K MEANS CLUSTERING

The data set contains 4 columns with the following information:

ID: A unique identifier for the observation x: Attribute corresponding to an x coordinate y: Attribute corresponding to a y coordinate Cluster: An identifier for the cluster the observation belongs to

We will discard column 4 for our analysis, but it may be useful to check the results of the application of -means. We will do this in our second example later on. Let us start by reading the dataset:

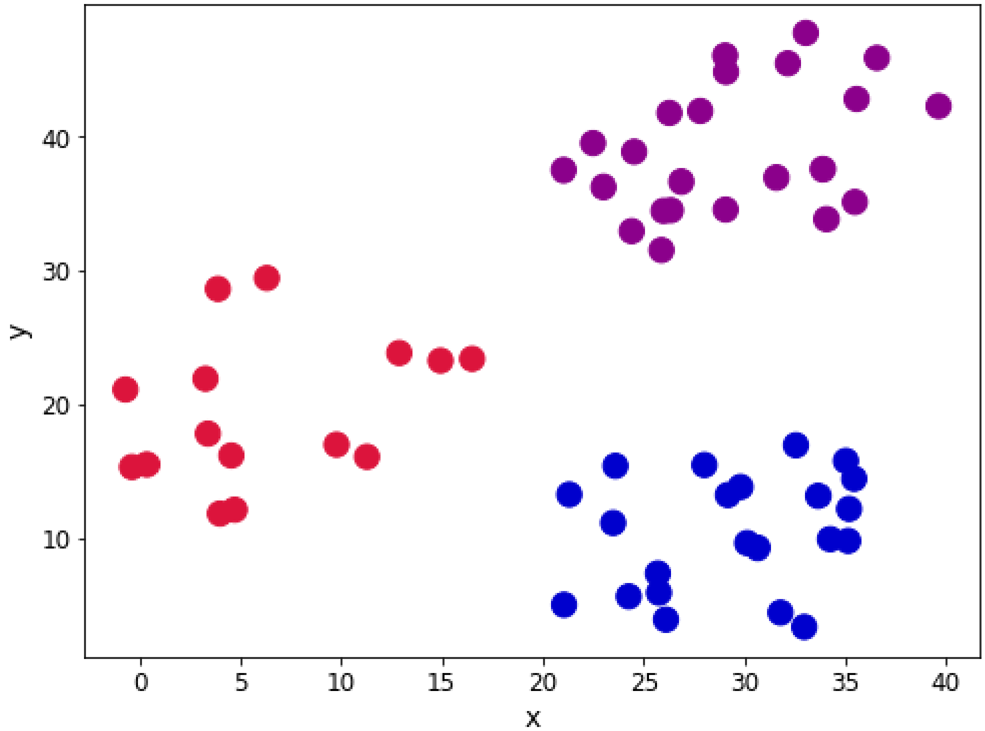
In [20]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from matplotlib.colors import ListedColormap
%matplotlib inline

blobs = pd.read_csv('kmeans_blobs.csv')
colnames = list(blobs.columns[1:-1])
blobs.head()
```

Out[20]:

	ID	x	y	cluster
0	0	24.412	32.932	2
1	1	35.190	12.189	1
2	2	26.288	41.718	2
3	3	0.376	15.506	0
4	4	26.116	3.963	1

Let us look at the observations in the dataset. We will use the Cluster column to show the different groups that are present in the dataset. Our aim will be to see if the application of the algorithm reproduces closely the groupings.

In [21]:
```
customcmap = ListedColormap(["crimson", "mediumblue", "darkmagenta"])

fig, ax = plt.subplots(figsize=(8, 6))
plt.scatter(x=blobs['x'], y=blobs['y'], s=150,
            c=blobs['cluster'].astype('category'),
            cmap = customcmap)
ax.set_xlabel(r'x', fontsize=14)
ax.set_ylabel(r'y', fontsize=14)
plt.xticks(fontsize=12)
plt.yticks(fontsize=12)
plt.show()
```



Steps 1 and 2 - Define and initiate the centroids

First we need

1) to decide how many groups we have and

2) assign the initial centroids randomly. In this case let us consider k=3, and as for the centroids, well, they have to be in the same range as the dataset itself. So one option is to randomly pick k observations and use their coordinates to initialise the centroids:

In [22]:
```
def initiate_centroids(k, dset):
    '''
    Select k data points as centroids
    k: number of centroids
    dset: pandas dataframe
    '''
    centroids = dset.sample(k)
    return centroids

np.random.seed(42)
k=3
df = blobs[['x','y']]
centroids = initiate_centroids(k, df)
centroids
```

Out[22]:

	x	y
0	24.412	32.932
5	25.893	31.515
36	26.878	36.609

Step 3 - Calculate distance

We now need to calculate the distance between each of the centroids and the data points. We will assign the data point to the centroid that gives us the minimum error. Let us create a function to calculate the root of square errors:

In [23]:
```
def rsserr(a,b):
    '''
    Calculate the root of sum of squared errors.
    a and b are numpy arrays
    '''
    return np.square(np.sum((a-b)**2))
```

Let us pick a data point and calculate the error so we can see how this works in practice. We will use point , which is in fact one of the centroids we picked above. As such, we expect that the error for that point and the third centroid is zero. We therefore would assign that data point to the second centroid. Let’s take a look:

In [24]:
```
for i, centroid in enumerate(range(centroids.shape[0])):
    err = rsserr(centroids.iloc[centroid,:], df.iloc[36,:])
    print('Error for centroid {0}: {1:.2f}'.format(i, err))
```

```
Error for centroid 0: 384.22
Error for centroid 1: 724.64
Error for centroid 2: 0.00
```

Step 4 - Assign centroids

We can use the idea from Step 3 to create a function that helps us assign the data points to corresponding centroids. We will calculate all the errors associated to each centroid, and then pick the one with the lowest value for assignation:

In [25]:
```
def centroid_assignation(dset, centroids):
    '''
    Given a dataframe `dset` and a set of `centroids`, we assign each
    data point in `dset` to a centroid.
    - dset - pandas dataframe with observations
    - centroids - pa das dataframe with centroids
    '''
    k = centroids.shape[0]
    n = dset.shape[0]
    assignation = []
    assign_errors = []

    for obs in range(n):
        # Estimate error
        all_errors = np.array([])
        for centroid in range(k):
            err = rsserr(centroids.iloc[centroid, :], dset.iloc[obs,:])
            all_errors = np.append(all_errors, err)

        # Get the nearest centroid and the error
```

```
        nearest_centroid =  np.where(all_errors==np.amin(all_errors))[0].tolist
        nearest_centroid_error = np.amin(all_errors)

        # Add values to corresponding lists
        assignation.append(nearest_centroid)
        assign_errors.append(nearest_centroid_error)

    return assignation, assign_errors
```

Let us add some columns to our data containing the centroid assignations and the error incurred. Furthermore, we can use this to update our scatter plot showing the centroids (denoted with squares) and we colour the observations according to the centroid they have been assigned to:

In [26]:

```
df['centroid'], df['error'] = centroid_assignation(df, centroids)
df.head()
```

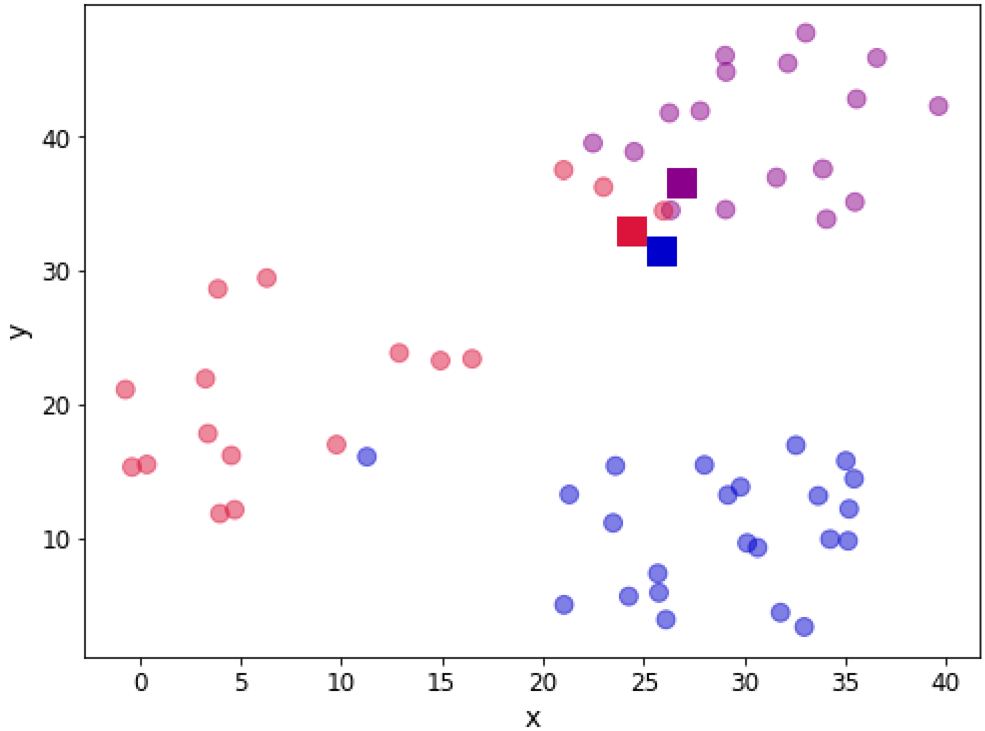
```
/var/folders/vr/1lbk5z1x3vldjtvbj2kx_8p80000gn/T/ipykernel_53577/3199595029.p
y:1: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/st
able/user_guide/indexing.html#returning-a-view-versus-a-copy
  df['centroid'], df['error'] = centroid_assignation(df, centroids)
```

Out[26]:

	x	y	centroid	error
0	24.412	32.932	0	0.000000
1	35.190	12.189	1	211534.211314
2	26.288	41.718	2	699.601495
3	0.376	15.506	0	776856.744109
4	26.116	3.963	1	576327.599678

In [27]:

```
fig, ax = plt.subplots(figsize=(8, 6))
plt.scatter(df.iloc[:,0], df.iloc[:,1],  marker = 'o',
            c=df['centroid'].astype('category'),
            cmap = customcmap, s=80, alpha=0.5)
plt.scatter(centroids.iloc[:,0], centroids.iloc[:,1],
            marker = 's', s=200, c=[0, 1, 2],
            cmap = customcmap)
ax.set_xlabel(r'x', fontsize=14)
ax.set_ylabel(r'y', fontsize=14)
plt.xticks(fontsize=12)
plt.yticks(fontsize=12)
plt.show()
```



Let us see the total error by adding all the contributions. We will take a look at this error as a measure of convergence. In other words, if the error does not change, we can assume that the centroids have stabilised their location and we can terminate our iterations. In practice, we need to be mindful of having found a local minimum

In [28]:
```
print("The total error is {0:.2f}".format(df['error'].sum()))
```

```
The total error is 11927659.01
```

Step 5 - Update centroid location

Now that we have a first attempt at defining our clusters, we need to update the position of the k centroids. We do this by calculating the mean of the position of the observations assigned to each centroid. Let take a look:

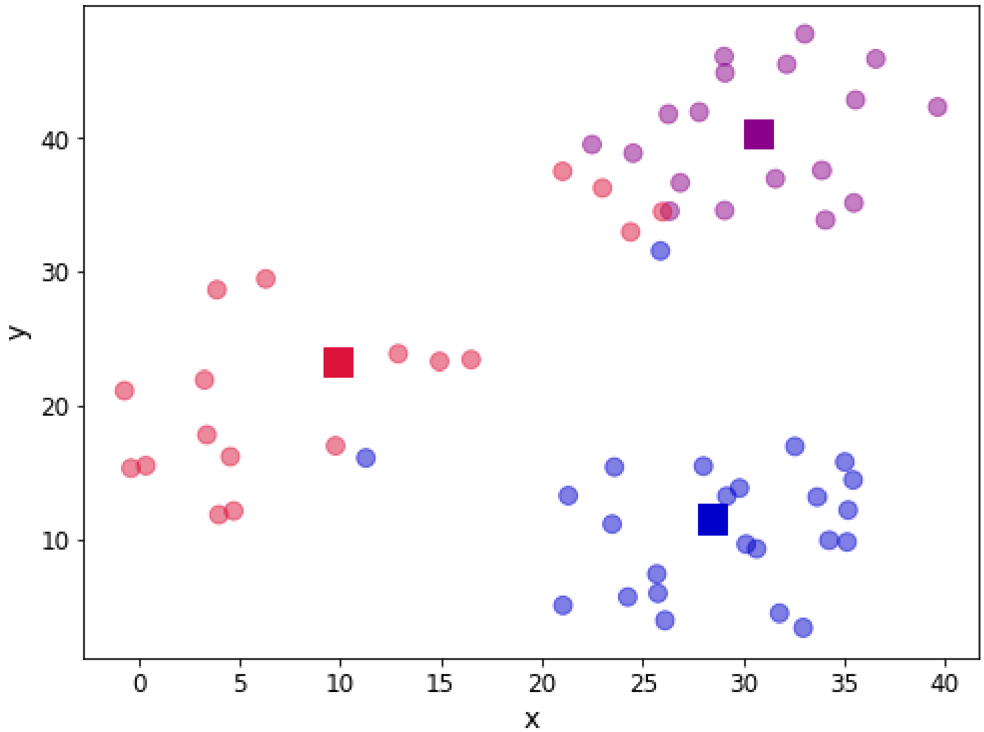
In [29]:
```
centroids = df.groupby('centroid').agg('mean').loc[:, colnames].reset_index(drc
centroids
```

Out[29]:

	x	y
0	9.889444	23.242611
1	28.435750	11.546250
2	30.759333	40.311167

In [30]:
```
fig, ax = plt.subplots(figsize=(8, 6))
plt.scatter(df.iloc[:,0], df.iloc[:,1],  marker = 'o',
            c=df['centroid'].astype('category'),
            cmap = customcmap, s=80, alpha=0.5)
plt.scatter(centroids.iloc[:,0], centroids.iloc[:,1],
```

```
             marker = 's', s=200,
             c=[0, 1, 2], cmap = customcmap)
ax.set_xlabel(r'x', fontsize=14)
ax.set_ylabel(r'y', fontsize=14)
plt.xticks(fontsize=12)
plt.yticks(fontsize=12)
plt.show()
```



Step 6 - Repeat steps 3-5

Now we go back to calculate the distance to each centroid, assign observations and update the centroid location. This calls for a function to encapsulate the loop:

In [31]:
```
def kmeans(dset, k=2, tol=1e-4):
    '''
    K-means implementationd for a
    `dset`:  DataFrame with observations
    `k`: number of clusters, default k=2
    `tol`: tolerance=1E-4
    '''
    # Let us work in a copy, so we don't mess the orginal
    working_dset = dset.copy()
    # We define some variables to hold the error, the
    # stopping signal and a counter for the iterations
    err = []
    goahead = True
    j = 0

    # Step 2: Initiate clusters by defining centroids
    centroids = initiate_centroids(k, dset)

    while(goahead):
        # Step 3 and 4 - Assign centroids and calculate error
```

```
        working_dset['centroid'], j_err = centroid_assignation(working_dset, ce
        err.append(sum(j_err))

        # Step 5 - Update centroid position
        centroids = working_dset.groupby('centroid').agg('mean').reset_index(dr

        # Step 6 - Restart the iteration
        if j>0:
            # Is the error less than a tolerance (1E-4)
            if err[j-1]-err[j]<=tol:
                goahead = False
        j+=1

    working_dset['centroid'], j_err = centroid_assignation(working_dset, centro
    centroids = working_dset.groupby('centroid').agg('mean').reset_index(drop =
    return working_dset['centroid'], j_err, centroids
```

OK, we are now ready to apply our function. We will clean our dataset first and let the algorithm run:

In [32]:
```
np.random.seed(42)
df['centroid'], df['error'], centroids =  kmeans(df[['x','y']], 3)
df.head()
```

Out[32]:

	x	y	centroid	error
0	24.412	32.932	2	3767.568743
1	35.190	12.189	1	1399.889001
2	26.288	41.718	2	262.961097
3	0.376	15.506	0	2683.086425
4	26.116	3.963	1	2723.650198

Let us see the location of the final centroids:

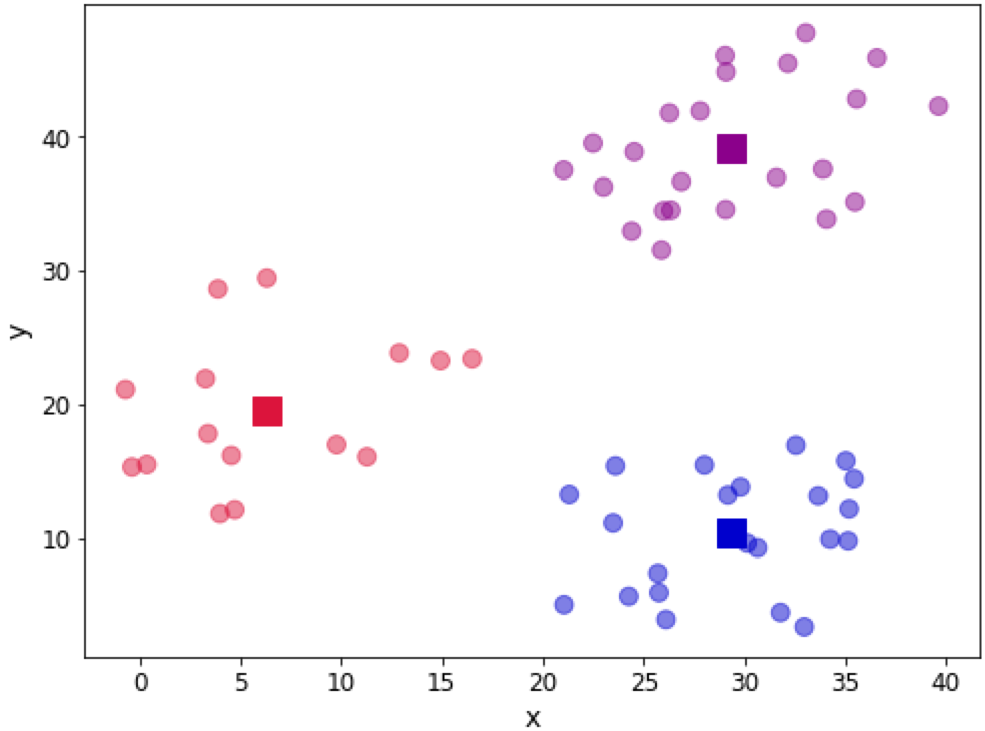
In [35]:
```
centroids = df.groupby('centroid').agg('mean').loc[:, colnames].reset_index(drc
centroids
```

Out[35]:

	x	y
0	6.322867	19.559800
1	29.330864	10.432409
2	29.304957	39.050783

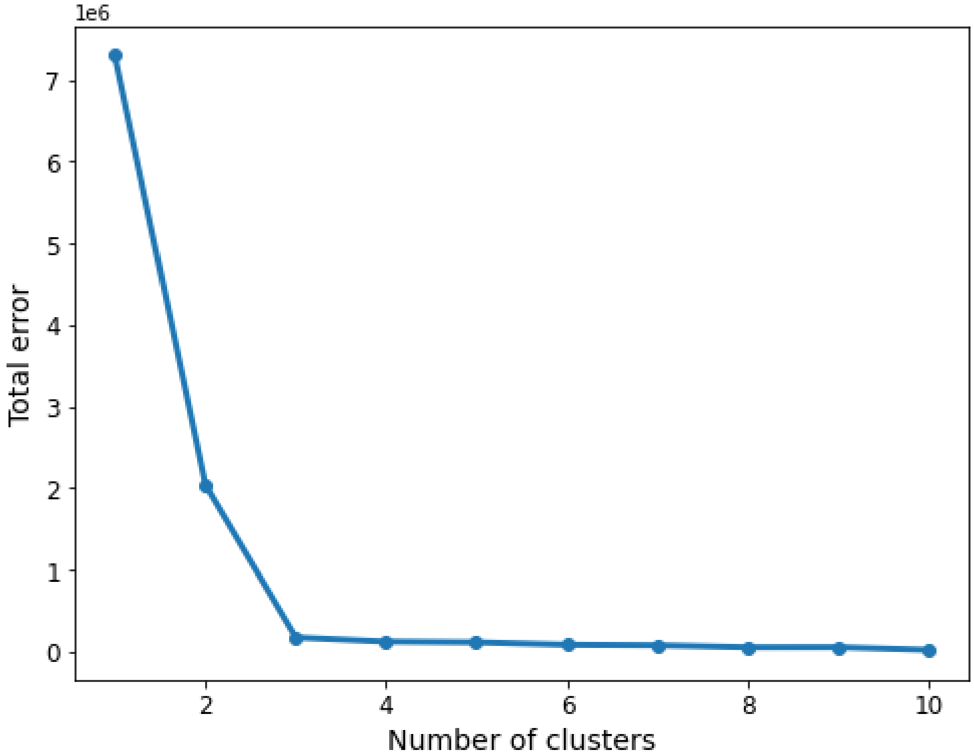
In [36]:
```
fig, ax = plt.subplots(figsize=(8, 6))
plt.scatter(df.iloc[:,0], df.iloc[:,1],  marker = 'o',
            c=df['centroid'].astype('category'),
            cmap = customcmap, s=80, alpha=0.5)
plt.scatter(centroids.iloc[:,0], centroids.iloc[:,1],
            marker = 's', s=200, c=[0, 1, 2],
            cmap = customcmap)
ax.set_xlabel(r'x', fontsize=14)
ax.set_ylabel(r'y', fontsize=14)
plt.xticks(fontsize=12)
```

```
plt.yticks(fontsize=12)
plt.show()
```



As we can see the three groups have been obtained. In this particular example the data is such that the distinction between the groups is clear. However, we may not be as lucky in every case. So the question about how many groups there are still remains. We can use a screen plot to help us with the error minimisation by looking at running the algorithm with a sequence k = 1,2,3,... and look for the “elbow” in the plot indicating a good number of clusters to use:

In [37]:
```
err_total = []
n = 10

df_elbow = blobs[['x','y']]

for i in range(n):
    _, my_errs, _ = kmeans(df_elbow, i+1)
    err_total.append(sum(my_errs))
fig, ax = plt.subplots(figsize=(8, 6))
plt.plot(range(1,n+1), err_total, linewidth=3, marker='o')
ax.set_xlabel(r'Number of clusters', fontsize=14)
ax.set_ylabel(r'Total error', fontsize=14)
plt.xticks(fontsize=12)
plt.yticks(fontsize=12)
plt.show()
```



In [ ]: