CS 6220 Data Mining — Assignment 5 — Clustering: K-Means — Samuel Steiner

In [ ]:

```
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#
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#
# SciPy function to compute the gap statistic for evaluating k-means clustering.
#
# The gap statistic is defined by Tibshirani, Walther, Hastie in:
#  Estimating the number of clusters in a data set via the gap statistic
#  J. R. Statist. Soc. B (2001) 63, Part 2, pp 411-423

import scipy as sp
import scipy as sp
import scipy.cluster.vq
import scipy.spatial.distance
import scipy.stats
import sklearn.cluster

import pylab as pl

from numpy.linalg import LinAlgError

dst = sp.spatial.distance.euclidean

def gap_statistics(data, refs=None, nrefs=20, ks=range(1,11)):
    """Computes the gap statistics for an nxm dataset.

    The gap statistic measures the difference between within-cluster dispersion on an input
    dataset and that expected under an appropriate reference null distribution.

    Computation of the gap statistic, then, requires a series of reference (null) distributions.
    One may either input a precomputed set of reference distributions (via the parameter refs)
    or specify the number of reference distributions (via the parameter nrefs) for automatic
    generation of uniform distributions within the bounding box of the dataset (data).

    Each computation of the gap statistic requires the clustering of the input dataset and of
    several reference distributions. To identify the optimal number of clusters k, the gap
    statistic is computed over a range of possible values of k (via the parameter ks).

    For each value of k, within-cluster dispersion is calculated for the input dataset and each
    reference distribution. The calculation of the within-cluster dispersion for the reference
    distributions will have a degree of variation, which we measure by standard deviation or
    standard error.

    The estimated optimal number of clusters, then, is defined as the smallest value k such that
    gap_k is greater than or equal to the sum of gap_k+1 minus the expected error err_k+1.

    Args:
      data ((n,m) SciPy array): The dataset on which to compute the gap statistics.
      refs ((n,m,k) SciPy array, optional): A precomputed set of reference distributions.
        Defaults to None.
      nrefs (int, optional): The number of reference distributions for automatic generation.
        Defaults to 20.
      ks (list, optional): The list of values k for which to compute the gap statistics.
        Defaults to range(1,11), which creates a list of values from 1 to 10.

    Returns:
      gaps: an array of gap statistics computed for each k.
      errs: an array of standard errors (se), with one corresponding to each gap computation.
      difs: an array of differences between each gap_k and the sum of gap_k+1 minus err_k+1.

    """
    shape = data.shape

    if refs==None:
        tops = data.max(axis=0) # maxima along the first axis (rows)
        bots = data.min(axis=0) # minima along the first axis (rows)
        dists = sp.matrix(sp.diag(tops-bots)) # the bounding box of the input dataset

        # Generate nrefs uniform distributions each in the half-open interval [0.0, 1.0)
        rands = sp.random.random_sample(size=(shape[0],shape[1], nrefs))

        # Adjust each of the uniform distributions to the bounding box of the input dataset
        for i in range(nrefs):
            rands[:,:,i] = rands[:,:,i]*dists+bots
    else:
        rands = refs

    gaps = sp.zeros((len(ks),))   # array for gap statistics (lenth ks)
```

```
    errs = sp.zeros((len(ks),))   # array for model standard errors (length ks)
    difs = sp.zeros((len(ks)-1,)) # array for differences between gaps (length ks-1)

    for (i,k) in enumerate(ks): # iterate over the range of k values
        # Cluster the input dataset via k-means clustering using the current value of k
        try:
            (kmc,kml) = sp.cluster.vq.kmeans2(data, k)
        except LinAlgError:
            kmeans = sklearn.cluster.KMeans(n_clusters=k).fit(data)
            (kmc, kml) = kmeans.cluster_centers_, kmeans.labels_

        # Generate within-dispersion measure for the clustering of the input dataset
        disp = sum([dst(data[m,:],kmc[kml[m],:]) for m in range(shape[0])])

        # Generate within-dispersion measures for the clusterings of the reference datasets
        refdisps = sp.zeros((rands.shape[2],))
        for j in range(rands.shape[2]):
            # Cluster the reference dataset via k-means clustering using the current value of k
            try:
                (kmc,kml) = sp.cluster.vq.kmeans2(rands[:,:,j], k)
            except LinAlgError:
                kmeans = sklearn.cluster.KMeans(n_clusters=k).fit(rands[:,:,j])
                (kmc, kml) = kmeans.cluster_centers_, kmeans.labels_

            refdisps[j] = sum([dst(rands[m,:,j],kmc[kml[m],:]) for m in range(shape[0])])

        # Compute the (estimated) gap statistic for k
        gaps[i] = sp.mean(sp.log(refdisps) - sp.log(disp))

        # Compute the expected error for k
        errs[i] = sp.sqrt(sum(((sp.log(refdisp)-sp.mean(sp.log(refdisps)))**2) \
                              for refdisp in refdisps)/float(nrefs)) * sp.sqrt(1+1/nrefs)

    # Compute the difference between gap_k and the sum of gap_k+1 minus err_k+1
    difs = sp.array([gaps[k] - (gaps[k+1]-errs[k+1]) for k in range(len(gaps)-1)])

    #print "Gaps: " + str(gaps)
    #print "Errs: " + str(errs)
    #print "Difs: " + str(difs)

    return gaps, errs, difs

def plot_gap_statistics(gaps, errs, difs):
    """Generates and shows plots for the gap statistics.

    A figure with two subplots is generated. The first subplot is an errorbar plot of the
    estimated gap statistics computed for each value of k. The second subplot is a barplot
    of the differences in the computed gap statistics.

    Args:
      gaps (SciPy array): An array of gap statistics, one computed for each k.
      errs (SciPy array): An array of standard errors (se), with one corresponding to each gap
        computation.
      difs (SciPy array): An array of differences between each gap_k and the sum of gap_k+1
        minus err_k+1.

    """
    # Create a figure
    fig = pl.figure(figsize=(16, 4))

    pl.subplots_adjust(wspace=0.35) # adjust the distance between figures

    # Subplot 1
    ax = fig.add_subplot(121)
    ind = range(1,len(gaps)+1) # the x values for the gaps

    # Create an errorbar plot
    rects = ax.errorbar(ind, gaps, yerr=errs, xerr=None, linewidth=1.0)

    # Add figure labels and ticks
    ax.set_title('Clustering Gap Statistics', fontsize=16)
    ax.set_xlabel('Number of clusters k', fontsize=14)
    ax.set_ylabel('Gap Statistic', fontsize=14)
    ax.set_xticks(ind)

    # Add figure bounds
    ax.set_ylim(0, max(gaps+errs)*1.1)
    ax.set_xlim(0, len(gaps)+1.0)

    # Subplot 2
    ax = fig.add_subplot(122)
```

```
    ind = range(1,len(difs)+1) # the x values for the difs

    max_gap = None
    if len(np.where(difs > 0)[0]) > 0:
        max_gap = np.where(difs > 0)[0][0] + 1 # the k with the first positive dif

    # Create a bar plot
    ax.bar(ind, difs, alpha=0.5, color='g', align='center')

    # Add figure labels and ticks
    if max_gap:
        ax.set_title('Clustering Gap Differences\n(k=%d Estimated as Optimal)' % (max_gap), \
                     fontsize=16)
    else:
        ax.set_title('Clustering Gap Differences\n', fontsize=16)
    ax.set_xlabel('Number of clusters k', fontsize=14)
    ax.set_ylabel('Gap Difference', fontsize=14)
    ax.xaxis.set_ticks(range(1,len(difs)+1))

    # Add figure bounds
    ax.set_ylim(min(difs)*1.2, max(difs)*1.2)
    ax.set_xlim(0, len(difs)+1.0)

    # Show the figure
    pl.show()

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#
# Function to compute the sum of squared distance (SSQ) for evaluating k-means clustering.

import numpy as np
import scipy as sp
import sklearn.cluster
from scipy.spatial.distance import cdist, pdist

import pylab as pl

def ssq_statistics(data, ks=range(1,11), ssq_norm=True):
    """Computes the sum of squares for an nxm dataset.

    The sum of squares (SSQ) is a measure of within-cluster variation that measures the sum of
    squared distances from cluster prototypes.

    Each computation of the SSQ requires the clustering of the input dataset. To identify the
    optimal number of clusters k, the SSQ is computed over a range of possible values of k
    (via the parameter ks). For each value of k, within-cluster dispersion is calculated for the
    input dataset.

    The estimated optimal number of clusters, then, is defined as the value of k prior to an
    "elbow" point in the plot of SSQ values.

    Args:
      data ((n,m) SciPy array): The dataset on which to compute the gap statistics.
      ks (list, optional): The list of values k for which to compute the gap statistics.
        Defaults to range(1,11), which creates a list of values from 1 to 10.

    Returns:
      ssqs: an array of SSQs, one computed for each k.

    """
    ssqs = sp.zeros((len(ks),)) # array for SSQs (lenth ks)

    #n_samples, n_features = data.shape # the number of rows (samples) and columns (features)
    #if n_samples >= 2500:
    #    # Generate a small sub-sample of the data
    #    data_sample = shuffle(data, random_state=0)[:1000]
    #else:
    #    data_sample = data

    for (i,k) in enumerate(ks): # iterate over the range of k values
        # Fit the model on the data
        kmeans = sklearn.cluster.KMeans(n_clusters=k, random_state=0).fit(data)

        # Predict on the data (k-means) and get labels
        #labels = kmeans.predict(data)

        if ssq_norm:
            dist = np.min(cdist(data, kmeans.cluster_centers_, 'euclidean'), axis=1)

            tot_withinss = sum(dist**2) # Total within-cluster sum of squares
            totss = sum(pdist(data)**2) / data.shape[0] # The total sum of squares
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```
            totss = sum(pdist(data)**2) / data.shape[0] # The total sum of squares
            betweenss = totss - tot_withinss # The between-cluster sum of squares
            ssqs[i] = betweenss/totss*100
        else:
            # The sum of squared error (SSQ) for k
            ssqs[i] = kmeans.inertia_

    return ssqs

def plot_ssq_statistics(ssqs):
    """Generates and shows plots for the sum of squares (SSQ).

    A figure with one plot is generated. The plot is a bar plot of the SSQ computed for each
    value of k.

    Args:
      ssqs (SciPy array): An array of SSQs, one computed for each k.

    """
    # Create a figure
    fig = pl.figure(figsize=(6.75, 4))

    ind = range(1,len(ssqs)+1) # the x values for the ssqs
    width = 0.5 # the width of the bars

    # Create a bar plot
    #rects = pl.bar(ind, ssqs, width)
    pl.plot(ind, ssqs)

    # Add figure labels and ticks
    pl.title('Clustering Sum of Squared Distances', fontsize=16)
    pl.xlabel('Number of clusters k', fontsize=14)
    pl.ylabel('Sum of Squared Distance (SSQ)', fontsize=14)
    pl.xticks(ind)

    # Add text labels
    #for rect in rects:
    #    height = rect.get_height()
    #    pl.text(rect.get_x()+rect.get_width()/2., 1.05*height, '%d' % int(height), \
    #            ha='center', va='bottom')

    # Add figure bounds
    pl.ylim(0, max(ssqs)*1.2)
    pl.xlim(0, len(ssqs)+1.0)

    pl.show()
```

Load the dataset, and remove features other than Annual Income and Spending Score.

In [ ]:
```
import pandas as pd
import warnings
warnings.filterwarnings('ignore')

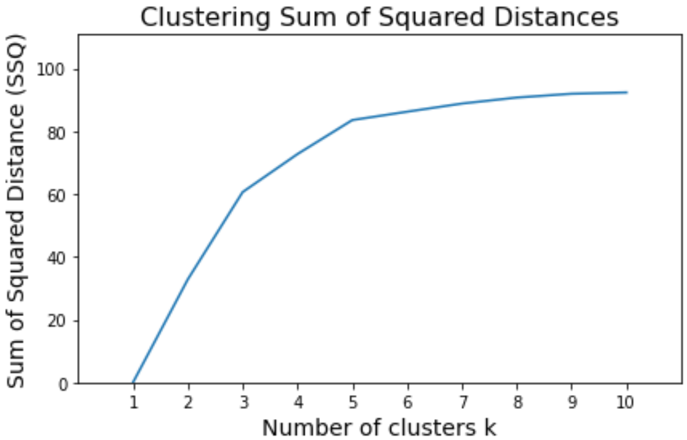
shopping_data = pd.read_csv('shopping-data.csv')[['Annual Income (k$)','Spending Score (1-100)']]
shopping_data.head()
```

Out[ ]:

	Annual Income (k$)	Spending Score (1-100)
0	15	39
1	15	81
2	16	6
3	16	77
4	17	40

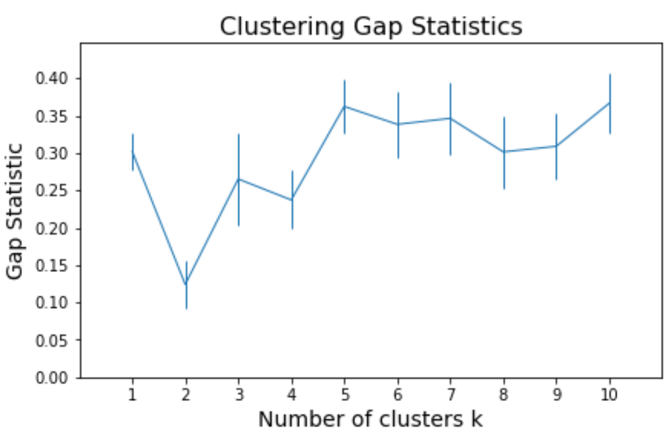
The SSQs computed for k values between 1 and 10 (inclusive). There should be one plot corresponding to the SSQs

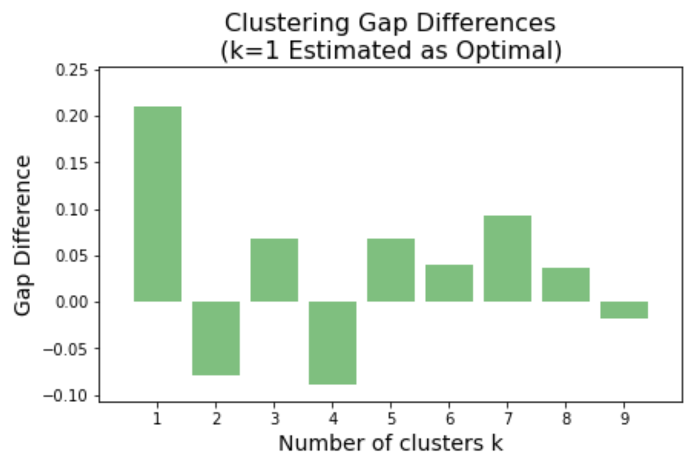
In [ ]:
```
ssqs = ssq_statistics(shopping_data, range(1,11))
plot_ssq_statistics(ssqs)
```

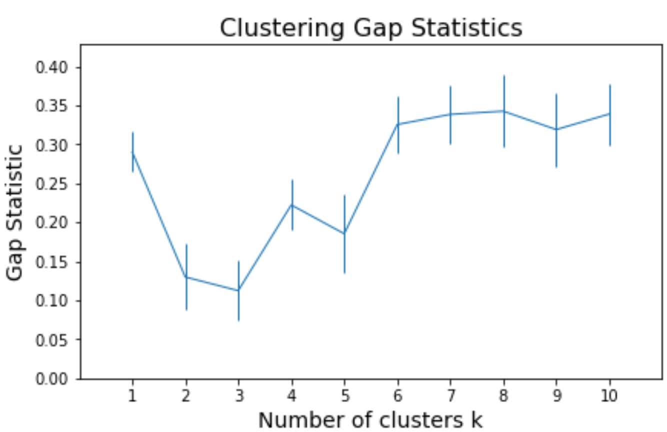


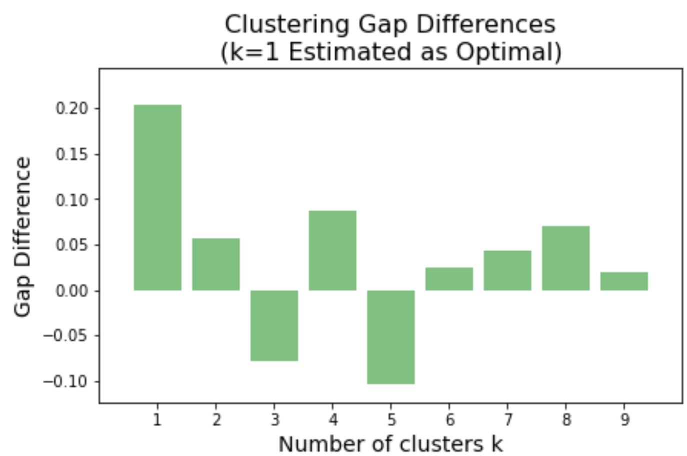
In [ ]:

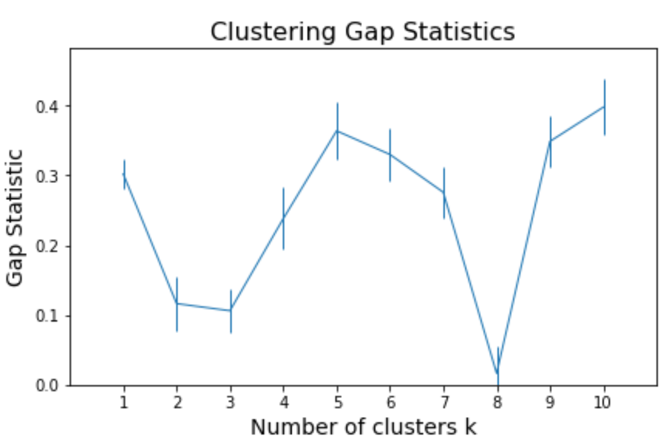
```
for _ in range(1,6):
    gaps, errs, difs = gap_statistics (shopping_data.to_numpy().astype(np.float64))
    plot_gap_statistics(gaps, errs , difs)
```

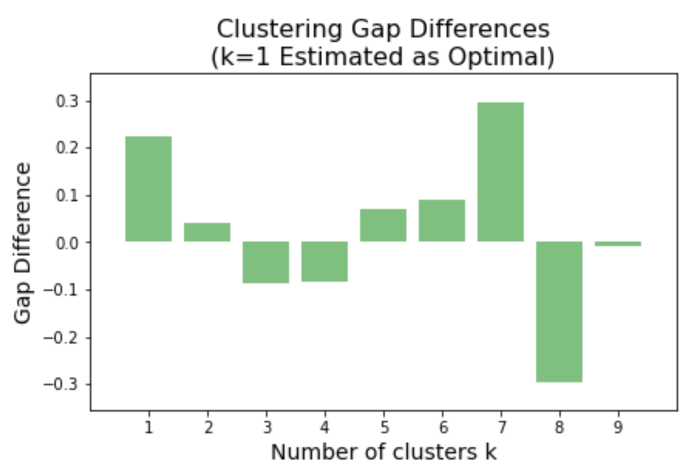


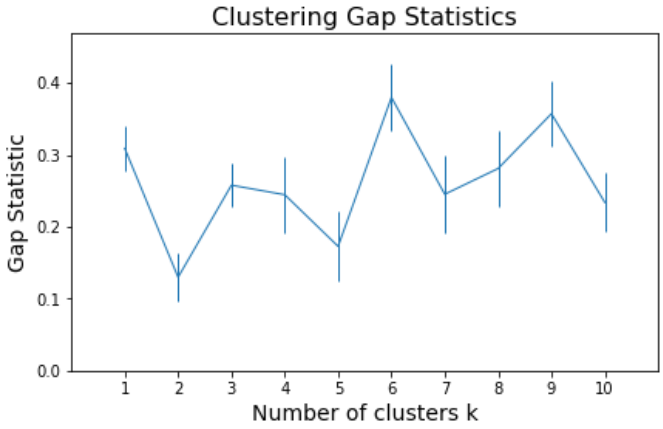


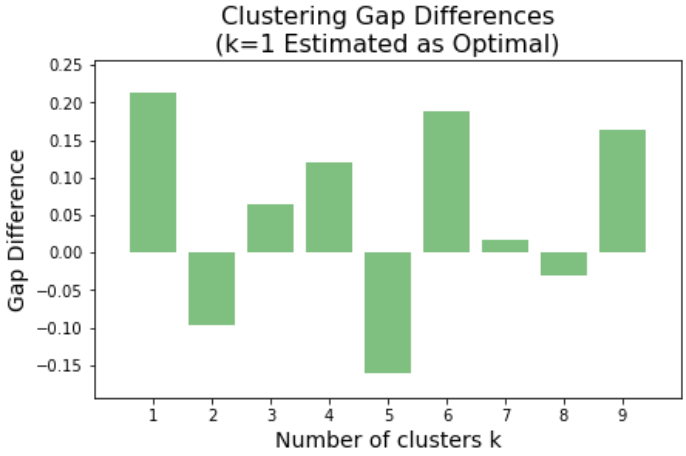


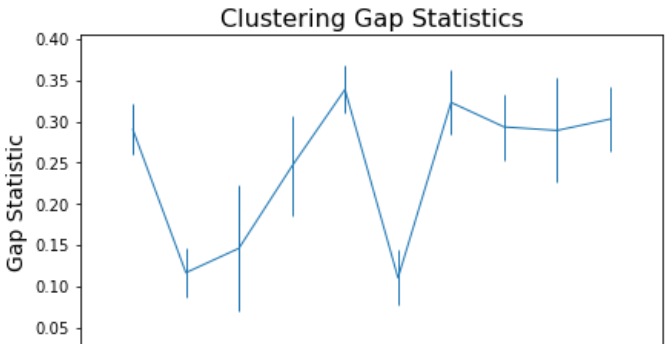


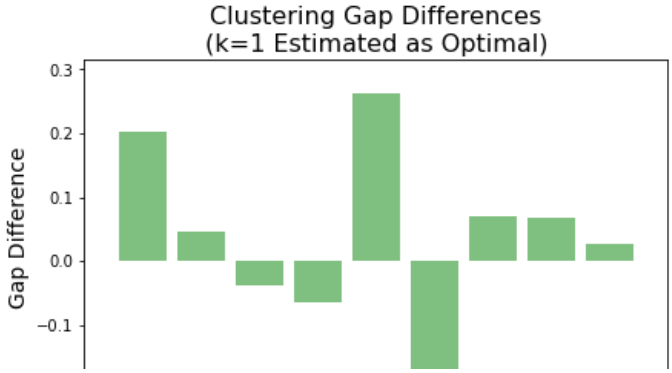












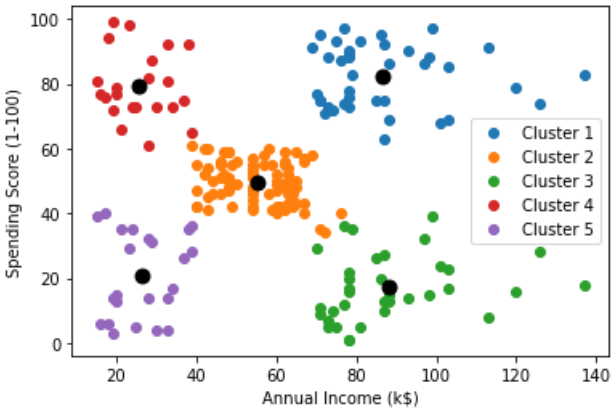
Plotting the clusters k=5 from the elbow, clustering gap gave k=1 for all clusters but 5, 6 came in as a close second many times using sklearn's Kmeans code

In [ ]:

```
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt
kmeans = KMeans(n_clusters=5)
labels = kmeans.fit_predict(shopping_data)

centroids = kmeans.cluster_centers_
u_labels = np.unique(labels)

for i in u_labels:
    plt.scatter(shopping_data[labels == i]['Annual Income (k$)'], shopping_data[labels == i]['Spending Score (1-100
plt.legend()
plt.scatter(centroids[:,0] , centroids[:,1] , s = 80, color ='black')
plt.xlabel('Annual Income (k$)')
plt.ylabel('Spending Score (1-100)')
plt.show()
```



Given this output, respond to the following questions:

1. Where did you estimate the elbow point to be (between what values of k)? What value of k was typically estimated as optimal by the gap statistic? To adequately answer this question, consider generating both measures several (atleast 5) times, as there may be some amount of variation in the value of k that they each estimate as optimal.

As stated above I estimated the elbow point to be somewhere around 5-6 and the value estiamted for k was 1 by the gap statistic, however this may have been caused by a problem with the code, and k=5 was always similar on the graphs above

2. Based on the scatter plot of the clustered data, what makes most sense? Give logical interpretation from visually inspecting the clusters.

Based on the scatter plot I think that k=5 makes the most sense, if you take the center chunk of points as 1 cluster you can clearly see there are 4 distinct clusters of points in each of the quandrents of the data. This to me is the biggest indication that there should be 5 clusters. This also looks correct when looking at the data colored with 5 clusters, the green cluster (cluster 3) and the blue cluster (cluster 1) have some outliers which may be other clusters but I still feel as though 5 clusters captures the information about the variations well and you can probably interpret much about the data with this. there is an intersting thing that there is 5 classes of shoppers presumably high income splits into high spening and low spending score, low income also splits into these categories while middle income only has one spending score group in the middle.

3. Between SSQ and Gap Statistics, does one measure seem to be a consistently better criterion for choosing the value of k than the other? Why or why not?

Between the two methods explored in this assignment I would have to say that SSQ is better at choosing the value of k. My reason for saying this is one that when looking at the value of K gathered from the the elbow 5-6 versus the optimal value the gap statisitc threw at me which was 1, there seems to be actual information we can gather from actually clustering the data vs not clustering it. On top of that Gap Statisitcs have a bit of randomness to them that, each run will have a different set of values calculated and this inherently adds some inconsistency, there could be a bad run where the gap statisitc does not give you the optimal value which is actually the most optimal but just the most optimal value for that run. This means that SSQ will give you more consistent values overall. Again my reasoning for better is that SSQ performed better here and showed more consistent results which garnered better information. There are probably applications in which the gap statisitc would be better but for this application and this data it seems SSQ is the better method.