HW4 Q1

November 17, 2018

1 CISC 6930 Assignment 4 Question 1

In [1]:
```
# Import packages
import numpy as np
import pandas as pd
from scipy.io import arff
import time
import matplotlib.pyplot as plt
```

Implement the *k*-means clustering algorithm and investigate the effects of different starting configurations. Work with the `segment.arff` dataset. This dataset is based on a set of images taken in color around the UMASS campus to which low-level image processing operators were applied. The goal is to find clusters in the data which define different types of objects (buildings, trees, sky, etc). Don't be concerned with understanding the meaning of each cluster.

Remember to *z*-score normalize the data as a preprocessing step before proceeding with the clustering. Again, *k* is a tuning parameter and should be abstracted from the core clustering subroutine; vary *k* and observe the effects.

Random Starting Positions

k-means is sensitive to the starting positions of the cluster centroids. To try to overcome this run *k*-means 25 times with randomized starting positions for the cluster centroids. For an actual application, the centroids would be selected though a randomization process. For this exercise, 300 instance numbers are provided to use (counting to start at the first instance in the dataset). To illustrate the approach, consider 5-means. This needs 5 centroid instances for each of 25 trials, or a total of 125 indices into the dataset. From the following list, select the first 5 items for the first iteration, the next 5 for the second iteration and so on.

The 300 indices are as follows:

In [2]:
```
# List of indices for centroid instances
indices = [775, 1020, 200, 127, 329, 1626, 1515, 651, 658, 328,
           1160, 108, 422, 88, 105, 261, 212, 1941, 1724, 704,
           1469, 635, 867, 1187, 445, 222, 1283, 1288, 1766, 1168,
           566, 1812, 214, 53, 423, 50, 705, 1284, 1356, 996,
           1084, 1956, 254, 711, 1997, 1378, 827, 1875, 424, 1790,
           633, 208, 1670, 1517, 1902, 1476, 1716, 1709, 264, 1,
           371, 758, 332, 542, 672, 483, 65, 92, 400, 1079,
           1281, 145, 1410, 664, 155, 166, 1900, 1134, 1462, 954,
           1818, 1679, 832, 1627, 1760, 1330, 913, 234, 1635, 1078,
```

```
               640, 833, 392, 1425, 610, 1353, 1772, 908,1964, 1260,
               784, 520, 1363, 544, 426, 1146, 987, 612, 1685, 1121,
               1740, 287, 1383, 1923, 1665, 19, 1239, 251, 309, 245,
               384, 1306, 786, 1814, 7, 1203, 1068, 1493, 859, 233,
               1846, 1119, 469, 1869, 609, 385, 1182, 1949, 1622, 719,
               643, 1692, 1389, 120, 1034, 805, 266, 339, 826, 530,
               1173, 802, 1495, 504, 1241, 427, 1555, 1597, 692, 178,
               774, 1623, 1641, 661, 1242, 1757, 553, 1377, 1419, 306,
               1838, 211, 356, 541, 1455, 741, 583, 1464, 209, 1615,
               475, 1903, 555, 1046, 379, 1938, 417, 1747, 342, 1148,
               1697, 1785, 298, 1485, 945, 1097, 207, 857, 1758, 1390,
               172, 587, 455, 1690, 1277, 345, 1166, 1367, 1858, 1427,
               1434, 953, 1992, 1140, 137, 64, 1448, 991, 1312, 1628,
               167, 1042, 1887, 1825, 249, 240, 524, 1098, 311, 337,
               220, 1913, 727, 1659, 1321, 130, 1904, 561, 1270, 1250,
               613, 152, 1440, 473, 1834, 1387, 1656, 1028, 1106, 829,
               1591, 1699, 1674, 947, 77, 468, 997, 611, 1776, 123,
               979, 1471, 1300, 1007, 1443, 164, 1881, 1935, 280, 442,
               1588, 1033, 79, 1686, 854, 257, 1460, 1380, 495, 1701,
               1611, 804, 1609, 975, 1181, 582, 816, 1770, 663, 737,
               1810, 523, 1243, 944, 1959, 78, 675, 135, 1381, 1472]

# Take length of above list to ensure there are enough indices
# for k-means clustering
len(indices)
```

Out[2]: 300

Running k-means entails iteratively moving the centroids to the best possible positions. For each value of k and for the 25 initial centroid sets, run k-means until either the clusters no longer change or the program has conducted 50 iterations over the dataset, whichever comes first.

In [3]:
```
# Import data and store in data frame
data, metadata = arff.loadarff("segment.arff")
n_data = pd.DataFrame(data)

# Separate the class label from the features
class_label = n_data.iloc[:, -1]
n_data = n_data.iloc[:, :-1]

# Normalize the features
for i in range(n_data.shape[1]):
    if n_data.iloc[:,i].std() != 0.0:
        n_data.iloc[:, i] = (n_data.iloc[:, i] - n_data.iloc[:,i].mean())
        / (n_data.iloc[:,i].std())

# Store the features in an easy to access array
df = np.array(n_data)
```

To evaluate the results, compute the sum of squared errors (SSE) for each of the 25 clustering runs. SSE measures the deviation of points from their cluster centroid and gives a simple measure of the cluster compactness:

$$SSE = \sum_{j=1}^{k} \sum_{x_i \in C_j} \|x_i - m_j\|^2$$

where the clusters are C_j ($j = 1, \ldots, k$), the final centroid for C_j is m_j, the x_i's are all the points assigned to C_j and $||a - b||$ is the distance from point a to point b.

In [4]:
```
# Return the euclidean distance between 2 points
def euclidean_distance(X,Y):
    return np.sqrt(np.sum((X - Y)**2))
```

In [5]:
```
# Return the length of intersecting elements from two lists
def intersection_length(lst1, lst2):
    return len(set(lst1).intersection(lst2))
```

In [6]:
```
# Classify each points in the dataframe into its cluster
# based on the euclidean distance
def findMembers(df, indices):

    # Store the number of data points in a variable
    n = df.shape[0]

    # Create an array of size n by 1 to store each data point's
    # cluster label
    Xs = np.zeros((n, 1))

    # For each data point, find the euclidean distance between it
    # and each indice and store the closest indice
    for j in range(n):
        dist = []
        for s in indices:
            dist.append([euclidean_distance(df[j], df[s]), s])
        Xs[j][0] = sorted(dist)[0][1]

    # Return the array of classified points
    return Xs
```

In [7]:
```
# Find the new mean point of each cluster
def findNewMean(df, points):

    # Create an empty list to store distances
    dist = []

    # To allow time complexity to be O(n) rather than O(n^2),
    # note that (n-a) + (n-b) + ... = (n*x) - (a + b + ...)
    # This simple manipulation is done below
    df_scaled = df * len(points)
```

```
        sum_points = sum(df[points])

        # Calculate the euclidean distance for all data points
        for i in range(df_scaled.shape[0]):
            dist.append([euclidean_distance(df_scaled[i], sum_points), i])

        # Return the new mean based on its shortest distance
        return sorted(dist)[0][1]
```

In [8]:
```
# Calculate the SSE of a cluster based on euclidean distance
def calculateSSE(df, points):

    # Create an empty list to store distances
    dist = []

    # To allow time complexity to be O(n) rather than O(n^2),
    # note that (n-a) + (n-b) + ... = (n*x) - (a + b + ...)
    # This simple manipulation is done below
    df_scaled = df * len(points)
    sum_points = sum(df[points])

    # Calculate the euclidean distance for all data points
    for i in range(df_scaled.shape[0]):
        dist.append([euclidean_distance(df_scaled[i], sum_points), i])

    # Return the SSE, or euclidean distance of the
    # cluster's points
    return sorted(dist)[0][0]
```

In [9]:
```
start = time.time()
# Create an array to store SSE values
SSE = np.zeros((25, 12))

# Allow only a maximum of 50 iterations
# and runs through 25 initial cluster indices
max_iter = 50
cluster_run = 25

# For each k from 1 to 12, perform k-means clustering
for k in range(1,13):

    # For each initial cluster index, perform k-means clustering
    for i in range(cluster_run):

        # Get the initial indices
        centroids = indices[i*k:(i+1)*k]
        relevant_c = centroids
```

```python
            # For each iteration, classify each data points
            # to its closest cluster mean and find the mean
            # of each cluster
            for b in range(max_iter):

                # Reclassify data points to its closest cluster
                memberList = findMembers(df, relevant_c)

                # Create a list to store new centroids
                new_c = []

                # For each indice, find the new centroid
                for m in relevant_c:
                    index = np.where(memberList == m)[0]
                    new_m = findNewMean(df, index)
                    new_c.append(new_m)

                # If the new centroids found have already appeared
                # before, meaning convergence has met, then
                # stop k-means clustering and calculate the SSE
                # Else add the new centroids to its list of
                # previous indices and let the new centroids
                # be recalculated
                if intersection_length(centroids, new_c) == k:
                    final_c = new_c
                    memberList = findMembers(df, final_c)
                    tempSSE = 0
                    for v in final_c:
                        w = np.where(memberList == v)[0]
                        tempSSE += calculateSSE(df, w)
                    SSE[i][k-1] = tempSSE
                    break
                else:
                    centroids = centroids + new_c
                    relevant_c = new_c
        print(k, "-means clustering is finished.")
    end = time.time()
    print("Time elapsed:", end - start)
```

```
1 -means clustering is finished.
2 -means clustering is finished.
3 -means clustering is finished.
4 -means clustering is finished.
5 -means clustering is finished.
6 -means clustering is finished.
7 -means clustering is finished.
8 -means clustering is finished.
9 -means clustering is finished.
```

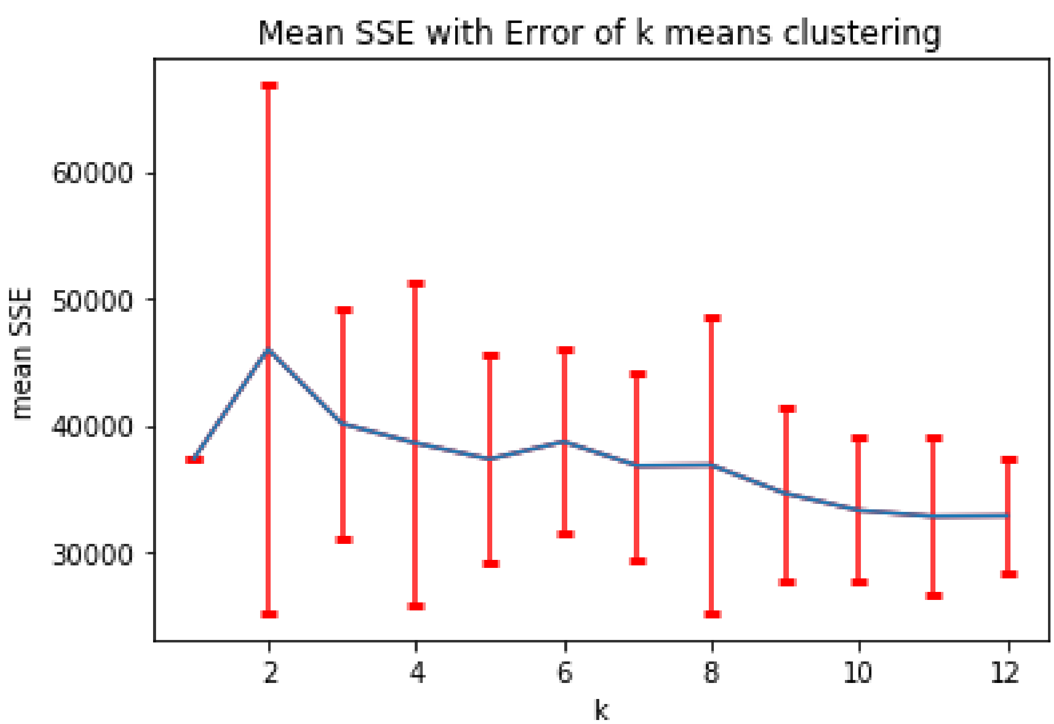
```
10 -means clustering is finished.
11 -means clustering is finished.
12 -means clustering is finished.
Time elapsed: 414.3130829334259
```

(a) For each $k = 1, 2, \ldots, 12$, compute the mean SSE, denoted μ_k and the sample standard deviation σ_k, over all 25 clustering runs for that value of k. Generate a line plot of the mean SSE (μ_k) as a function of k. Include error bars that indicate the 95% confidence interval: ($\mu_k - 2\sigma_k$ to $\mu_k + 2\sigma_k$)

In [10]:
```python
# Calculate the mean SSE and sample standard deviation
# over all 25 clustering runs for each k
avgSSE = np.mean(SSE, axis = 0).round(4)
stdSSE = np.std(SSE, axis = 0).round(4)

# Calculate the error to be 2 times the sd
error = 2 * stdSSE
```

In [11]:
```python
# Create a plot of the mean SSEs with error bars showing
# the 95% confidence interval
plt.plot(range(1,13), avgSSE, color = 'r')
plt.errorbar(x = range(1,13), y = avgSSE, yerr = error,
             ecolor = 'r', capsize = 3,  markeredgewidth = 3)
plt.title("Mean SSE with Error of k means clustering")
plt.xlabel("k")
plt.ylabel("mean SSE")
plt.show()
```



(b) Produce a table containing the 4 columns: k, μ_k, $\mu_k - 2\sigma_k$ and $\mu_k + 2\sigma_k$ for each of the values of $k = 1, 2, \ldots, 12$.

In [12]:
```
# Produce all values for the table
k_vals = pd.DataFrame(list(range(1,13)))
avg = pd.DataFrame(avgSSE)
left = pd.DataFrame(avgSSE - error)
right = pd.DataFrame(avgSSE + error)
table = pd.concat([k_vals, avg, left, right], axis = 1)
table.columns = ['k', "$\mu_k$", "$\mu_k-2\sigma_k$", "$\mu_k+2\sigma_k$"]
table
```

Out[12]:

	k	\$\mu_k\$	\$\mu_k-2\sigma_k\$	\$\mu_k+2\sigma_k\$
0	1	37371.1346	37371.1346	37371.1346
1	2	45995.1453	25191.9437	66798.3469
2	3	40118.1075	31090.0833	49146.1317
3	4	38586.1462	25810.1842	51362.1082
4	5	37322.3845	29090.5615	45554.2075
5	6	38700.8073	31411.7667	45989.8479
6	7	36804.2022	29389.0682	44219.3362
7	8	36855.6613	25246.0181	48465.3045
8	9	34628.2882	27773.7948	41482.7816
9	10	33292.5657	27608.4379	38976.6935
10	11	32821.8159	26622.0909	39021.5409
11	12	32867.1319	28434.7341	37299.5297

In [13]:
```
# For viewing the table in terminal
print("Table of k, mu_k, mu_k - 2sigma_k, mu_k + 2sigma_k")
for i in range(table.shape[0]):
    print(list(table.loc[i]))
```

```
Table of k, mu_k, mu_k - 2sigma_k, mu_k + 2sigma_k
[1.0, 37371.134599999998, 37371.134599999998, 37371.134599999998]
[2.0, 45995.145299999996, 25191.943699999996, 66798.346900000004]
[3.0, 40118.107499999998, 31090.083299999998, 49146.131699999998]
[4.0, 38586.146200000003, 25810.184200000003, 51362.108200000002]
[5.0, 37322.3845, 29090.5615, 45554.207500000004]
[6.0, 38700.8073, 31411.7667, 45989.847900000001]
[7.0, 36804.2022, 29389.068200000002, 44219.336199999998]
[8.0, 36855.6613, 25246.018100000001, 48465.304499999998]
[9.0, 34628.288200000003, 27773.794800000003, 41482.781600000002]
[10.0, 33292.565699999999, 27608.437899999997, 38976.693500000001]
[11.0, 32821.815900000001, 26622.090900000003, 39021.5409]
[12.0, 32867.1319, 28434.734100000001, 37299.529699999999]
```

(c) As k increases and approaches the total number of examples N, what value does the SSE approach? What problems does this cause in terms of using SSE to choose an optimal k?

Answer: As k increases and approaches the total number of examples N, the SSE approaches 0. This causes a problem in choosing an optimal k because it would mean that $k = N$ would be the optimal k and its SSE would effectively be 0. But by having $k = N$, it means there N clusters, each having a single data point. This is a meaningless set of clusters.

(d) Suggest another measure of cluster compactness and separation that might be more useful than SSE?

Answer: Another measure of cluster compactness and separation that might be more useful than SSE is the Dunn Index. It is equal to the minimal inter-cluster distance divided by the maximal cluster size. A high Dunn Index is good; it means minimal inter-cluster distance is maximized and maximal cluster size is minimized. A large inter-cluster distance means that separation is maxed. A small cluster size means clusters are well compacted.