In [2]:
```
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#
# Modified from:
# (c) 2013 Mikael Vejdemo-Johansson
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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

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.
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    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)
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        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:
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      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), \
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                 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.
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        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
            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 [3]:
```
import csv
from sklearn.cluster import KMeans
import warnings
warnings.filterwarnings('ignore')
def load_dataset(filename):
    '''Loads an example of market basket transactions from a provided csv file.

    Returns: A list (database) of lists (transactions). Each element of a transaction is
    an item.
    '''
    with open(filename,'r') as dest_f:
        data_iter = csv.reader(dest_f, delimiter = ',', quotechar = '"')
        data = [data for data in data_iter]
        data_array = np.asarray(data)

    # Remove features other than Annual Income and Spending Score.
    new_table = []
    for i in range(1, len(data_array)):
        new_table.append([data_array[i][3], data_array[i][4]])
    dataset = np.asarray(new_table).astype(float)
    return dataset
```

In [4]:
```
# Load the data
data = load_dataset('shopping-data.csv')
D = list(map(set, data))
print(D[0])
```

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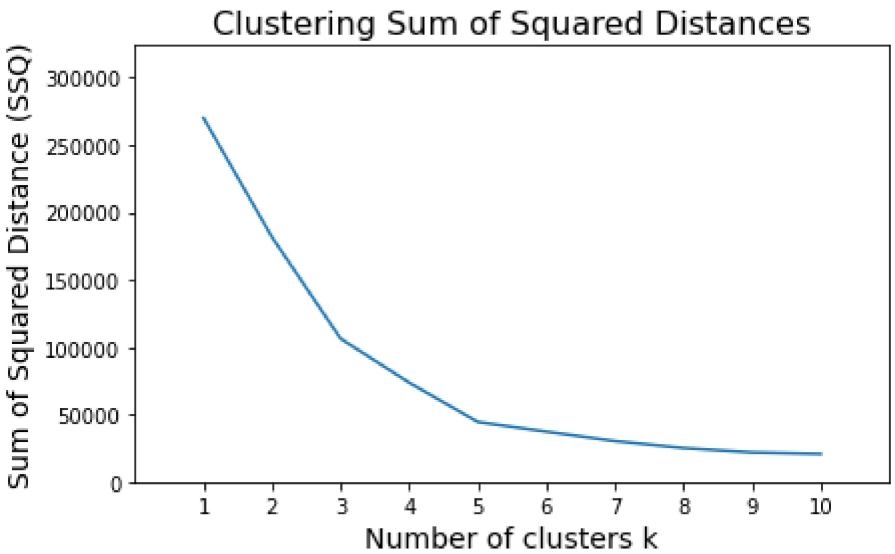
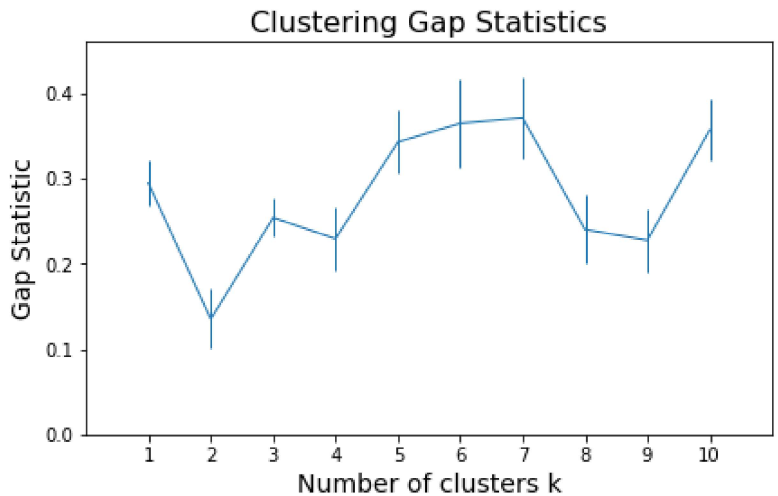
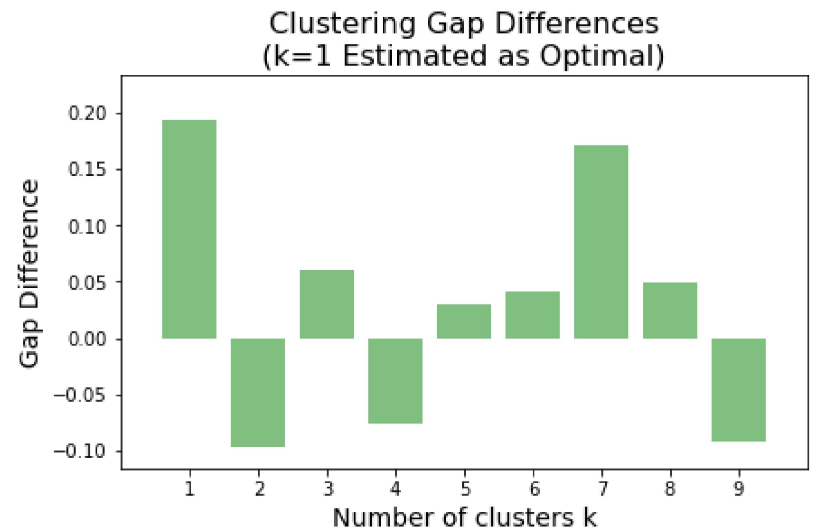
{39.0, 15.0}
```

In [5]:
```
# Generate and plot the SSQ statistics
ssqs = ssq_statistics(data, ks=range(1,11), ssq_norm=False)
plot_ssq_statistics(ssqs)
```



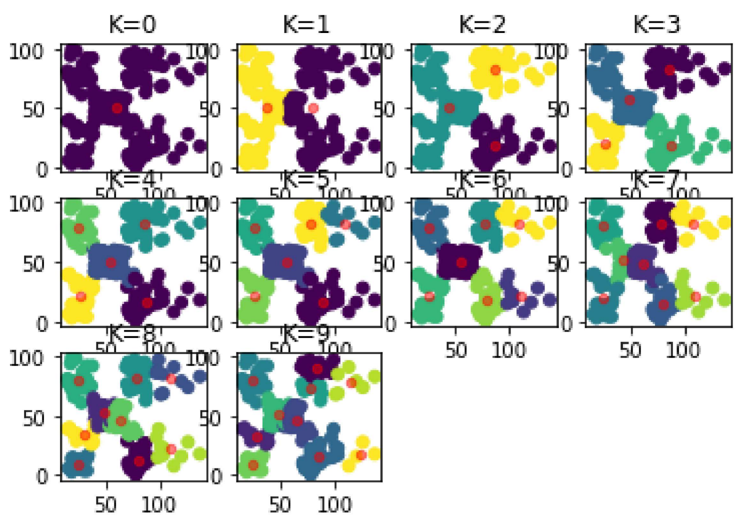
In [6]:
```
# Generate and plot the gap statistics
gaps,errs,difs = gap_statistics (data, nrefs=20, ks=range(1,11))
plot_gap_statistics(gaps,errs,difs)
```





In [7]:
```
def KMeans_data(data,ks):
    pl.figure()
    for (i, k) in enumerate(ks):  # iterate over the range of k values
        # Fit the model on the data
        km = KMeans(n_clusters = k, random_state = 0)
        y_pre = km.fit_predict(data)
        pl.subplot(3, 4, i+1)
        pl.title("K=" + str(i))
        pl.scatter(data[:, 0], data[:, 1], c = y_pre)
        centers = km.cluster_centers_
        pl.scatter(centers[:, 0], centers[:, 1], c='red', s=20, alpha=0.5);
    pl.show()

KMeans_data(data,ks=range(1,11))
```



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 (at least 5) times, as there may be some amount of variation in the value of k that they each estimate as optimal.

```
After generating both measures serveral times, here is my answer:

The estimate elbow point is k = 5.

And k = 1 is the typically estimated as optimal by the gap statistic.
```

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 of the clustered data, the elbow way makes more sense. In the figure, we can clearly see that the data can be divided into upper left part, lower left part, upper right part, lower right part and middle part.

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?

I think Gap Statistics seems to be a consistently better criterion for choosing the value of k than SSQ.

Because the disadvantage of the elbow method is that it is not automatic enough, and Gap Statistics no longer needs the eye to judge the “Elbow point”, but only needs to find the K value that makes the Gap Statistic maximum. Therefore, Gap Statistics is suitable for batch operation.