.93295108e+01
2  -3.34838281e-15
3  7.47833227e-16]
4  <class 'numpy.ndarray'>
5  eigenvector= [[-0.16492942 -0.95539856  0.24497323 -0.54001979
6  -0.78501713]
7  [-0.47164732 -0.03481209 -0.45330644 -0.62022234  0.30294097]
8  [-0.33647055  0.27076072  0.82943965 -0.12704172  0.2856551 ]
9  [-0.00330585  0.04409532  0.16974659  0.16015949  0.43709105]
10 [-0.79820031  0.10366268 -0.13310656  0.53095405 -0.13902319]]
11 <class 'numpy.matrix'>

```

```

1 # (d) Method 1
2
3 # Find the SVD for the original matrix M from parts (b) and (c)
4
5 # d-1: Find the sigma of matrix M
6 # The result is the same when replacing MMT_E with MTM_E,
  because MTM and MMT have same non-zero eigenvalues, index=0,2
7 M_sigma = np.array([math.sqrt(MMT_E[0]),math.sqrt(MMT_E[2])])
8 print ("sigma=", M_sigma)
9
10 # check the number of non-zero eigenvalues, = the rank of
   matrix
11 M_rank = np.linalg.matrix_rank(M)
12 print (M_rank) # M is rank 2.

```

```

1 sigma= [14.65163776  8.32643446]
2 2

```

```

1 # d-2: Find the VT of matrix M, VT is a 2*2 matrix
2
3 rows_V = [0,1] # get row 0 and 1
4 cols_V = [0,2] # get column 0 and 2
5 M_V = MTM_V[rows_V,:][:,cols_V]
6 M_VT = M_V.T
7 print ("VT=", M_VT)

```

```

1 VT= [[ 0.42615127  0.61500884]
2      [-0.01460404 -0.72859799]]

```

```

1 # d-3: Find the U of matrix M, U is a 5*2 matrix
2
3 cols_U = [0,2] # get column 0 and 2
4 M_U = MMT_V[:,cols_U]
5 print ("U=", M_U)

```

```
1 U= [[-0.16492942  0.24497323]
2      [-0.47164732 -0.45330644]
3      [-0.33647055  0.82943965]
4      [-0.00330585  0.16974659]
5      [-0.79820031 -0.13310656]]
```

```
1 # (e) Method 1
2
3 # e-1: keep only one non-zero singular value, by setting the
4     smaller singular value to 0
5
6 sigma_max = max(M_sigma)
7 print (sigma_max)
8 M_sigma_new = np.array([sigma_max])
9 #M_sigma_new = np.mat(M_sigma_new)
10 print (M_sigma_new)
```

```
1 14.651637764976883
2 [14.65163776]
```

```
1 # e-2: Compute the 1D approximation to M
2
3 k=1
4 u,d,vt = M_U[:, :k], M_sigma[:k], M_VT[:, :k][:k, :]
5 print("-----U-----")
6 print(u)
7 print("-----S-----")
8 print(d)
9 print("-----VT-----")
10 print(vt)
11
12 # Compute the 1D approximation to M
13
14 A = np.zeros([1,1])
15 for i in range(1):
16     A[i][i] = d[i]
17 print (A)
```



```

18 tmp = np.dot(u,A)
19 print("1D approximation to M:")
20 print(np.dot(tmp,vt))

```

```

1  -----U-----
2  [[-0.16492942]
3   [-0.47164732]
4   [-0.33647055]
5   [-0.00330585]
6   [-0.79820031]]
7  -----S-----
8  [14.65163776]
9  -----VT-----
10 [[0.42615127]]
11 [[14.65163776]]
12 1D approximation to M:
13 [[-1.02978864]
14  [-2.94487812]
15  [-2.10085952]
16  [-0.02064112]
17  [-4.9838143  ]]

```

```

1  # (d) Method 2
2
3  U,sigma,VT = np.linalg.svd(M)
4
5  print ("U=", U)
6  print ("sigma=", sigma)
7  print ("VT=", VT)
8
9  k=2
10 u,d,vt = U[:, :k], sigma[:k], VT[:, :k][:k, :]
11 print("-----U-----")
12 print(u)
13 print("-----S-----")
14 print(d)
15 print("-----VT-----")
16 print(vt)

```

```

1  U= [[-0.16492942 -0.24497323  0.9482579   0.09864471
      -0.06214956]
2      [-0.47164732  0.45330644 -0.02261948  0.08103373 -0.75165416]
3      [-0.33647055 -0.82943965 -0.27341434 -0.18350729 -0.3006445 ]
4      [-0.00330585 -0.16974659 -0.14522096  0.97468061  0.00915155]
5      [-0.79820031  0.13310656 -0.06671416  0.00505374  0.58368021]]
6  sigma= [1.46516378e+01 8.32643446e+00 2.99921582e-16]
7  VT= [[-0.42615127 -0.61500884 -0.66344497]
8        [ 0.01460404  0.72859799 -0.68478587]
9        [-0.90453403  0.30151134  0.30151134]]
10 -----U-----
11 [[-0.16492942 -0.24497323]
12    [-0.47164732  0.45330644]
13    [-0.33647055 -0.82943965]
14    [-0.00330585 -0.16974659]
15    [-0.79820031  0.13310656]]
16 -----S-----
17 [14.65163776  8.32643446]
18 -----VT-----
19 [[-0.42615127 -0.61500884]
20    [ 0.01460404  0.72859799]]

```

```

1  # (e) Method 2
2
3  k=1
4  u,d,v,t = u[:, :k], d[:k], vt[:, :k][:k, :]
5  print("-----U-----")
6  print(u)
7  print("-----S-----")
8  print(d)
9  print("-----VT-----")
10 print(vt)
11
12 # Compute the 1D approximation to M
13 A = np.zeros([1,1])
14 for i in range(1):
15     A[i][i] = d[i]
16 tmp = np.dot(u,A)
17 print("1D approximation to M:")
18 print(np.dot(tmp,vt))

```

```
1  -----U-----
2  [[-0.16492942]
3   [-0.47164732]
4   [-0.33647055]
5   [-0.00330585]
6   [-0.79820031]]
7  -----S-----
8  [14.65163776]
9  -----VT-----
10 [[-0.42615127]]
11 1D approximation to M:
12 [[1.02978864]
13  [2.94487812]
14  [2.10085952]
15  [0.02064112]
16  [4.9838143  ]]
```



