K-means clustering: intuitive explanation

The notebook provides an intuitive description and explanation of the k-means clustering technique. A synthetic dataset will be used to identify clusters manually.

Acknowledgments

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Importing libraries

```
# Import the packages that we will be using
import numpy as np                  # For arrays, matrices, and functions to operate on the
import pandas as pd                 # For data handling
import seaborn as sns               # For advanced plotting
import matplotlib.pyplot as plt     # For showing plots
```

Importing data

```
# Create synthetic data that consists of 5 points and 2 variables
d = {'x1': [2, 4, 2, 6, 6],
     'x2': [2, 3, 4, 6, 5]}

# Construct the dataframe
df = pd.DataFrame(data=d)
```

Undertanding and preprocessing the data

1. Get a general 'feel' of the data

```
# Print the dataset
df
```

	x1	x2
0	2	2

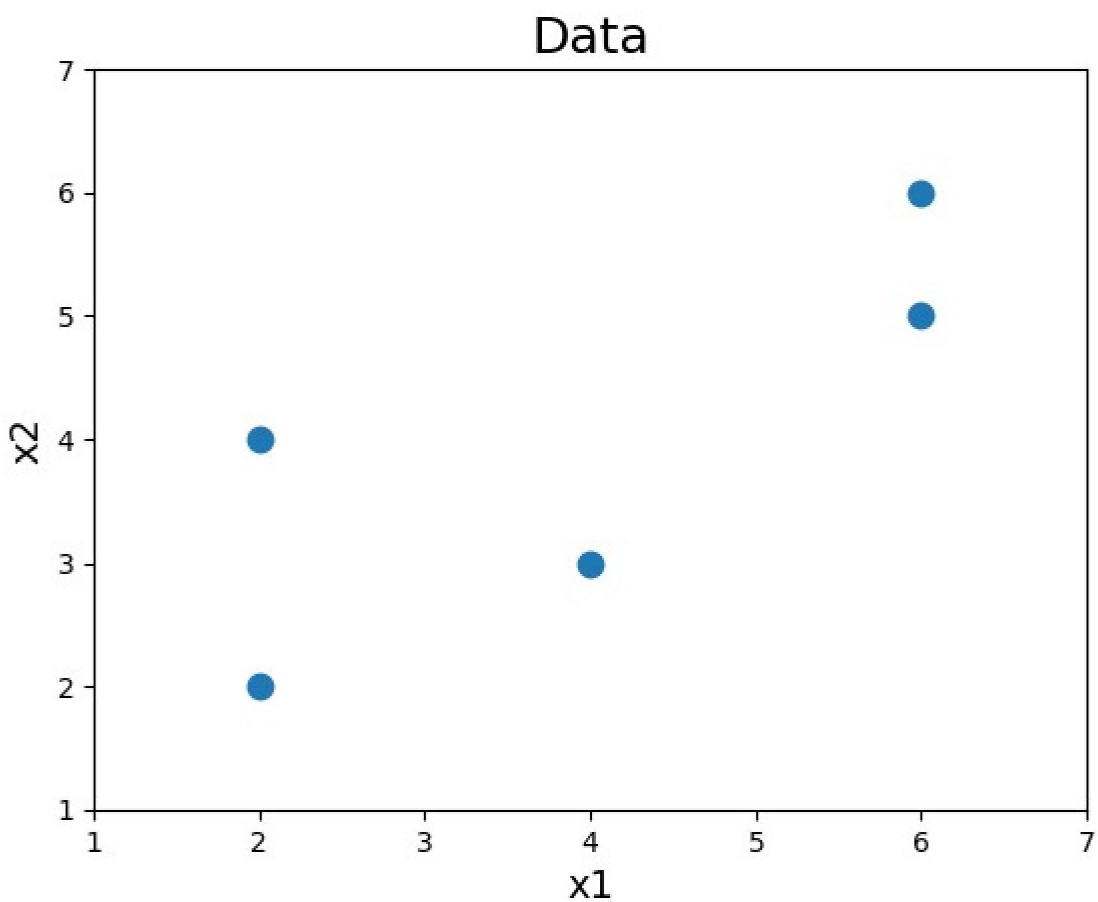
1	4	3
2	2	4
3	6	6
4	6	5

2. Scatter plot of the data

```
# Plot scatter plot
plt.scatter(df.x1,df.x2, s=80)
plt.title("Data", fontsize=18)
plt.xlabel("x1", fontsize=14)
plt.ylabel("x2", fontsize=14)

plt.xlim(1,7)
plt.ylim(1,7)

plt.show()
```



Note that for this dataset we do not know in advance the cluster/group/class to which each point belongs to, and that is what we want to do: to identify the existing cluster/group/class, i.e., to assing each point to a cluster/group/class

3. Preprocessing the data

No preprocessing is required

Kmeans clustering

Intuitive explanation

Initialize/Preliminaries

```
# Compute the number of points in the dataset
index=df.index
Npoints=len(index)

print("The number of points is: ", Npoints)
```

```
The number of points is:  5
```

1: Specify the number of clusters

Define the number K of clusters

```
# Let's assume our data has two clusters (note that the rest of the code is for K=2)
K  = 2
```

2: Initialize the centroids of the clusters

Randomly initialize the centroids of the clusters $C_1, C_2, \cdots, C_K$

```
# Let's initialize the centroids for the K=2 clusters (this has to be done randomly)

# Let's do it manually
C1new =  np.array([1.5, 3.0])
C2new =  np.array([3.0, 3.0])

# Print centroids
print("Centroide 1: ", C1new)
```

```
print("Centroide 2: ", C2new)
```

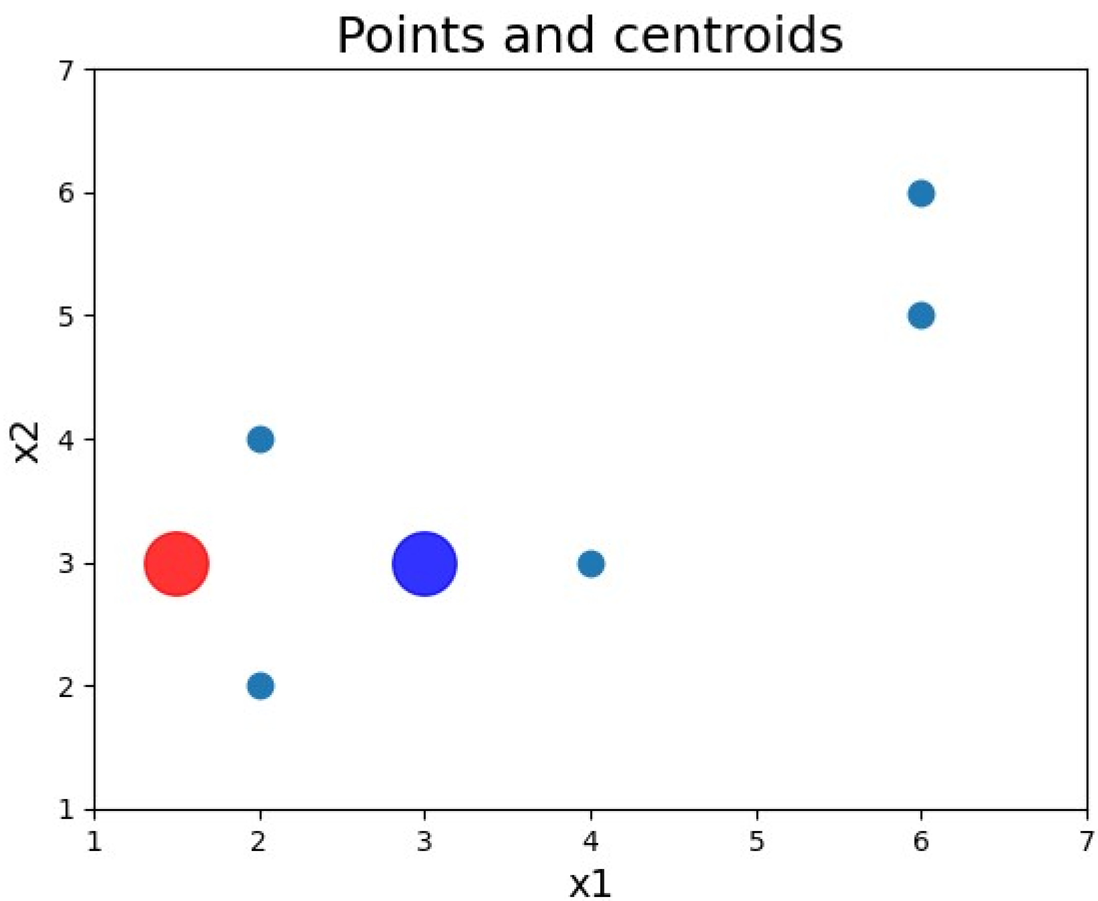
```
Centroide 1:  [1.5 3. ]
Centroide 2:  [3. 3.]
```

```
# Plot the points and the centroids
plt.scatter(df.x1,df.x2, s=80)
plt.scatter(C1new[0], C1new[1], color='r', marker='o', label='Centroide 1', s=512, alpha=
plt.scatter(C2new[0], C2new[1], color='b', marker='o', label='Centroide 2', s=512, alpha=

plt.title("Points and centroids", fontsize=18)
plt.xlabel("x1", fontsize=14)
plt.ylabel("x2", fontsize=14)

plt.xlim(1,7)
plt.ylim(1,7)

plt.show()
```



3: Repeat the following

Define the current centroids

```
# Define centrode 1
C1 = C1new.copy()
C1
```

```
array([2.66666667, 3.        ])
```

```
# Define centrode 2
C2 = C2new.copy()
C2
```

```
array([6. , 5.5])
```

4: Assign each point to its closest centroid

Compute the distance of each data point to each centroid

Assign each point to the centroid with the minimum Euclidean distance

Euclidean distance:

- Consider two points $x = (x_1, x_2)$ and $y = (y_1, y_2)$.
- The Euclidean distance between these two points is $d = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$

```
# Compute the distance of each data point to each centroid

# Variable to save the distance of each point ot each centroid
Dis2Centroids = np.zeros((Npoints,K))

# Let's compute the distances manually
ipoint, x1, x2 = 0, 2, 2
Dis2Centroids[ipoint,0]=np.sqrt((x1-C1[0])**2+(x2-C1[1])**2)
Dis2Centroids[ipoint,1]=np.sqrt((x1-C2[0])**2+(x2-C2[1])**2)

ipoint, x1, x2 = 1, 4, 3
Dis2Centroids[ipoint,0]=np.sqrt((x1-C1[0])**2+(x2-C1[1])**2)
Dis2Centroids[ipoint,1]=np.sqrt((x1-C2[0])**2+(x2-C2[1])**2)

ipoint, x1, x2 = 2, 2, 4
Dis2Centroids[ipoint,0]=np.sqrt((x1-C1[0])**2+(x2-C1[1])**2)
Dis2Centroids[ipoint,1]=np.sqrt((x1-C2[0])**2+(x2-C2[1])**2)

ipoint, x1, x2 = 3, 6, 6
Dis2Centroids[ipoint,0]=np.sqrt((x1-C1[0])**2+(x2-C1[1])**2)
Dis2Centroids[ipoint,1]=np.sqrt((x1-C2[0])**2+(x2-C2[1])**2)

ipoint, x1, x2 = 4, 6, 5
```

```
    Dis2Centroids[ipoint,0]=np.sqrt((x1-C1[0])**2+(x2-C1[1])**2)
    Dis2Centroids[ipoint,1]=np.sqrt((x1-C2[0])**2+(x2-C2[1])**2)

# Print result 0s
print(Dis2Centroids)
```

```
[[1.20185043 5.31507291]
 [1.33333333 3.20156212]
 [1.20185043 4.27200187]
 [4.48454135 0.5       ]
 [3.88730126 0.5       ]]
```

```
# Assign each point to the centroid with the minimum Euclidean distance

# Let's do this manually
#cluster=np.array([1,2,1,2,2])
#cluster=np.array([1,1,1,2,2])
cluster=np.array([1,1,1,2,2])
#cluster =
#cluster =
#cluster =


# Print results
print(cluster)
```

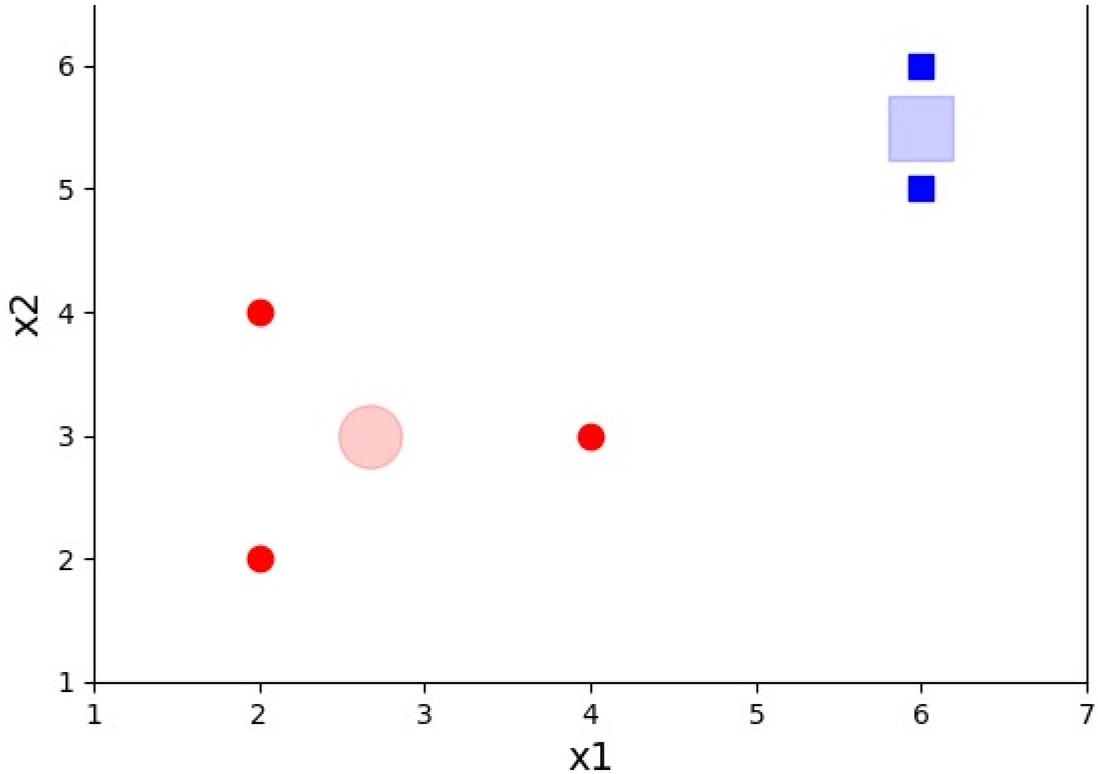
```
[1 1 1 2 2]
```

```
# Scatter plot of the data asigning each point to the cluster it belongs to ¡¡
#plt.scatter(df.x1,df.x2, s=80, c=cluster)
df1=df[cluster==1]
df2=df[cluster==2]
plt.scatter(df1.x1,df1.x2, s=80, color='r', marker='o', label='Cluster 1')
plt.scatter(df2.x1,df2.x2, s=80, color='b', marker='s', label='Cluster 2')
plt.scatter(C1[0], C1[1], color='r', marker='o', label='Centroide 1', s=512, alpha=0.2)
plt.scatter(C2[0], C2[1], color='b', marker='s', label='Centroide 2', s=512, alpha=0.2)

plt.title("Points and centroids", fontsize=18)
plt.xlabel("x1", fontsize=14)
plt.ylabel("x2", fontsize=14)

plt.xlim(1,7)
plt.ylim(1,7)

plt.show()
```



5: Compute the new centroid (mean) of each cluster

Compute the new centroid of each cluster

```
# Let's compute the 1st Centroid
print(df1)
C1new[0]=df1.x1.mean()
C1new[1]=df1.x2.mean()

print(C1new)
```

```
   x1  x2
0   2   2
1   4   3
2   2   4
[2.66666667 3.        ]
```

```
# Let's compute the 2nd Centroid
print(df2)
C2new[0]=df2.x1.mean()
C2new[1]=df2.x2.mean()


print(C2new)
```

```
   x1  x2
3   6   6
```

```
4   6   5
[6.  5.5]
```

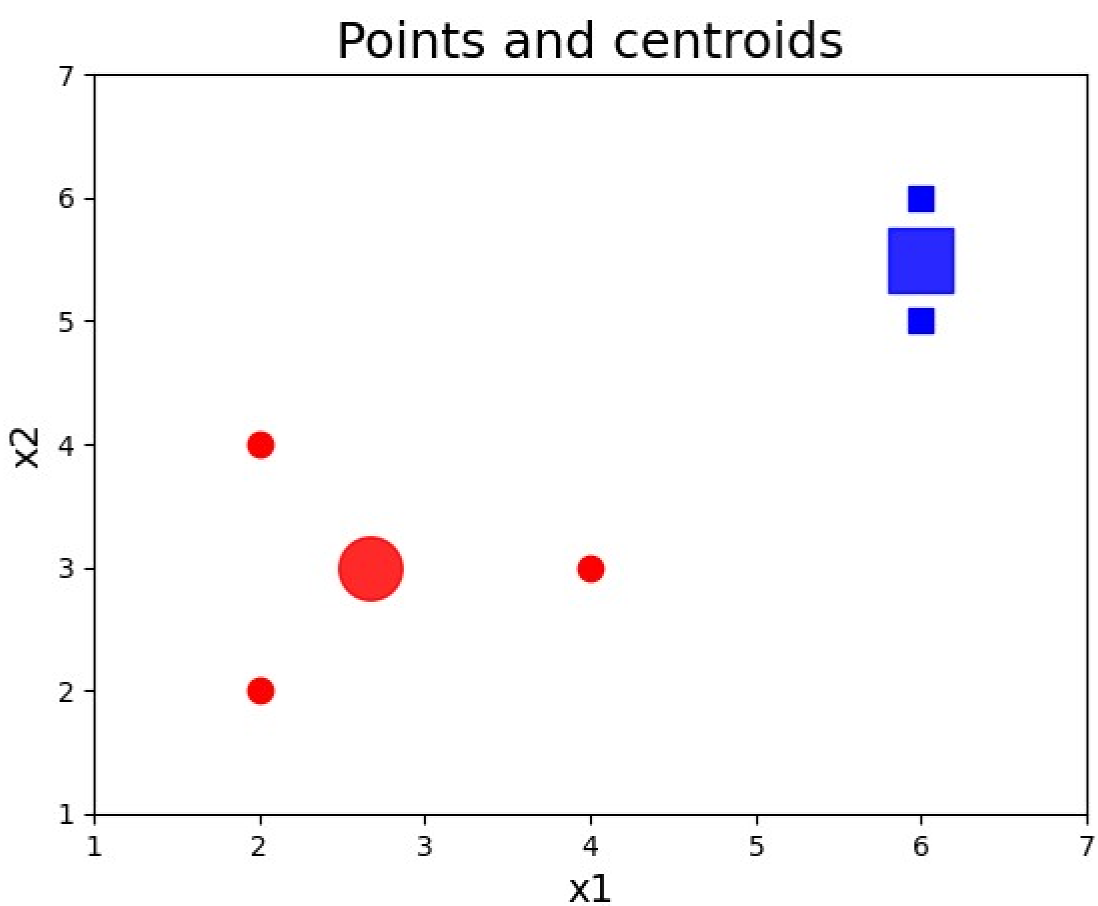
```
# Scatter plot of the data asigning each point to the cluster it belongs to ¡¡
df1=df[cluster==1]
df2=df[cluster==2]
plt.scatter(df1.x1,df1.x2, s=80, color='r', marker='o', label='Cluster 1')
plt.scatter(df2.x1,df2.x2, s=80, color='b', marker='s', label='Cluster 2')
plt.scatter(C1[0], C1[1], color='r', marker='o', label='Centroide 1', s=512, alpha=0.2)
plt.scatter(C2[0], C2[1], color='b', marker='s', label='Centroide 2', s=512, alpha=0.2)

plt.scatter(C1new[0], C1new[1], color='r', marker='o', label='Centroide 1', s=512, alpha=
plt.scatter(C2new[0], C2new[1], color='b', marker='s', label='Centroide 2', s=512, alpha=

plt.title("Points and centroids", fontsize=18)
plt.xlabel("x1", fontsize=14)
plt.ylabel("x2", fontsize=14)

plt.xlim(1,7)
plt.ylim(1,7)

plt.show()
```



6: Until the centroids do not change

If the centroids do not change, then, none of the data points change of the assigned cluster

```
print(C1)
print(C1new)
```

```
[2.66666667 3.        ]
[2.66666667 3.        ]
```

```
print(C2)
print(C2new)
```

```
[6.  5.5]
[6.  5.5]
```

If the centroids do change... go to 3 (recall to use the new centroids)

If the centroids do not change... done ¡¡