Problem 4

In [1]:
```
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
import sys
import random
random.seed(0)
np.random.seed(0)
```

In [2]:
```
column_names = ['sepal length','sepal width','petal length','petal width', 'class']
```

In [3]:
```
# read iris dataset
iris = pd.read_csv('iris.data',names=column_names,index_col=False)
```

In [4]:
```
iris.head()
```

Out[4]:

	sepal length	sepal width	petal length	petal width	class
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa

In [5]:
```
iris_df_new = pd.DataFrame() # creating new dataframe
```

In [6]:
```
# this function assigns values
def get_class(x):
    if x=='Iris-setosa': #  Iris-setosa =0
        return 0
    elif(x=='Iris-versicolor'): # Iris-versicolor =1
        return 1
    else:
        return 2 # Iris Virginica =3
```

In [7]:
```
# Assgning x1 and x2
iris_df_new['x1']=iris['sepal length']/iris['sepal width']
iris_df_new['x2']=iris['petal length']/iris['petal width']
iris_df_new['class']=iris['class']
iris_df_new['class_enc']=iris_df_new['class'].apply(lambda x: get_class(x))
```

In [8]:
```
iris_df_new.head()
```

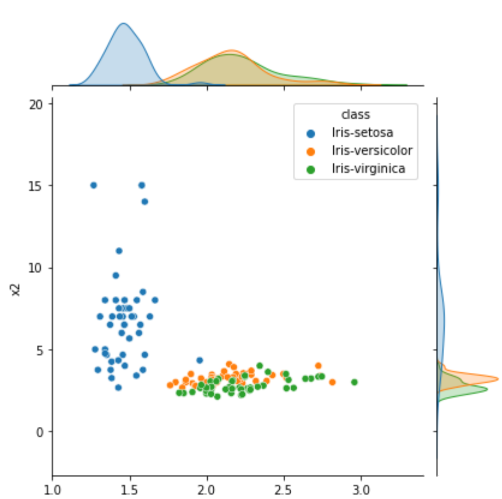
Out[8]:

	x1	x2	class	class_enc
0	1.457143	7.0	Iris-setosa	0
1	1.633333	7.0	Iris-setosa	0
2	1.468750	6.5	Iris-setosa	0
3	1.483871	7.5	Iris-setosa	0
4	1.388889	7.0	Iris-setosa	0

In [9]:
```
# showing the clusters
plt.figure(figsize=(12,8))
data = iris_df_new.drop('class_enc',axis=1)
sns.jointplot(x='x1',y='x2',data=data,hue='class')
```

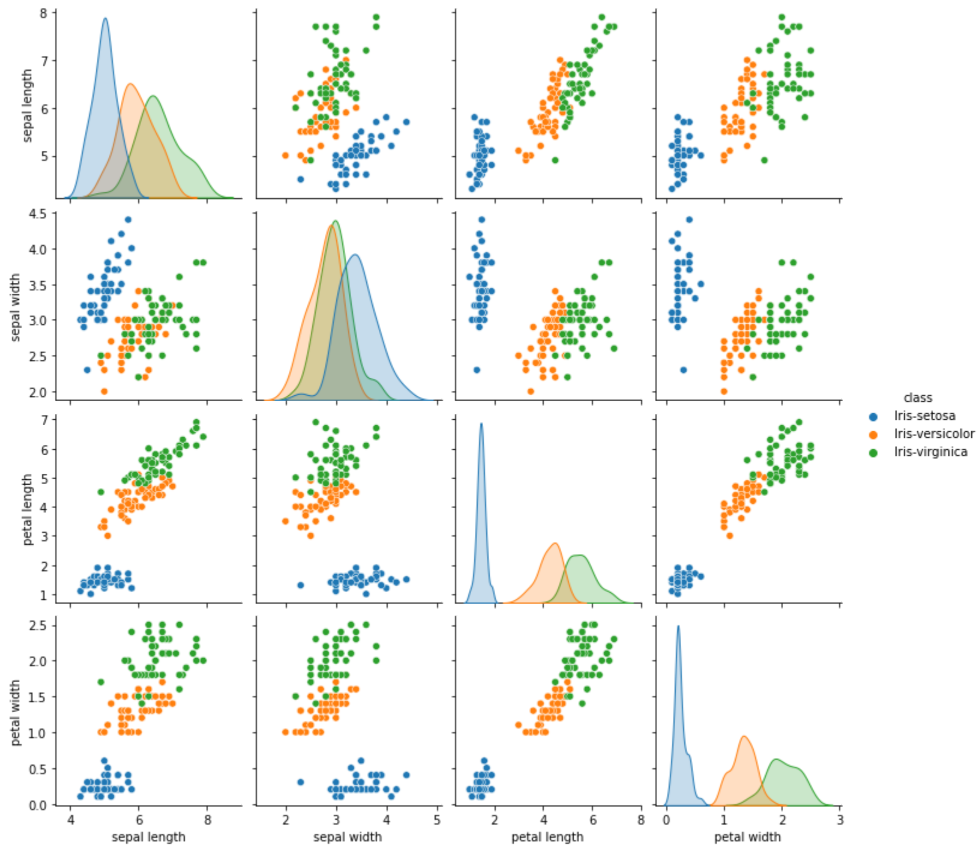
Out[9]: <seaborn.axisgrid.JointGrid at 0x7fb85005bcd0>

<Figure size 864x576 with 0 Axes>



In [10]:
```
sns.pairplot(data=iris,hue='class')
```

Out[10]: <seaborn.axisgrid.PairGrid at 0x7fb85005be90>



2) KMeans++ Source Code Documentation:

1. **Using Euclidean Distance for calculating distance between data points (get_distance function)**
2. **initialize_kmeans_plus_plus -> Initializes Centroids (takes "K" as argument) and returns initial K centroids**

   We initialize a list of centroids

   centroids=[]

   a. First we randomly select a point and append to the centroids list b. Then for rest (K-1) times,

   ```
   i. We loop through all the points
       .> Then determine minimum distance of the point from all current centroids in the centroids list
   ii. Among those minimum distances, we now select the distance with max value
        and select the corresponding data point as new centroid.
   iv. Append the new centroid data point to centroids list
   ```

3. **KMeans Plus Plus Algorithm:**

   kmeans_plus_plus -> (takes current centroids, "K" value), (returns new centroids,point to cluster centroids mapping)

   a. (initialization)

   ```
   cent_map=[] stores centroids and corresponding assigned points mapping
   sums_x1=[] # stores sum of x1 feature of all points within a cluster
   sums_x2=[] # stores sum of x2 feature of all points within a cluster
   ```

   b. For each of the points,

   ```
   i. we calculate the distance from all the current centroids.
   ii. we map the data point to the centroid with which it has minimum distance
   ```

   c. For each of the cluster, we calculate the new centroids by

   ```
   new_cx1[k] = sums_x1[k]/length(cent_map[k])
   new_cx2[k] = sums_x2[k]/length(cent_map[k])
   append this values to new centroids list
   ```

   d. Returns the new centroids list and mapping of points to centroids.

In [11]:
```
# Euclidean Distance - to calculate distance
def get_distance(x1,x2,y1,y2):
    d1=(y1-x1)**2
    d2=(y2-x2)**2
    return (d1+d2)
```

In [12]:
```python
## Initialize the centroids function
num_rows = iris_df_new.shape[0]
def initialize_kmeans_plus_plus(k):
    centroids_x1=[]
    centroids_x2=[]
    # first point is selected randomly
    rand_num = np.random.randint(num_rows-1)
    first_centroid_x1 = iris_df_new['x1'].iloc[rand_num]
    first_centroid_x2 = iris_df_new['x2'].iloc[rand_num]
    centroids_x1.append(first_centroid_x1)
    centroids_x2.append(first_centroid_x2)

    for k_id in range(k-1):
        dist=[]
        # for each of the point
        for ind in range(num_rows):
            x1=iris_df_new['x1'].iloc[ind]
            x2=iris_df_new['x2'].iloc[ind]
            min_dist = sys.maxsize
            # we determine the minimum distance from current all centroids
            for cd in range(len(centroids_x1)):
                y1=centroids_x1[cd]
                y2=centroids_x2[cd]
                distance = get_distance(x1,x2,y1,y2)
                min_dist = min(min_dist,distance)
            dist.append(min_dist)
        # then select the data point which is at maximum distance,
        # and assign that data point as new centroid
        mx_ind = np.argmax(np.array(dist))
        centroids_x1.append(iris_df_new['x1'].iloc[mx_ind])
        centroids_x2.append(iris_df_new['x2'].iloc[mx_ind])

    return centroids_x1,centroids_x2
```

In [13]:
```python
## Kmean++ algorithm
def kmeans_plus_plus(k,centroids_x1,centroids_x2):
    # number of datapoints
    num_rows = iris_df_new.shape[0]
    cent_map=[] # stores centroids and corresponding assigned points mapping
    sums_x1=[] # stores sum of x1 feature of all points within a cluster
    sums_x2=[] # stores sum of x2 feature of all points within a cluster
    for ind in range(k):
        cent_map.append([])
        sums_x1.append(0)
        sums_x2.append(0)
    # for each data point
    for ind in range(num_rows):
        x1=iris_df_new['x1'].iloc[ind]
        x2=iris_df_new['x2'].iloc[ind]
        min_dist = sys.maxsize
        mid=-1
        # we calculate the distances between point and all centroids
        # point will be mapped to the centroid with minimum distance from it
        for cd in range(len(centroids_x1)):
            y1=centroids_x1[cd]
            y2=centroids_x2[cd]
            distance = get_distance(x1,x2,y1,y2)
            if mid==-1:
                mid=cd
                min_dist = distance
            else:
                if(distance<min_dist):
                    mid=cd
                    min_dist = distance
        cent_map[mid].append(ind)
    # calculating new centroids
    for ind in range(len(cent_map)):
        for cd in range(len(cent_map[ind])):
            index = cent_map[ind][cd]
            sums_x1[ind]+=iris_df_new['x1'].iloc[index]
            sums_x2[ind]+=iris_df_new['x2'].iloc[index]

    for ind in range(len(cent_map)):
        length = len(cent_map[ind])
        #print(length)
        if(length>0):
            sums_x1[ind]=sums_x1[ind]/float(length)
            sums_x2[ind]=sums_x2[ind]/float(length)

    centroids_x1=sums_x1
    centroids_x2=sums_x2
    # returning new centroids, mapping of points to corresponding centroids
    return centroids_x1,centroids_x2,cent_map
```

In [14]:
```
# 3. K=1 to 5 and 50 iterations for each
maps_of_points=[]
final_centroids=[]
initial_centroids=[]
for k_value in range(1,6):
    centroids_x1,centroids_x2=initialize_kmeans_plus_plus(k_value)
    first_cent=[]
    first_cent.append(centroids_x1)
    first_cent.append(centroids_x2)
    initial_centroids.append(first_cent)
    final_map=[]
    for turn in range(50):
        centroids_x1,centroids_x2,cent_map = kmeans_plus_plus(k_value,centroids_x1,centroids_x2)
        final_map=cent_map
    maps_of_points.append(final_map)
    centroids =[]
    centroids.append(centroids_x1)
    centroids.append(centroids_x2)
    final_centroids.append(centroids)
```

In [15]:
```python
for k in range(len(final_centroids)):
    print("centroids for k_value = ",k+1)
    print("Initial Centroids")
    for t in range(len(initial_centroids[k][0])):
        print(initial_centroids[k][0][t],initial_centroids[k][1][t])
    print("\nFinal Centroids")
    for t in range(len(final_centroids[k][0])):
        print(final_centroids[k][0][t],final_centroids[k][1][t])
    print("\n\n*******\n\n")
```

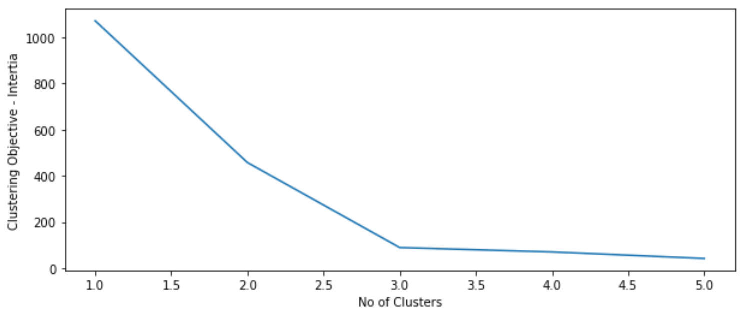
```
centroids for k_value =  1
Initial Centroids
1.4374999999999998 6.999999999999999

Final Centroids
1.9551444308694617 4.367166423691872


*******


centroids for k_value =  2
Initial Centroids
2.0263157894736845 3.0454545454545454
1.2682926829268295 15.0

Final Centroids
1.9777366323385024 3.920104640236229
1.4936180294304975 13.5


*******


centroids for k_value =  3
Initial Centroids
2.148148148148148 4.1
1.2682926829268295 15.0
1.411764705882353 9.499999999999998

Final Centroids
2.0928950450949397 3.1673129041992576
1.5220456333595596 14.8
1.4788141804347774 7.3678160919540225


*******


centroids for k_value =  4
Initial Centroids
2.1724137931034484 3.1111111111111107
1.2682926829268295 15.0
1.411764705882353 9.499999999999998
1.5714285714285714 6.5

Final Centroids
2.1066310718427834 3.1351604990097712
1.5220456333595596 14.8
1.4838758832268053 8.625
1.4623690090317294 6.724637681159421


*******


centroids for k_value =  5
Initial Centroids
1.5806451612903227 15.0
2.0714285714285716 2.125
1.5882352941176472 8.5
1.2777777777777777 5.0
1.4333333333333333 11.0

Final Centroids
1.5220456333595596 14.8
2.172285144648706 2.984749635537806
1.48232743051511 7.211538461538462
1.5910182803613162 4.3882352941176475
1.4225490196078432 10.25


*******
```

In [16]:
```
# calculating inertia (sum of square of distance of points from their cluster centroids)
acc=[]
for u in range(len(maps_of_points)):
    fmap=maps_of_points[u]
    centroids = final_centroids[u]
    sum_dist=0
    for t in range(len(fmap)):
        pts = fmap[t]
        mn_dist=0
        for y in range(len(pts)):
            dist = get_distance(centroids[0][t],centroids[1][t],
                                iris_df_new['x1'].iloc[pts[y]],iris_df_new['x2'].iloc[pts[y]])
            mn_dist+=dist
        sum_dist+=mn_dist
    acc.append(sum_dist)
    print("mean =", sum_dist, "for K = ",u+1)
```

```
mean = 1071.228686156884 for K =  1
mean = 457.22352154601197 for K =  2
mean = 89.17750273047949 for K =  3
mean = 70.1996474420087 for K =  4
mean = 42.03957396126128 for K =  5
```

In [17]:
```
plt.figure(figsize=(10,4))
index=range(1,6)
sns.lineplot(x=index, y=acc)
plt.xlabel('No of Clusters')
plt.ylabel('Clustering Objective - Intertia')
```

Out[17]:
```
Text(0, 0.5, 'Clustering Objective - Intertia')
```



4) From K =1 to 3, the inertia (sum of square of distance of points from their cluster centroids) decreases highly, then the decrease rate is very less. So, I will choose K=3

In [18]:
```
#chosen cluster = 3
centroids_x13,centroids_x23=initialize_kmeans_plus_plus(3)
print("initial chosen centroids with k=3 ")
for u in range(len(centroids_x13)):
        print(centroids_x13[u],centroids_x23[u])
```

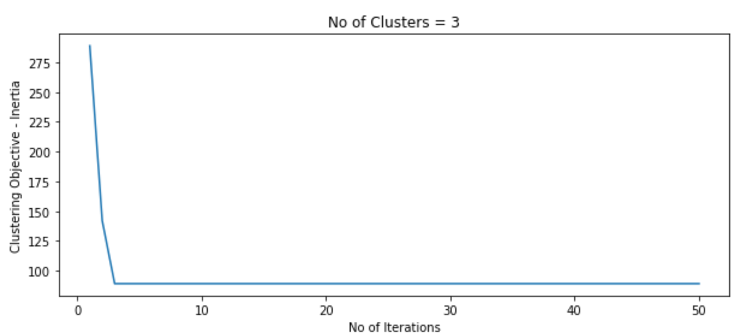
```
initial chosen centroids with k=3
1.3783783783783783 3.75
1.5806451612903227 15.0
1.411764705882353 9.499999999999998
```

In [19]:
```python
final_map3=[]
cent_map3=[]
accuracy3=[]
for u in range(3):
    cent_map3.append([])
num_rows = iris_df_new.shape[0]
# initial assignment of points to initial cluster centers
for ind in range(num_rows):
        x1=iris_df_new['x1'].iloc[ind]
        x2=iris_df_new['x2'].iloc[ind]
        min_dist = sys.maxsize
        mid=-1
        for cd in range(len(centroids_x13)):
            y1=centroids_x13[cd]
            y2=centroids_x23[cd]
            distance = get_distance(x1,x2,y1,y2)
            if mid==-1:
                mid=cd
                min_dist = distance
            else:
                if(distance<min_dist):
                    mid=cd
                    min_dist = distance
        cent_map3[mid].append(ind)

for turn in range(50):
    #print("iteration = ",turn+1)
    sum_dist=0
    for u in range(len(cent_map3)):
        pts=cent_map3[u]
        mn_dist=0
        for j in range(len(pts)):
            x1=iris_df_new['x1'].iloc[pts[j]]
            x2=iris_df_new['x2'].iloc[pts[j]]
            dist = get_distance(centroids_x13[u],centroids_x23[u],x1,x2)
            mn_dist+=dist
        sum_dist+=mn_dist
    #print(sum_dist,"\n\n")
    accuracy3.append(sum_dist)
    centroids_x13,centroids_x23,cent_map3 = kmeans_plus_plus(3,centroids_x13,centroids_x23)
    final_map3=cent_map3
print("objective function (accuracy) changes for 50 iterations and K =3")
print(accuracy3)
```

```
objective function (accuracy) changes for 50 iterations and K =3
[288.86800513774403, 142.09234821590687, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273
047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.177
50273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 8
9.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.177502730479
49, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.1775027
3047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949, 89.17
750273047949, 89.17750273047949, 89.17750273047949, 89.17750273047949]
```

In [20]:
```python
plt.figure(figsize=(10,4))
index3=range(1,51)
sns.lineplot(x=index3, y=accuracy3)
plt.xlabel('No of Iterations')
plt.ylabel('Clustering Objective - Inertia')
plt.title('No of Clusters = 3')
```

Out[20]:
```
Text(0.5, 1.0, 'No of Clusters = 3')
```

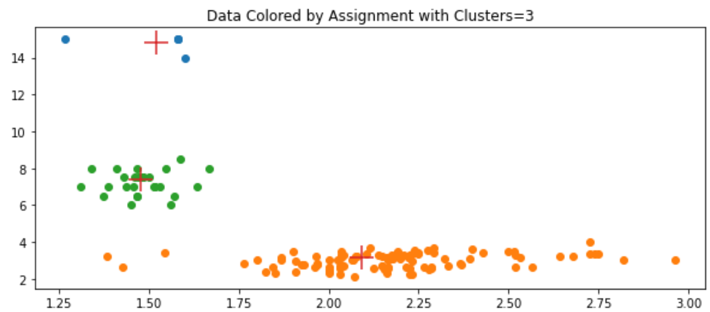


In [21]:
```python
print(final_map3)
print("Final Cluster Centers for K=3")
for u in range(len(centroids_x13)):
    print(centroids_x13[u],centroids_x23[u])
```

```
[[5, 6, 15, 16, 17, 19, 21, 22, 23, 26, 31, 40, 41, 43, 44, 45, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70,
71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 1
06, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 13
5, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149], [9, 12, 32, 34, 37], [0, 1, 2, 3, 4, 7, 8, 10, 11, 13, 14, 18, 20, 24, 2
5, 27, 28, 29, 30, 33, 35, 36, 38, 39, 42, 46, 47, 48, 49]]
Final Cluster Centers for K=3
2.0928950450949397 3.1673129041992576
1.5220456333595596 14.8
1.4788141804347774 7.3678160919540225
```

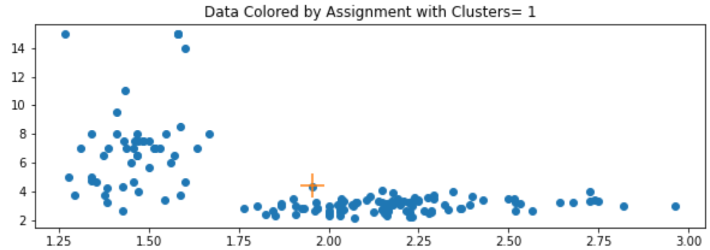
In [22]:
```
x3=[]
y3=[]
for t in range(len(final_map3)):
    pts = fmap[t]
    lx=[]
    ly=[]
    for y in range(len(pts)):
        lx.append(iris_df_new['x1'].iloc[pts[y]])
        ly.append(iris_df_new['x2'].iloc[pts[y]])
    x3.append(lx)
    y3.append(ly)
```

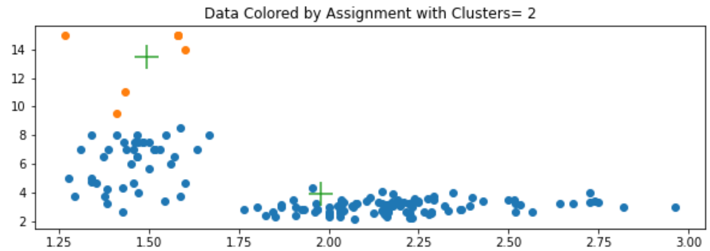
In [23]:
```
# centroids are in + sign

plt.figure(figsize=(10,4))
for u in range(len(x3)):
    plt.scatter(x3[u],y3[u])
plt.scatter(centroids_x13,centroids_x23,marker='+',s=400)
plt.title('Data Colored by Assignment with Clusters=3')
plt.show()
```

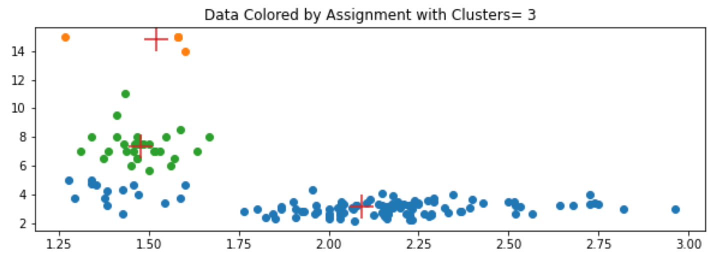


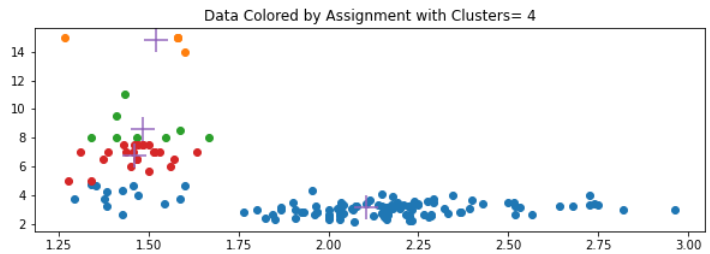
In [24]:
```
X=[]
Y=[]
for u in range(len(maps_of_points)):
    fmap=maps_of_points[u]
    centroids = final_centroids[u]
    mx=[]
    my=[]
    for t in range(len(fmap)):
        pts = fmap[t]
        mn_dist=0
        lx=[]
        ly=[]
        for y in range(len(pts)):
            lx.append(iris_df_new['x1'].iloc[pts[y]])
            ly.append(iris_df_new['x2'].iloc[pts[y]])
        mx.append(lx)
        my.append(ly)
    X.append(mx)
    Y.append(my)
```

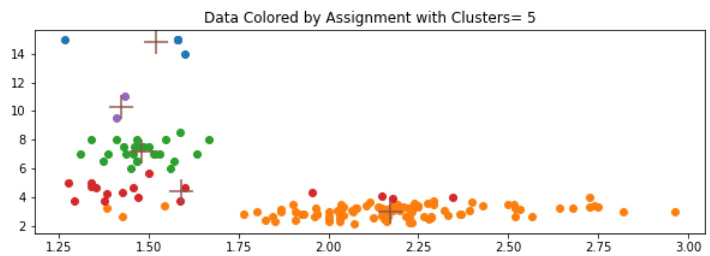
In [25]:
```
for y in range(5):
    plt.figure(figsize=(10,18))
    plt.subplot(5,1,y+1)
    for u in range(len(X[y])):
        plt.scatter(X[y][u],Y[y][u])
    plt.scatter(final_centroids[y][0],final_centroids[y][1],marker='+',s=400)
    plt.title('Data Colored by Assignment with Clusters= '+str(y+1))
    plt.show()
```











In [ ]: