Exercise10SebastianPineda

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Machine Learning Lab - Exercise Sheet 10
Author: Sebastian Pineda Arango ID: 246098 Universität Hildesheim - Data Analytics Master

0.1 Exercise 1

In this exercise we want to aply clusterin methods to two differente datasets:

- Dataset 1: Iris dataset (in sparse format) https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/multic
- Dataset 2: 20 news dataset: http://qwone.com/~jason/20Newsgroups/

Firstly, we want to cluster Iris dataset. The dataset is well-known tdataset, with four features, 150 samples and three classes. However, in this case we are going to neglect the classes, since we want to work only in an unsupervised way.

Step 1: Importing libraries

```
In [1]: #Importing libraries
        import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        from sklearn.datasets import load_svmlight_file

        %matplotlib inline
```

Step 2: Reading file The file is in sparse format, however the function load_svm_light_file returns the design matrix and the label vectors. We also transform the returned design matrix (which is in sparse compressed format) to dense matrix.

```
In [2]: #Reading file
        data = load_svmlight_file("iris.scale.txt")
        X = data[0]
        y = data[1]

        #transforming to dense matrix
        X_dense = X.todense()
```

Step 3: Implementing K-Means algorithm To implement k-means algorhtm, four functions are defined:

- find_assignation: to find the cluster to which each sample belongs to.
- find_center: to update the center after and assignation step
- find_MSE: to evaluate the clustering

```
In [3]: def find_assignation(X,C):

            '''Finds the cluster represented by centers in C to which each
               sample of X belongs. Returns the number of the cluster for
               each sample.'''

            assignation=[]
            for i in range(X.shape[0]):

                #Look for the closes center for each data point
                assignation.append(np.argmin(np.linalg.norm(X[i,]-C,axis=1)))

            return assignation

        def find_center(X, assignation, k):

            '''Returns the new centers according to the assignation. '''

            d = X.shape[1]
            C = np.zeros([k, d])

            for i in list(set(assignation)):

                #calculate the new center with assgination index given by i
                C[i,:] = X[np.array(assignation)==i,:].mean(axis=0)

            return C

        def find_MSE(X,C,assignation):

            '''Returns the RMSE for a given clustering configuration: (data and centers)'''

            q = []

            for i, a in enumerate(assignation):
                q.append(np.linalg.norm(X[i,]-C[a,])**2)

            return np.mean(q)


        def K_means(X, k, max_iter = 50):
```

```python
    '''Performs K-Means clustering, where K is the number of cluster to return'''

    #Initialization of variables
    d = X.shape[1] #dimension of the problem
    C= np.random.random((k,d)) #random centers initialization
    MSE_list = []

    #First run of assignation
    assignation = find_assignation(X,C)
    MSE = find_MSE(X, C, assignation)
    MSE_list.append(MSE)

    for i in range(4):

        #updating centers
        C = find_center(X, assignation, k)

        #assignation of data to cluster accordint to centers
        assignation = find_assignation(X,C)

        #computing RMSE
        last_MSE = MSE
        MSE = find_MSE(X, C, assignation)

        #saving data for plotting
        MSE_list.append(MSE)

        #convergence criterion: if MSE change is small
        if(np.abs(last_MSE-MSE)<0.0001):
            break


    return C, np.array(assignation), MSE_list
```

Step 4: Evaluating the performance of the algorithm Evaluating the clustering is a though task, since no data classes are given a priori. Therefore, some methodologies and heuristics have been developed to assess the quality of the clustering. Maybe, one of the most well known is the elbow criteria, which states that the number of cluster should be located near to the point where the curve RMSE vs. Number of clusters change a lot. A reinterpretation of that is: where the second derivative is maximal.

Another criteria is also the index Silhouette. This index aims to minimize the intracluster distance (distance between points of the same cluster) and, at the same time, to maximize the intercluster distance (distance between clusters centers) [2].

The silhouette index for a sample i is given by:

$s(i) = \frac{b(i)-a(i)}{max\{a(i),b(i)\}}$

The silhouette index of a clustering setting is therefore the mean of the cluster indeces of the individual samples.

```
In [17]: def silhouette(X, A, k):

             '''This function evaluates the silhouette index for a dataset X, given
             an assignation A (this includes information of clustering).'''

             print("Trying k=",k)
             sil= []
             for i in range(X.shape[0]):
                 dist_to_k = []
                 for k_i in range(k):

                     dist= np.mean(np.linalg.norm(X[i,]-X[A==k_i,], axis=1))

                     if(k_i == A[i]):
                         a = dist
                     else:
                         dist_to_k.append(dist)

                 m_min = min(dist_to_k)
                 sil_x = (m_min-a)/max((a, m_min))
                 sil.append(sil_x)

             return np.mean(sil)


         def find_K_with_silhouette (X, max_k):

             '''This function iterates over a set of K values and pick the k
             with the most apporpiate silhouette index'''
             max_iter=100
             sil_list = []
             for i in range(2,max_k):

                 #cluster data using k-means
                 C, A, MSE_list = K_means(X,i, max_iter)

                 #find the silhouette index of the clustering
                 sil = silhouette(X, A, i)

                 #append index to indeces list
                 sil_list.append(sil)

             return sil_list, np.argmax(sil_list)+2

         #find best K
```

```
max_k = 20
sil_list, best_k = find_K_with_silhouette(X_dense, max_k)
print("The best number of k is", best_k)
```

```
Trying k= 2
Trying k= 3
Trying k= 4
Trying k= 5
Trying k= 6
Trying k= 7
Trying k= 8
Trying k= 9
Trying k= 10
```

```
C:\Users\User\Anaconda3\lib\site-packages\numpy\core\fromnumeric.py:2909: RuntimeWarning: Mean
  out=out, **kwargs)
C:\Users\User\Anaconda3\lib\site-packages\numpy\core\_methods.py:80: RuntimeWarning: invalid va
  ret = ret.dtype.type(ret / rcount)
```

```
Trying k= 11
Trying k= 12
Trying k= 13
Trying k= 14
Trying k= 15
Trying k= 16
Trying k= 17
Trying k= 18
Trying k= 19
The best number of k is 2
```

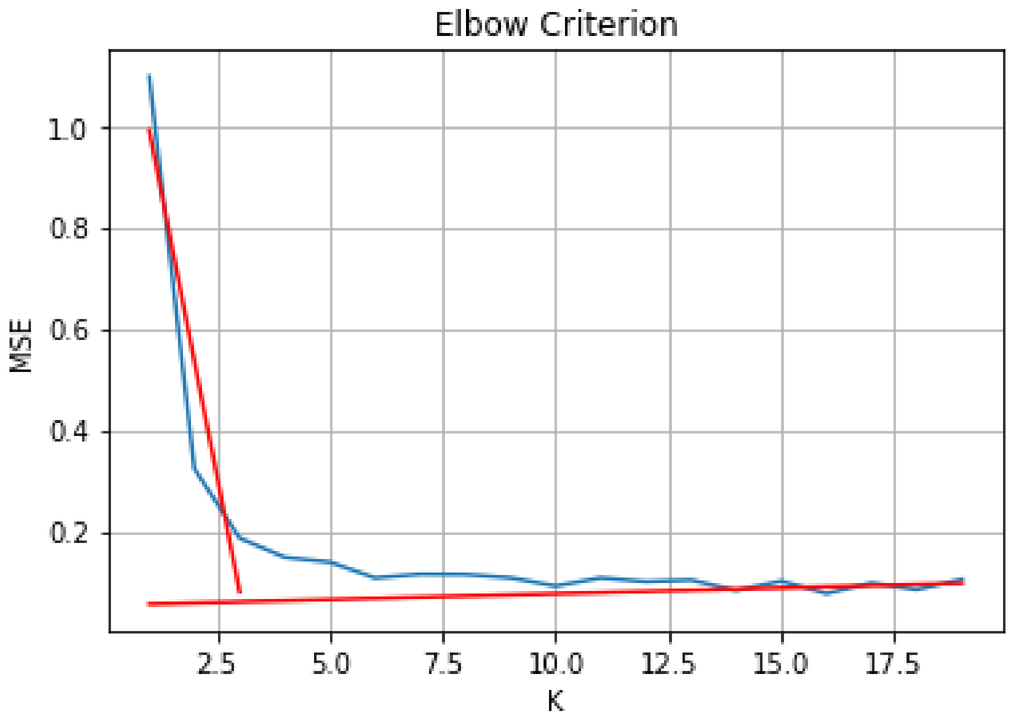
In [48]:
```
def find_K_with_derivative(X, max_k):

    '''Iterates over different K and pick the one with
    the highest second derivative (elbow criterion)'''

    k_list = list(range(1,max_k))
    MSE_k_list  = []
    max_iter = 100

    for k in k_list:
        print("Trying with k=",k)
        C, A, MSE_list = K_means(X, k, max_iter)
        MSE_k_list.append(MSE_list[-1])

    second_derivative = [MSE_k_list[i+1] + MSE_k_list[i-1] - 2 * MSE_k_list[i] for i 
    best_k = np.argmax(second_derivative)+2
```

```
        return second_derivative, best_k, MSE_k_list

    sd, best_k, MSE_list = find_K_with_derivative(X_dense, max_k)

    print("Best k for clustering:", best_k)
```

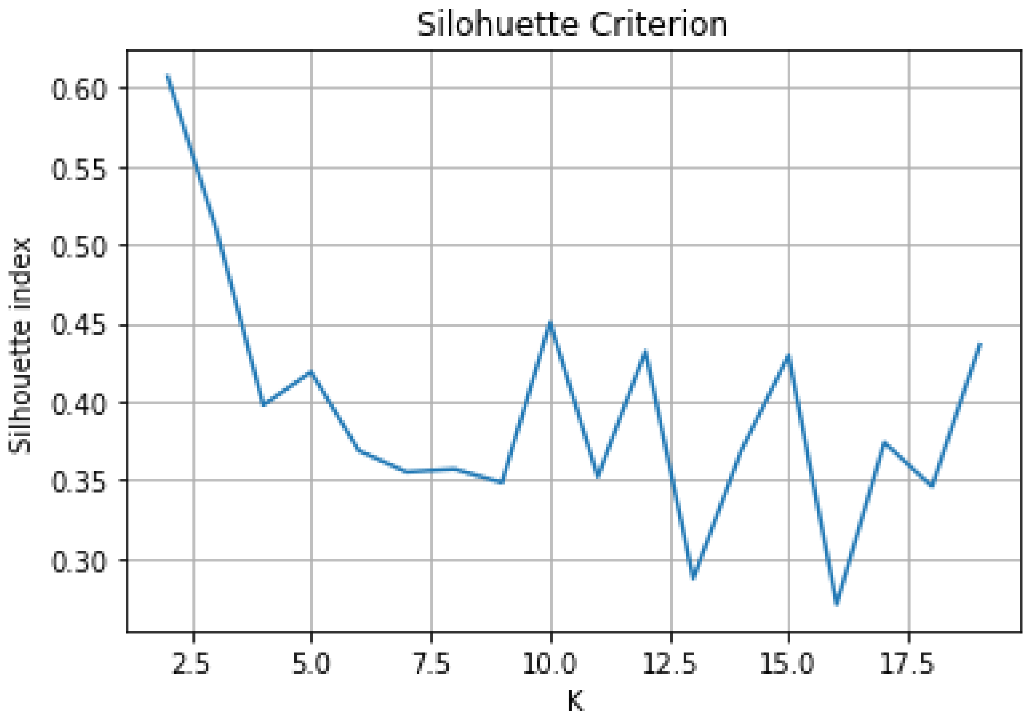
```
Trying with k= 1
Trying with k= 2
Trying with k= 3
Trying with k= 4
Trying with k= 5
Trying with k= 6
Trying with k= 7
Trying with k= 8
Trying with k= 9
Trying with k= 10
Trying with k= 11
Trying with k= 12
Trying with k= 13
Trying with k= 14
Trying with k= 15
Trying with k= 16
Trying with k= 17
Trying with k= 18
Trying with k= 19
Best k for clustering: 2
```

Now we put all the graphs together to pick the cluster size:

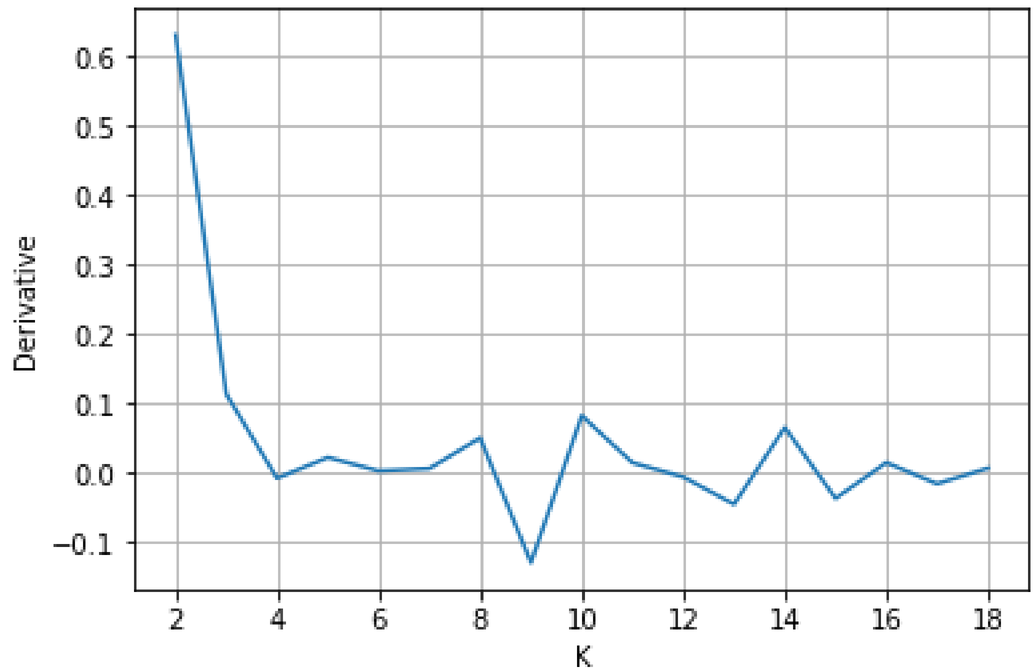
```
In [40]: plt.plot(range(1, max_k), MSE_list)
         plt.xlabel("K")
         plt.ylabel("MSE")
         plt.title("Elbow Criterion")

         x1 = range(1,4)
         y1 = MSE_list[:3]
         m1,b1 = np.polyfit(x1, y1, 1)

         x2 = range(max_k-6,max_k)
         y2 = MSE_list[-6:]
         m2,b2 = np.polyfit(x2, y2, 1)

         x = range(1, max_k)
         plt.plot(x, m2*x+b2, 'red')
         plt.plot(x1, m1*x1+b1, 'red')
         plt.grid()
```




```
In [46]: plt.plot(range(2,max_k),sil_list)
         plt.grid()
         plt.xlabel("K")
         plt.ylabel("Silhouette index")
         plt.title("Silohuette Criterion")

Out[46]: Text(0.5,1,'Silohuette Criterion')
```




```
In [56]: plt.plot(range(2,max_k-1), sd)
         plt.grid()
         plt.xlabel("K")
         plt.ylabel("Derivative")

Out[56]: Text(0,0.5,'Derivative')
```

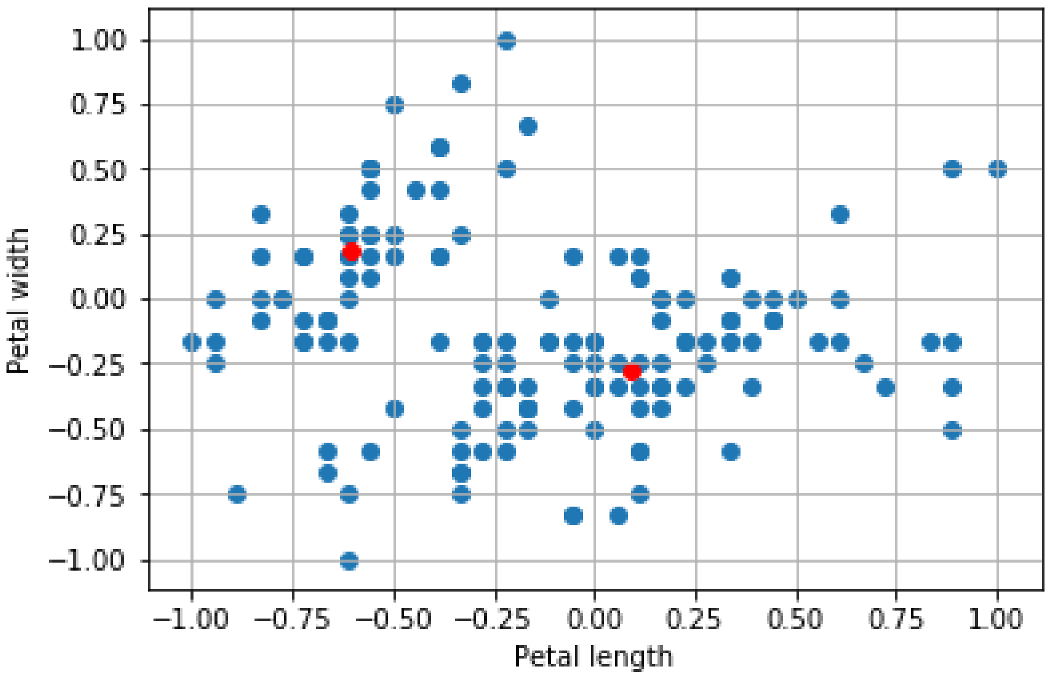


To get the exact number of optimal cluster is nearly impossible but there criterions somewhat give a closer insight. According to the elbow criterion, the number of cluster should be 3. By referring to second derviative and sihlouette, the decision would be for 2 clusters.

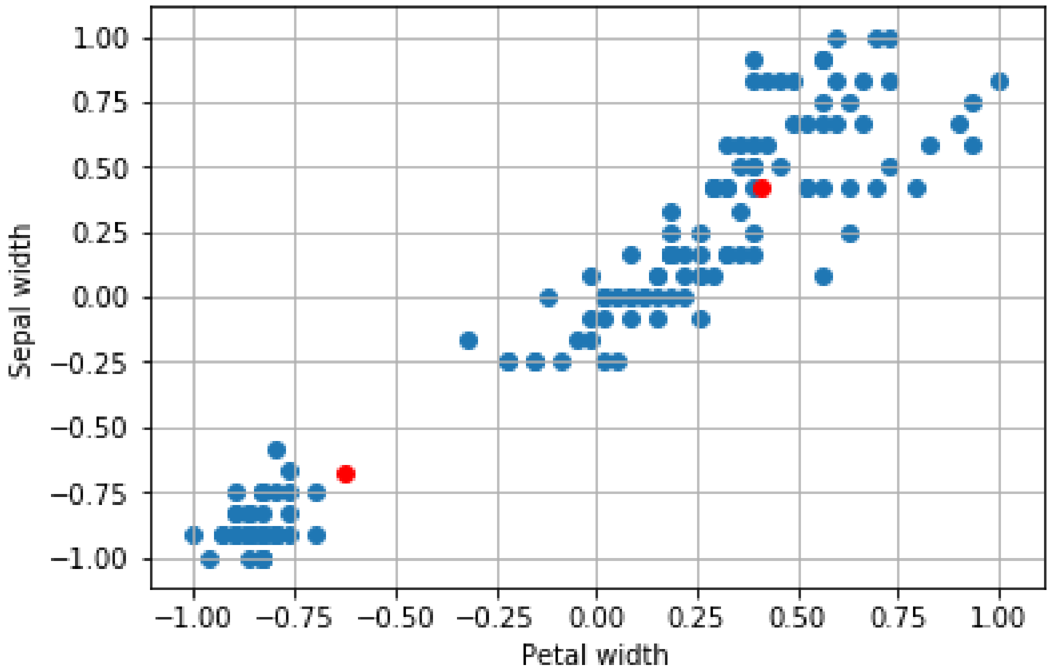
It is, therefore, aceptable to claim that the proper number of cluster is 2. In the following we create different plots to get an idea of how the data is being clustered along different dimensions. The clusters center are colored with red.Two centers turns to be a reasoable decision.

In [57]:
```
#Graphs
X= X_dense
k = 2
C, A, MSE_list = K_means(X_dense,k, 120)

plt.scatter(np.array(X[:,0]), np.array(X[:,1]))
plt.scatter(np.array(C[:,0]), np.array(C[:,1]), c= "red")
plt.grid()
plt.xlabel("Petal length")
plt.ylabel("Petal width")
```

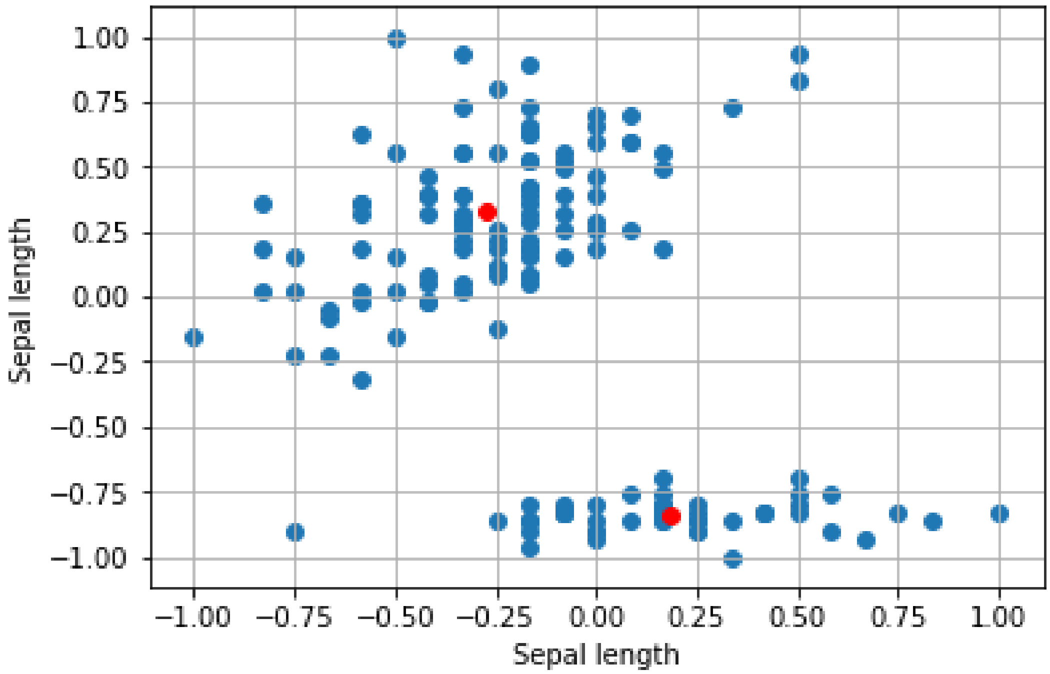
Out[57]:
```
Text(0,0.5,'Petal width')
```




```
In [61]: #Graphs
         X= X_dense
         k = 2
         C, A, MSE_list = K_means(X_dense,k, 120)

         plt.scatter(np.array(X[:,2]), np.array(X[:,3]))
         plt.scatter(np.array(C[:,2]), np.array(C[:,3]), c= "red")
         plt.grid()
         plt.xlabel("Petal width")
         plt.ylabel("Sepal width")

Out[61]: Text(0,0.5,'Sepal width')
```




```
In [62]: #Graphs
         X= X_dense
         k = 2
         C, A, MSE_list = K_means(X_dense,k, 120)

         plt.scatter(np.array(X[:,1]), np.array(X[:,2]))
         plt.scatter(np.array(C[:,1]), np.array(C[:,2]), c= "red")
         plt.grid()
         plt.xlabel("Sepal length")
         plt.ylabel("Sepal length")

Out[62]: Text(0,0.5,'Sepal length')
```



1 Exercise 2

The second dataset consist in a set of news which belongs to 20 different topics. However, in this clustering task, we won't use the label. The main objective, then, is to perform cluster analysis and to find the best possible K for this data set.

Step 1: Readin dataset As the dataset are raw texts, we should list them and read them. Then we put it toggether in list to further processing.

```
In [69]: #importing library to get data
         import os

         #path to th data
         path_to_train = "20news-bydate/20news-bydate-train"
         path_to_test = "20news-bydate/20news-bydate-test"


         def read_news(path):

             '''Function to read news located in given path folder'''

             class_list = []
             text_list = []
             folders = os.listdir(path)
```

```
        for folder in folders:
            files = os.listdir(path+"/"+folder)

            print("Reading", folder, "folder")

            for file_name in files:
                file = open(path+"/"+folder+"/"+file_name, 'r')
                text = file.read()

                class_list.append(folder)
                text_list.append(text)

        data = pd.DataFrame({'Text': text_list,
                             'Label': class_list})

        return data

    print("Gathering all news data...")
    train_news = read_news(path_to_train)
    test_news = read_news(path_to_test)

    print("Shape of training set:", train_news.shape)
    print("Shape of test set:", test_news.shape)
```

```
Gathering all news data...
Reading alt.atheism folder
Reading comp.graphics folder
Reading comp.os.ms-windows.misc folder
Reading comp.sys.ibm.pc.hardware folder
Reading comp.sys.mac.hardware folder
Reading comp.windows.x folder
Reading misc.forsale folder
Reading rec.autos folder
Reading rec.motorcycles folder
Reading rec.sport.baseball folder
Reading rec.sport.hockey folder
Reading sci.crypt folder
Reading sci.electronics folder
Reading sci.med folder
Reading sci.space folder
Reading soc.religion.christian folder
Reading talk.politics.guns folder
Reading talk.politics.mideast folder
Reading talk.politics.misc folder
Reading talk.religion.misc folder
Reading alt.atheism folder
Reading comp.graphics folder
```

```
Reading comp.os.ms-windows.misc folder
Reading comp.sys.ibm.pc.hardware folder
Reading comp.sys.mac.hardware folder
Reading comp.windows.x folder
Reading misc.forsale folder
Reading rec.autos folder
Reading rec.motorcycles folder
Reading rec.sport.baseball folder
Reading rec.sport.hockey folder
Reading sci.crypt folder
Reading sci.electronics folder
Reading sci.med folder
Reading sci.space folder
Reading soc.religion.christian folder
Reading talk.politics.guns folder
Reading talk.politics.mideast folder
Reading talk.politics.misc folder
Reading talk.religion.misc folder
Shape of training set: (11314, 2)
Shape of test set: (7532, 2)
```

Step 2: Preprocessing of text After reading the text, we process it using regular expression in oder to eliminate non-alpahnumeric characters and common stop words.

```
In [70]: from stop_words import  get_stop_words
         import re

         def preprocess_text (x, stop_words):

             '''This function preprocess a string, eliminateing sop words and
             non-alphanumeric characters.'''

             x = x.lower()
             x = re.sub(r'[^\w\s]','',x)
             x = re.sub(r'[0-9]','',x)
             x = re.sub(r'\n','',x)

             for stop_word in stop_words:
                 x = re.sub(r' '+stop_word+' ',' ', x)

             return x
```

```
In [72]: en_stop = get_stop_words('en')

         print("Preprocessing data... ")
         train_news.Text = train_news.Text.apply(lambda x: preprocess_text(x, en_stop))
```

```
        test_news.Text = test_news.Text.apply(lambda x: preprocess_text(x, en_stop))
        print("Preprocessing finished... ")
```

```
Preprocessing data...
Preprocessing finished...
```

We separate the design matrix (X) from the label vector (y) for training and test.

```
In [74]: #saving in libsvm format
         train_news.to_csv("train_news.csv", sep ="\t")
         test_news.to_csv("test_news.csv", sep="\t")

         #separating features and labels
         X_train = train_news.Text
         y_train = train_news.Label

         X_test = test_news.Text
         y_test = test_news.Label
```

Step 3: Transforming data We want now to convert the data to numeric format so that we can use it in a given model. We first tried count vectorizer, but we see that the number of dimensions turns out to be very high. So we use a Doc2Vec model, to embed the documents in fewer dimensions. We also standarize data.

```
In [75]: from sklearn.feature_extraction.text import CountVectorizer

         #getting the frequency of terms
         count_vect = CountVectorizer()
         X_train_counts = count_vect.fit_transform(X_train)
         print("Design matrix for training has following dimensions:", X_train_counts.shape)

         X_test_counts = count_vect.transform(X_test)
         print("Design matrix for training has following dimensions:", X_test_counts.shape)
```

```
Design matrix for training has following dimensions: (11314, 209498)
Design matrix for training has following dimensions: (7532, 209498)
```

```
In [76]: #importing Doc2Vec library
         from gensim.models.doc2vec import Doc2Vec, TaggedDocument

         d = 30 #dimensions to embeded

         #creating the list of words (one word for each sentence)
         lists_of_words = [x.split(" ") for x in X_train]

         #create documents to create embedding model
         documents = [TaggedDocument(doc, [i]) for i, doc in enumerate(lists_of_words)]
```

```
    model = Doc2Vec(documents, vector_size=d, window=2, min_count=1)

    #transforming the data
    embedding = np.zeros((len(lists_of_words),d))
    for i in range(embedding.shape[0]):
        embedding[i, ] =model.infer_vector(lists_of_words[i])
```

```
In [78]: #standarizing data
         from sklearn.preprocessing import StandardScaler

         X_transformed = embedding
         scaler = StandardScaler()
         X_tr2 = scaler.fit_transform(X_transformed)
```

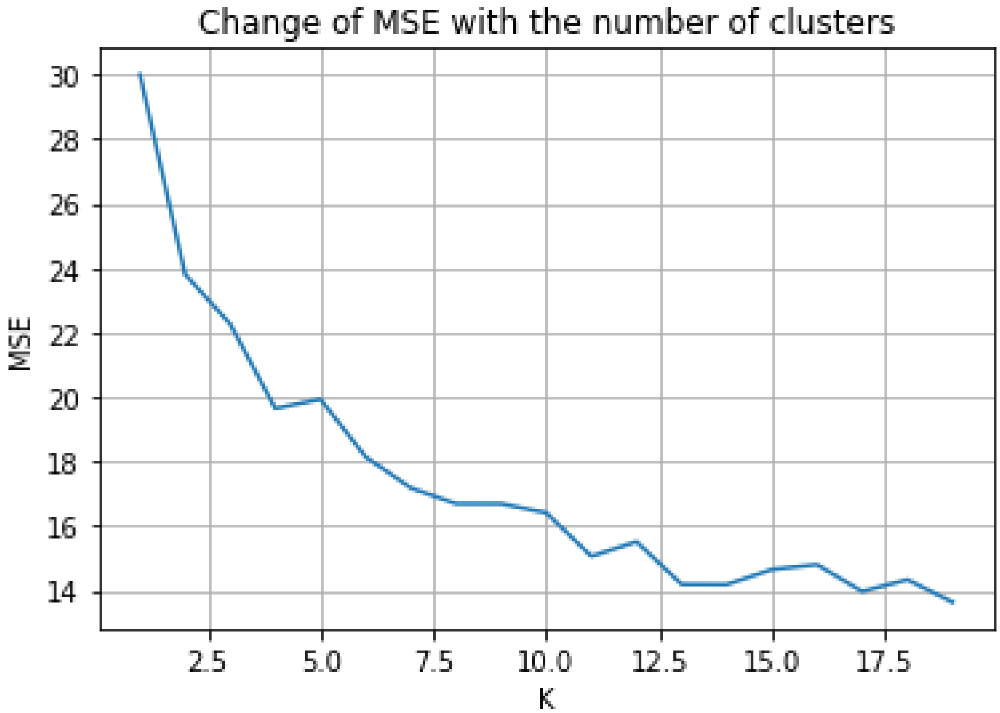
Step 4: Choosing the best k As before, using the K-Means for Iris dataset, we try different criteria to get the best K.

```
In [104]: max_k = 20
          sd, best_k, MSE_list = find_K_with_derivative(X_tr2, max_k)
          print("Best k according to derivatives:",best_k)
```

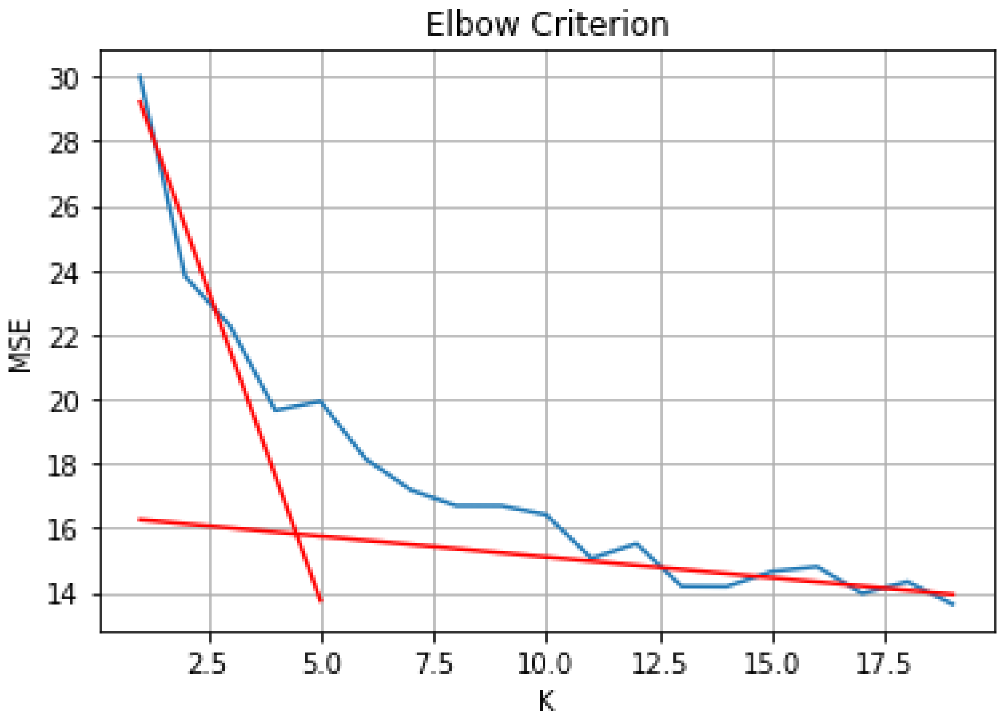
```
Trying with k= 1
Trying with k= 2
Trying with k= 3
Trying with k= 4
Trying with k= 5
Trying with k= 6
Trying with k= 7
Trying with k= 8
Trying with k= 9
Trying with k= 10
Trying with k= 11
Trying with k= 12
Trying with k= 13
Trying with k= 14
Trying with k= 15
Trying with k= 16
Trying with k= 17
Trying with k= 18
Trying with k= 19
Best k according to derivatives: 2
```

```
In [105]: plt.plot(range(1, max_k), MSE_list)
          plt.xlabel("K")
          plt.ylabel("MSE")
          plt.grid()
          plt.title("Change of MSE with the number of clusters")
```

Out[105]: Text(0.5,1,'Change of MSE with the number of clusters')

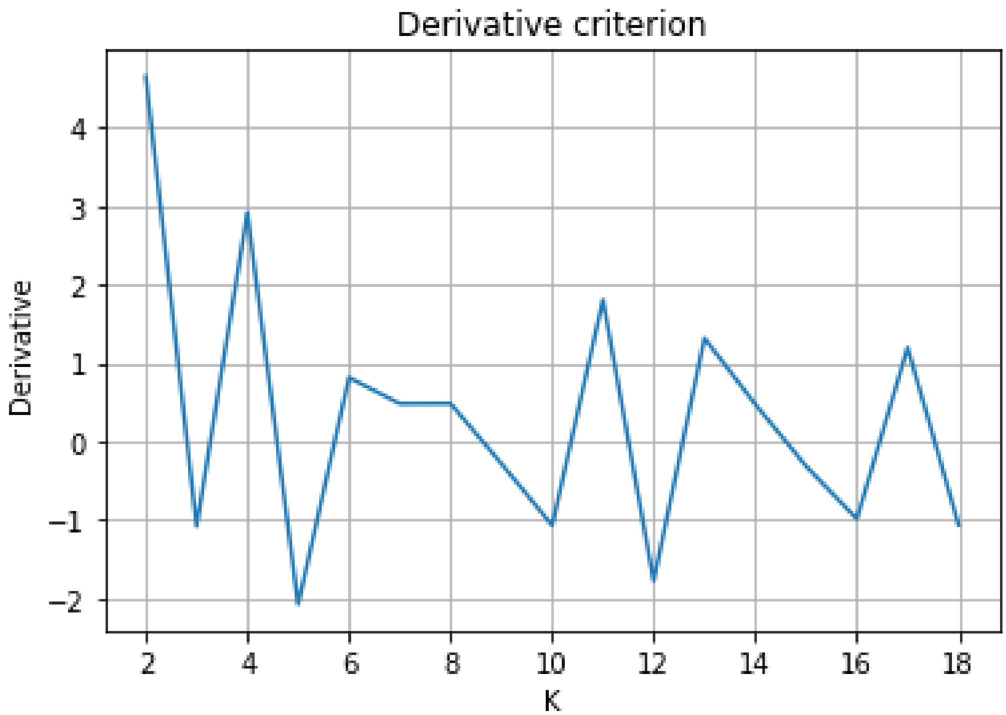


In [108]:
```
plt.plot(range(1, max_k), MSE_list)
plt.xlabel("K")
plt.ylabel("MSE")
plt.title("Elbow Criterion")

x1 = range(1,4)
y1 = MSE_list[:3]
m1,b1 = np.polyfit(x1, y1, 1)

x2 = range(max_k-6,max_k)
y2 = MSE_list[-6:]
m2,b2 = np.polyfit(x2, y2, 1)

x = range(1, max_k)
plt.plot(x, m2*x+b2, 'red')
plt.plot(x[:5], m1*x[:5]+b1, 'red')
plt.grid()
```



In [109]:
```
plt.plot(range(2,max_k-1), sd)
plt.grid()
plt.xlabel("K")
plt.ylabel("Derivative")
plt.title("Derivative criterion")
```

Out[109]:
```
Text(0.5,1,'Derivative criterion')
```



We also apply silhouette cristerion to get the best K. However, since Silhouette criterion is too complex to calculate, we use a subset of the data.

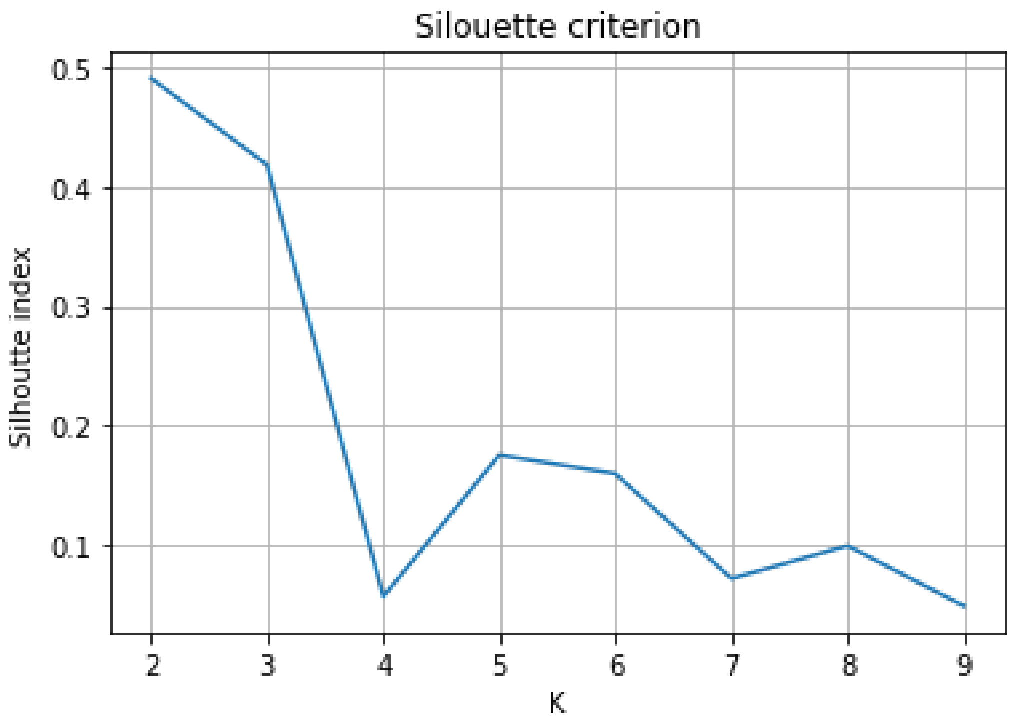
```
In [110]: X = X_tr2
          max_k=10

          sil_list = []

          for i in range(2,max_k):
              C, A, MSE_list = K_means(X,i, 100)
              idx = np.random.randint(0,X.shape[0],2000)
              sil = silhouette(X[idx,], A[idx,], i)
              sil_list.append(sil)
```

```
Trying k= 2
Trying k= 3
Trying k= 4
Trying k= 5
Trying k= 6
Trying k= 7
Trying k= 8
Trying k= 9
```

```
In [148]: plt.plot(range(2, max_k),sil_list)
          plt.grid()
```

```
plt.xlabel("K")
plt.ylabel("Silhoutte index")
plt.title("Silouette criterion")
```

Out[148]: Text(0.5,1,'Silouette criterion')



Step 5: Interpreting results According to the different plots (and the elbow criterion) the best k is between three and four. The silhouette index for k=2 and k=3 is high, whereas the derivative for k=2 and k = 4 is also high. The elbow criterion show that the "elbow" could approximately be find in 4.

We want now to see how many train samples of each new type fall into each cluster, so that we can interpretate the cluster as identifying a news class. After creating cross tabulations of the distribution of samples given a cluster and a type of new, we see that is somewhat difficult to differentiate clearly each cluster class. It means indeed, that the classes are not so easily separable with spherical clusters.

In [120]:
```
#interpreting clustering with 3 centers
C, A, MSE_list = K_means(X_tr2,3, 1000)

pd.crosstab(y_train, A)
```

Out[120]:

col_0	0	1	2
Label			
alt.atheism	3	374	103

comp.graphics	50	519	15
comp.os.ms-windows.misc	52	531	8
comp.sys.ibm.pc.hardware	37	550	3
comp.sys.mac.hardware	23	546	9
comp.windows.x	108	474	11
misc.forsale	43	519	23
rec.autos	5	517	72
rec.motorcycles	3	521	74
rec.sport.baseball	3	509	85
rec.sport.hockey	2	487	111
sci.crypt	106	424	65
sci.electronics	28	522	41
sci.med	12	442	140
sci.space	66	451	76
soc.religion.christian	1	395	203
talk.politics.guns	10	371	165
talk.politics.mideast	6	320	238
talk.politics.misc	17	310	138
talk.religion.misc	2	271	104

In [117]:
```
#interpreting clustering with 4 centers
C, A, MSE_list = K_means(X_tr2,4, 1000)

pd.crosstab(y_train, A)
```

Out[117]:

col_0	0	1	2	3
Label				
alt.atheism	137	93	245	5
comp.graphics	445	11	114	14
comp.os.ms-windows.misc	509	3	70	9
comp.sys.ibm.pc.hardware	510	3	72	5
comp.sys.mac.hardware	442	8	127	1
comp.windows.x	426	9	141	17
misc.forsale	442	17	119	7
rec.autos	237	56	298	3
rec.motorcycles	229	52	315	2
rec.sport.baseball	271	58	265	3
rec.sport.hockey	228	60	293	19
sci.crypt	260	70	229	36
sci.electronics	339	26	223	3
sci.med	164	105	310	15
sci.space	222	53	282	36
soc.religion.christian	156	183	256	4
talk.politics.guns	129	132	273	12
talk.politics.mideast	112	179	241	32
talk.politics.misc	115	112	222	16
talk.religion.misc	117	97	160	3

We also want to compare how it performs in test data.

```
In [121]: #transforming test data
          lists_of_words = [x.split(" ") for x in X_test]

          #embedding test data
          embedding = np.zeros((len(lists_of_words),d))
          for i in range(embedding.shape[0]):
              embedding[i, ] =model.infer_vector(lists_of_words[i])

          X_test_tr = embedding
          X_test_tr2 = scaler.fit_transform(X_test_tr)
```

```
In [137]: C, A, MSE_list = K_means(X_tr2,4, 1000)

          assignation = find_assignation(X_test_tr2, C)
          MSE_test = find_MSE(X_test_tr2, C, assignation)

          print("Train MSE:", MSE_list[-1])
          print("Test MSE:", MSE_test)
```

```
Train MSE: 18.7925189411
Test MSE: 19.9126719911
```

We can see that, in fact, the MSE for test is very close to the MSE of train. It is reasonable, since both data come from the same distribution, therefore the clustering of a train set should be valid for new data sampled from the same distribution. However, this result also shows that we didn't overfit the data. As K increase, the clustering model gets more complex and more prone to overfit.

Step 6: Comparison with Scikit-learn K-Means We wnat to compare MSE and speed of our implementation with the one of Scikit learn. To make it comparable, we must note that Scikit-learn outputs the inertia, which is the sum of the square distance of samples to the cluster centers.

```
In [145]: from sklearn.cluster import KMeans
          import numpy as np

          n_samples = X_tr2.shape[0]

          kmeans = KMeans(n_clusters=4, random_state=0, n_init=1).fit(X_tr2)

          print("MSE Scikit-learn:", kmeans.inertia_/n_samples)
          print("MSE self implementation:" , MSE_list[-1])
```

```
MSE Scikit-learn: 18.5196837336
MSE self implementation: 18.7925189411
```

We see that both results are very close, what shows that both implementations are funcional comparable. But, what happen with the execution speed? We want to measure it now.

```
In [147]: import time

          start_sk = time.time()
          kmeans = KMeans(n_clusters=20, random_state=2, n_init=1).fit(X_tr2)
          end_sk = time.time()

          print("Time Elapsed with Scikit-Learn:", end_sk-start_sk)

          start_m = time.time()
          C, A, MSE_list = K_means(X_tr2, 20, 100)
          end_m = time.time()

          print("Time Elapsed with self implementation:",end_m - start_m)
```

```
Time Elapsed with Scikit-Learn: 0.40576720237731934
Time Elapsed with self implementation: 1.5191280841827393
```

For scikit-learn, we execute with the parameter n_init=1, since the function runs K-Mean several times to get the lower MSE (to avoid possible local minima). This, therefore, affect computation time. The times are scale comparable, however, the scikit learn implementation is three times faster than our implementations. This is due to the possible optimizations that they do computing the centers or assignations, which we did not approach here.

1.1 References

[1] Elbow criterion: https://en.wikipedia.org/wiki/Elbow_method_(clustering)
[2] Silhouette index paper: https://pdfs.semanticscholar.org/f168/41e022038e94a59f7e0a82002102b78d79a4.p