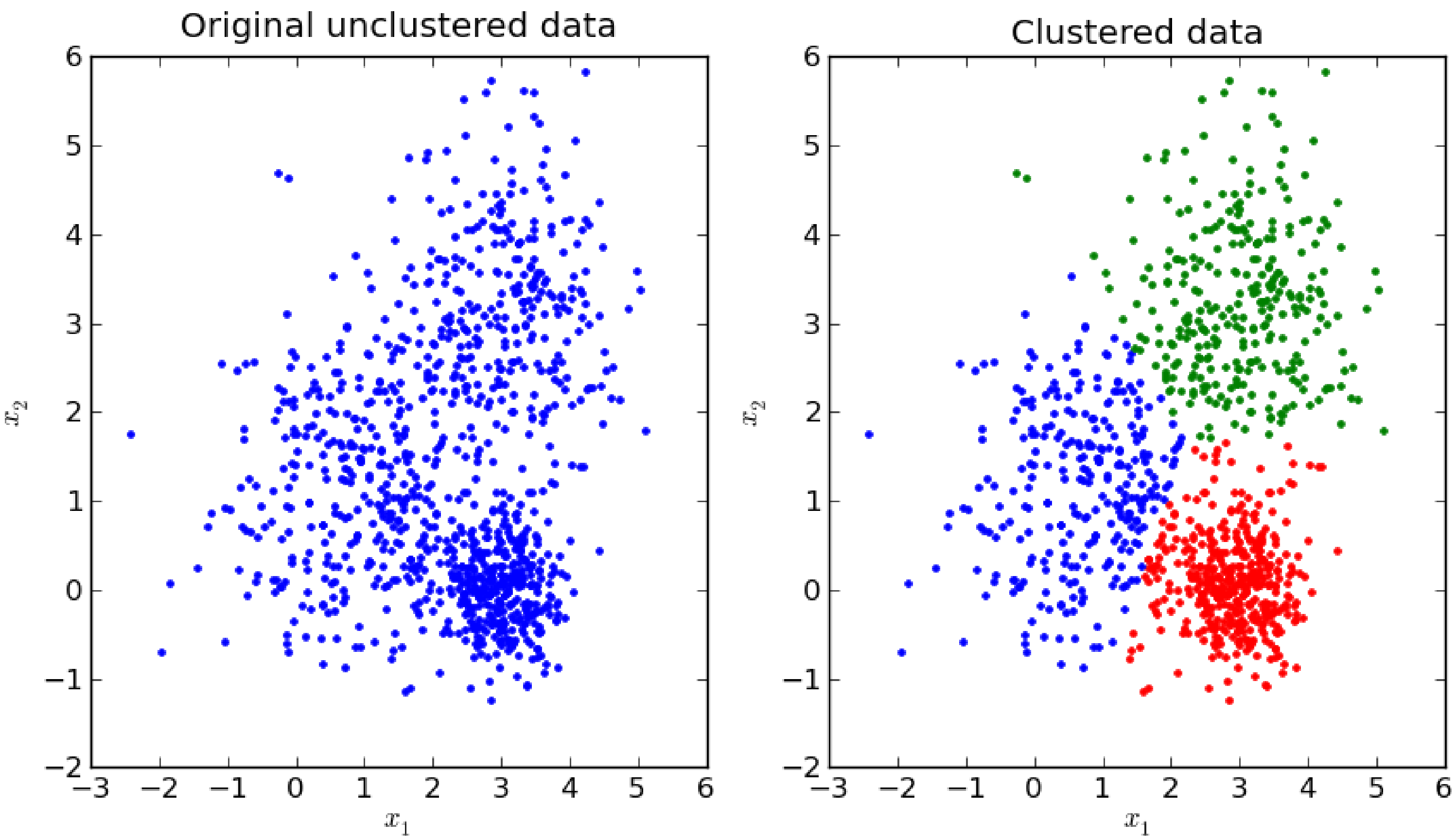
K-Means Clustering in Python

Clustering is a type of Unsupervised learning. This is very often used when you don't have labeled data. K-Means Clustering is one of the popular clustering algorithm. The goal of this algorithm is to find groups(clusters) in the given data. In this post we will implement K-Means algorithm using Python from scratch.

K-Means Clustering

K-Means is a very simple algorithm which clusters the data into *K* number of clusters. The following image from PyPR is an example of K-Means Clustering.



Use Cases

applications.

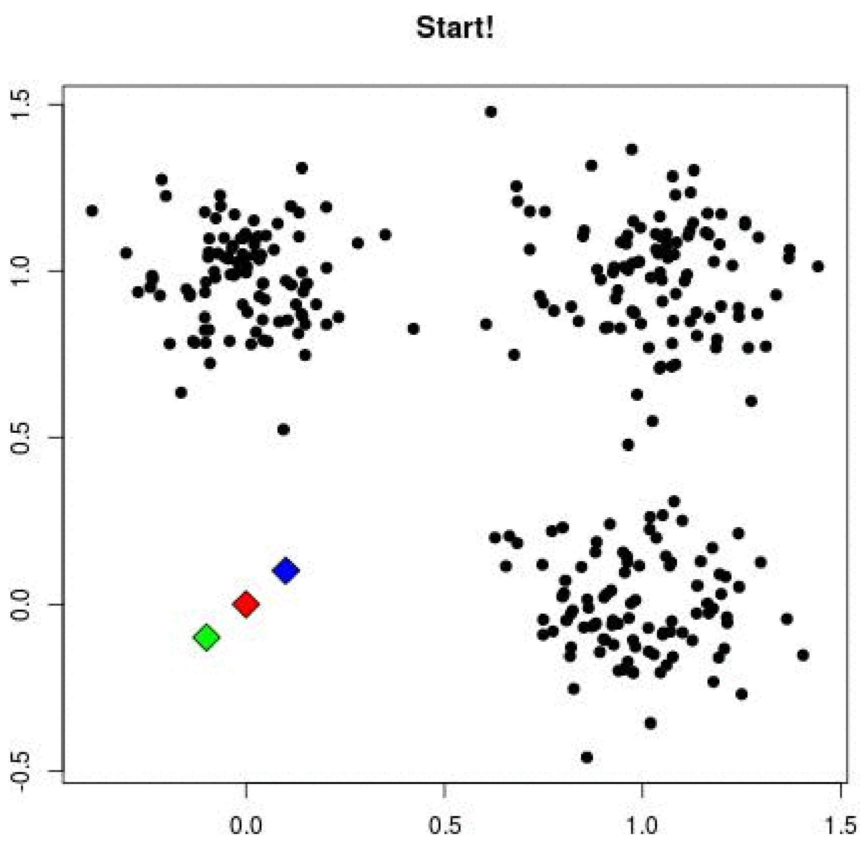
on Data

- News Article Clustering
- Clustering Languages
- Species Clustering
- Anomaly Detection

Algorithm

Our algorithm works as follows, assuming we have inputs $x_1, x_2, x_3, \ldots, x_n$ and value of K

- Step 1 - Pick K random points as cluster centers called centroids.
- Step 2 - Assign each x_i to nearest cluster by calculating its distance to each centroid.
- Step 3 - Find new cluster center by taking the average of the assigned points.
- Step 4 - Repeat Step 2 and 3 until none of the cluster assignments change.



The above animation is an example of running K-Means Clustering on a two dimensional data.

rs(centroids). Let's assume these are $c_1, c_2, \ldots, c_k$, and we can say that;

$$C = c_1, c_2, \ldots, c_k$$

C is the set of all centroids.

Step 2

In this step we assign each input value to closest center. This is done by calculating Euclidean(L2) distance between the point and the each centroid.

$$\arg\min_{c_i \in C} dist(c_i, x)^2$$

Where $dist(.)$ is the Euclidean distance.

Step 3

In this step, we find the new centroid by taking the average of all the points assigned to that cluster.

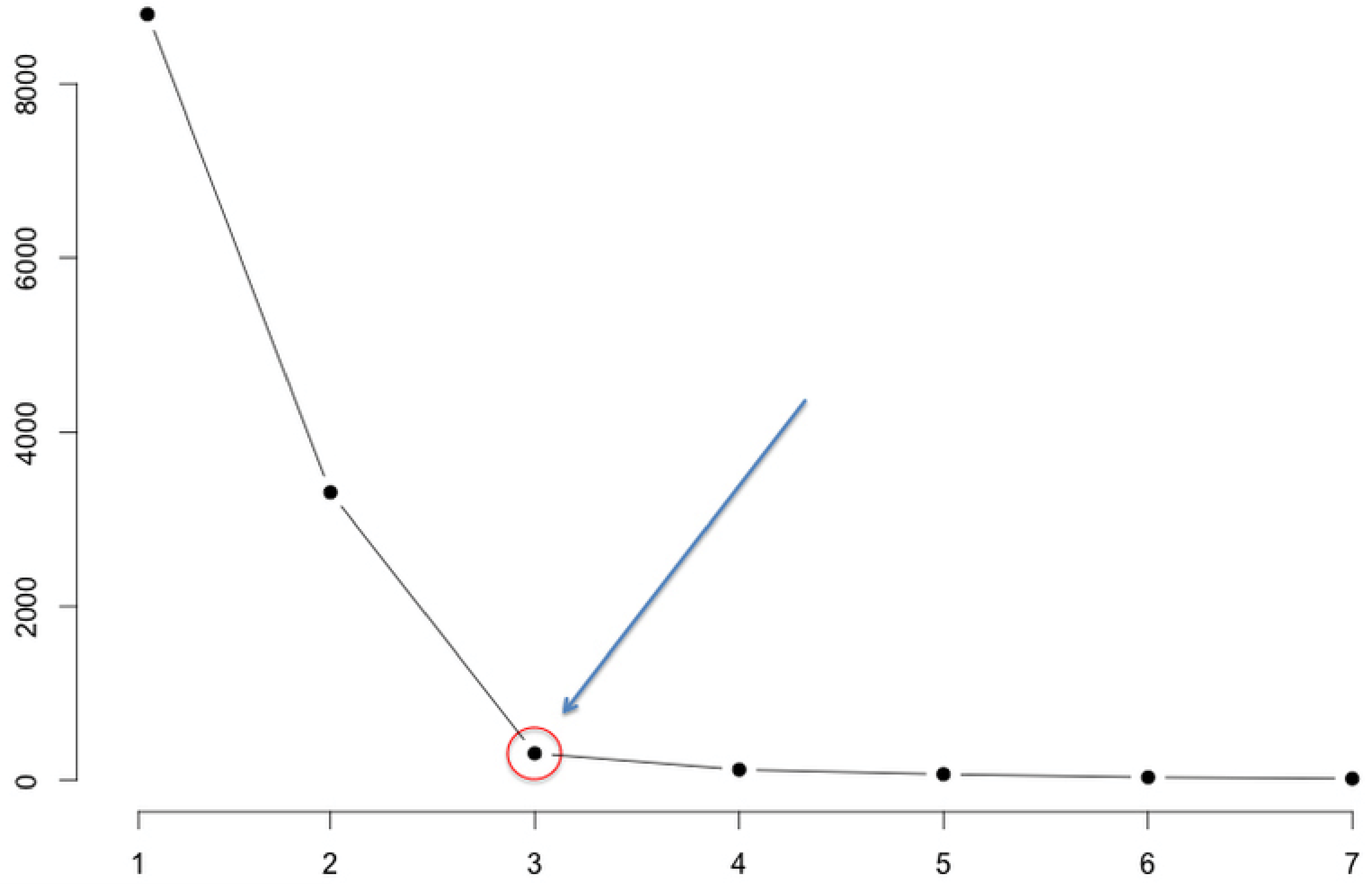
$$c_i = \frac{1}{|S_i|} \sum_{x_i \in S_i} x_i$$

S_i is the set of all points assigned to the i^{th} cluster.

3 until none of the cluster assignments change. That means until our clusters remain stable, we repeat the algorithm.

Choosing the Value of K

We often know the value of K. In that case we use the value of K. Else we use the Elbow Method.



…t values of K(say K = 10 to 1) and plot the K values against SSE(Sum of Squared Errors).
…lbow point as shown in the figure.

Implementation using Python

The dataset we are gonna use has 3000 entries with 3 clusters. So we already know the value of K.

Checkout this [Github Repo](#) for full code and dataset.

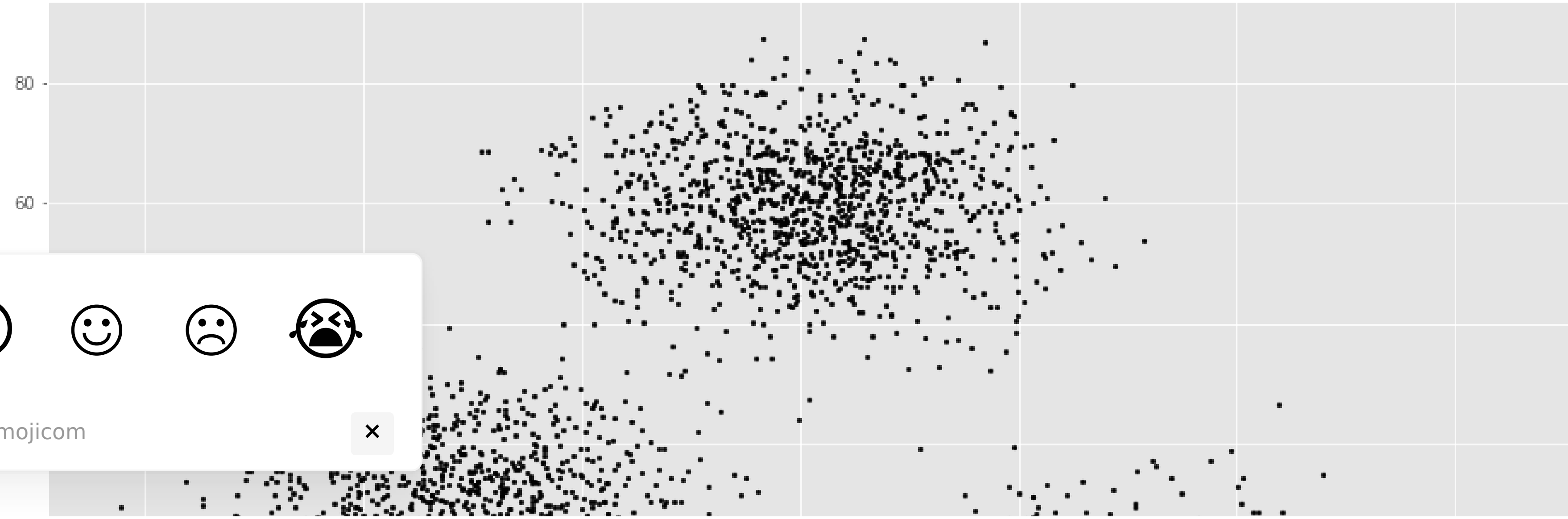
We will start by importing the dataset.

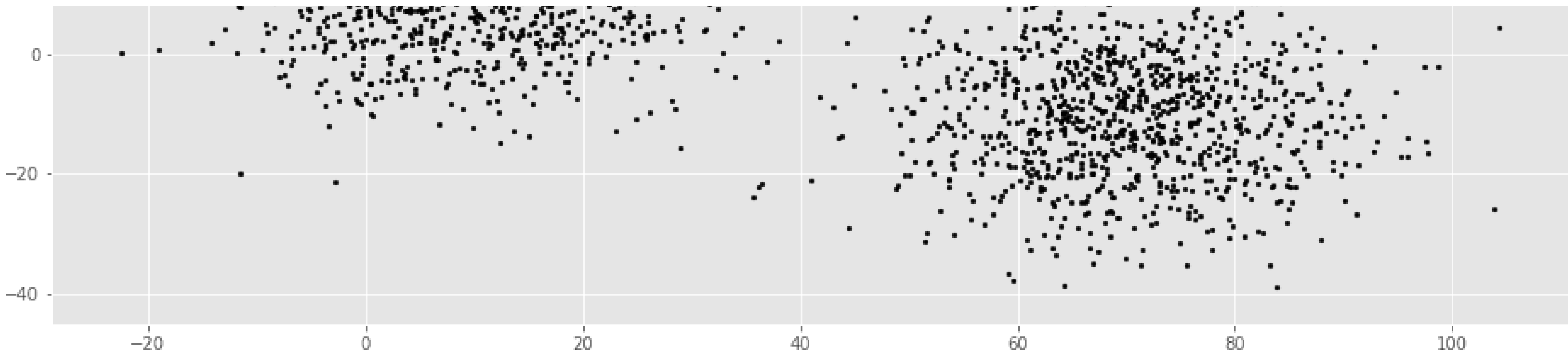
```
%matplotlib inline
from copy import deepcopy
import numpy as np
import pandas as pd
from matplotlib import pyplot as plt
plt.rcParams['figure.figsize'] = (16, 9)
plt.style.use('ggplot')
```

```
# Importing the dataset
data = pd.read_csv('xclara.csv')
print(data.shape)
data.head()
```

	V1	V2
0	2.072345	-3.241693
1	17.936710	15.784810
2	1.083576	7.319176
3	11.120670	14.406780
4	23.711550	2.557729

```
# Getting the values and plotting it
f1 = data['V1'].values
f2 = data['V2'].values
X = np.array(list(zip(f1, f2)))
plt.scatter(f1, f2, c='black', s=7)
```






```python
# Euclidean Distance Caculator
def dist(a, b, ax=1):
    return np.linalg.norm(a - b, axis=ax)
```

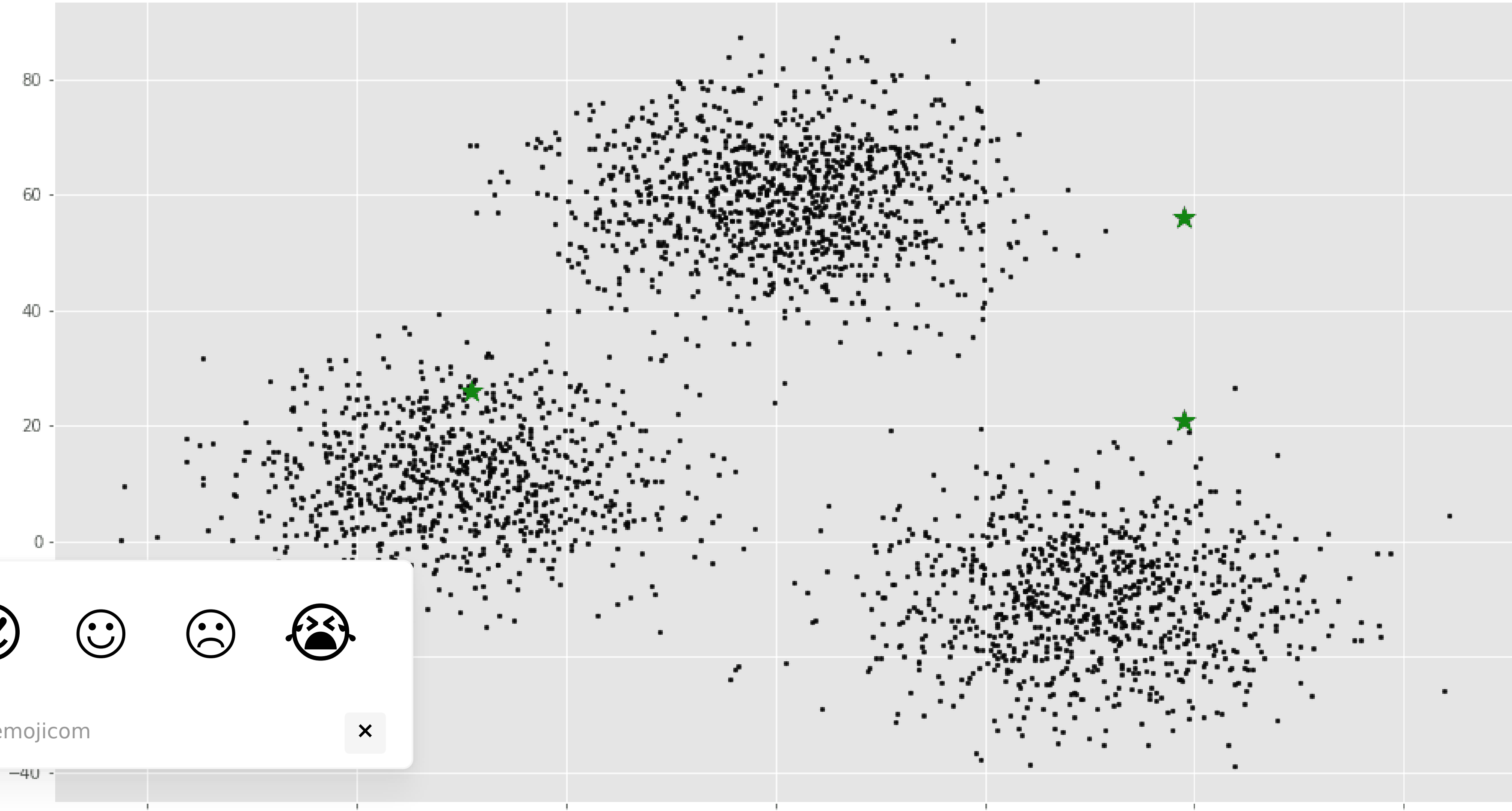
```python
# Number of clusters
k = 3
# X coordinates of random centroids
C_x = np.random.randint(0, np.max(X)-20, size=k)
# Y coordinates of random centroids
C_y = np.random.randint(0, np.max(X)-20, size=k)
C = np.array(list(zip(C_x, C_y)), dtype=np.float32)
```



```
 [ 79.   56.]
```

```
 [ 79.   21.]]
```

```
# Plotting along with the Centroids
plt.scatter(f1, f2, c='#050505', s=7)
plt.scatter(C_x, C_y, marker='*', s=200, c='g')
```



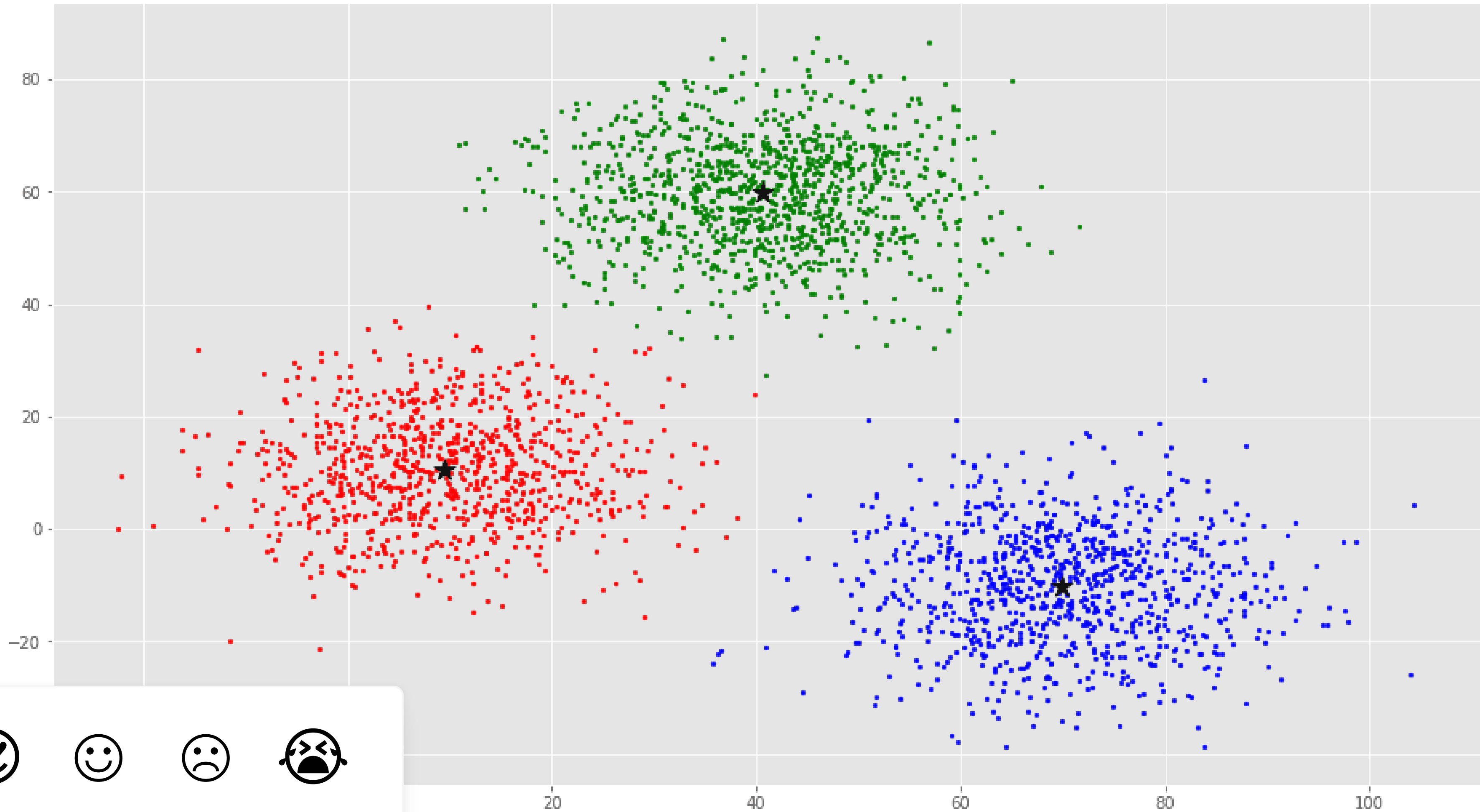
−20 0 20 40 60 80 100

```python
# To store the value of centroids when it updates
C_old = np.zeros(C.shape)
# Cluster Lables(0, 1, 2)
clusters = np.zeros(len(X))
# Error func. - Distance between new centroids and old centroids
error = dist(C, C_old, None)
# Loop will run till the error becomes zero
while error != 0:
    # Assigning each value to its closest cluster
    for i in range(len(X)):
        distances = dist(X[i], C)
        cluster = np.argmin(distances)
        clusters[i] = cluster
    # Storing the old centroid values
    C_old = deepcopy(C)
    # Finding the new centroids by taking the average value
    for i in range(k):
        points = [X[j] for j in range(len(X)) if clusters[j] == i]
        C[i] = np.mean(points, axis=0)
    error = dist(C, C_old, None)
```



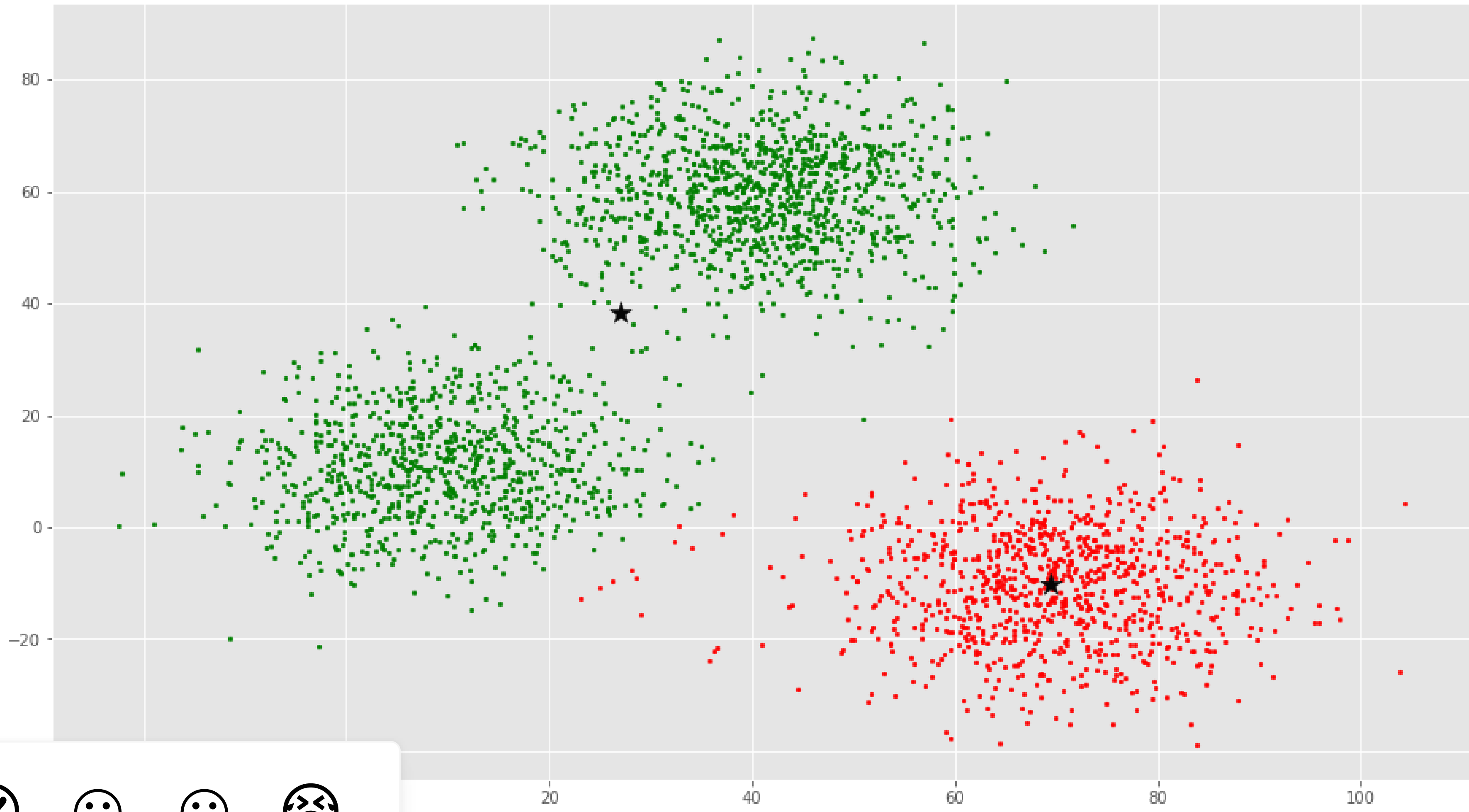
```python
'y', 'c', 'm']

for i in range(k):
```

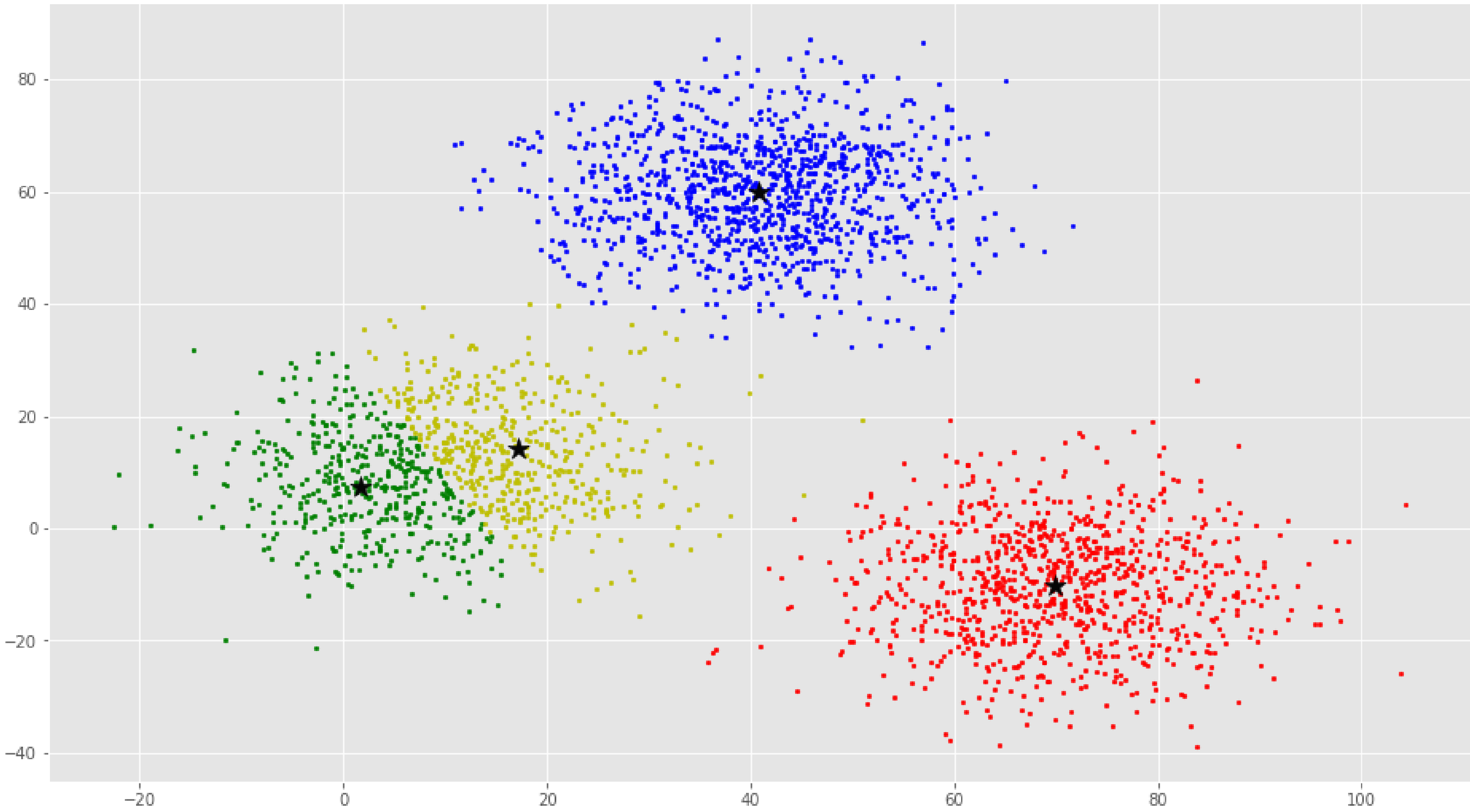
```
        points = np.array([X[j] for j in range(len(X)) if clusters[j] == i])
        ax.scatter(points[:, 0], points[:, 1], s=7, c=colors[i])
ax.scatter(C[:, 0], C[:, 1], marker='*', s=200, c='#050505')
```



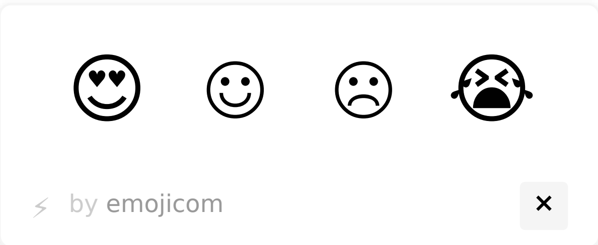
From this visualization it is clear that there are 3 clusters with black stars as their centroid.

If you run K-Means with wrong values of K, you will get completely misleading clusters. For example, if you run K-Means on this with values 2, 4, 5 and 6, you will get the following clusters.

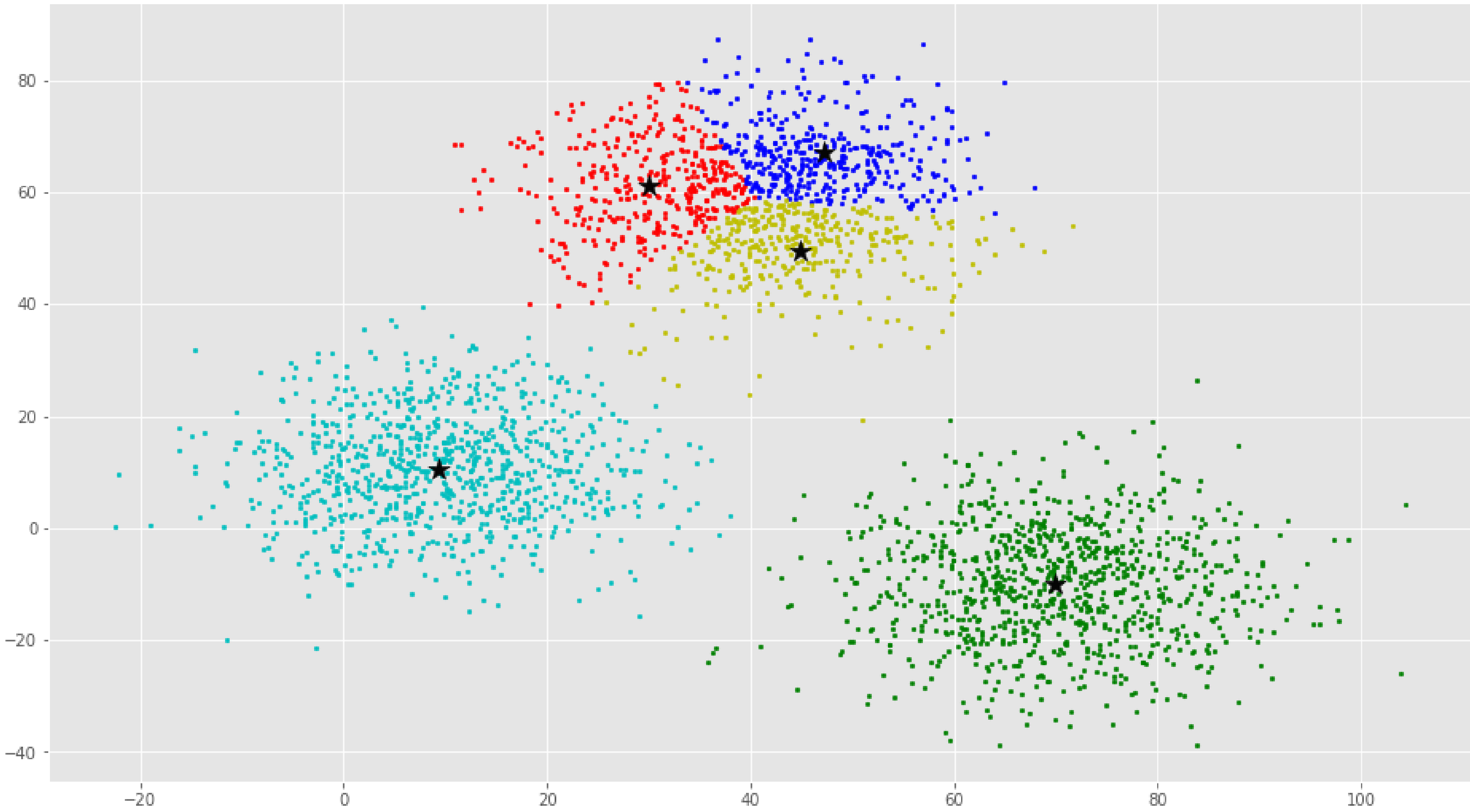


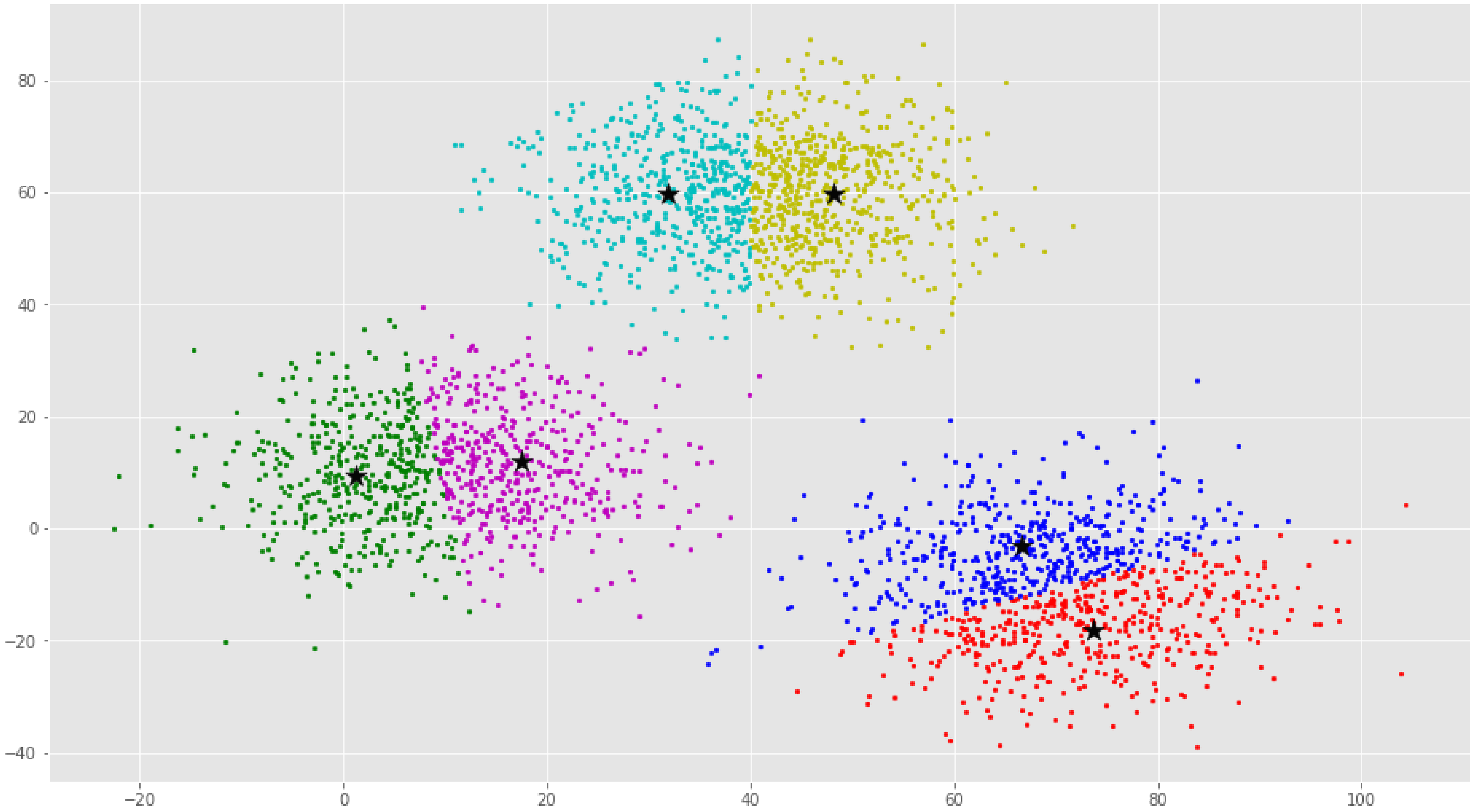


80
60
40
20
0
−20
−40
−20
0
20
40
60
80
100



by emojicom


80
60
40
20
0
−20
−40
−20
0
20
40
60
80
100



😍 ☺ ☹ 😫

by emojicom

×

t K-Means Clustering using scikit-learn

h

Example 1

We will use the same dataset in this example.

```
from sklearn.cluster import KMeans

# Number of clusters
kmeans = KMeans(n_clusters=3)
# Fitting the input data
kmeans = kmeans.fit(X)
# Getting the cluster labels
labels = kmeans.predict(X)
# Centroid values
centroids = kmeans.cluster_centers_
```

```
# Comparing with scikit-learn centroids
print(C) # From Scratch
print(centroids) # From sci-kit learn
```

```
5232]
9279]
413 ]]
52  ]
```

```
 [ 69.92418447 -10.11964119]
 [ 40.68362784  59.71589274]]
```

You can see that the centroid values are equal, but in different order.

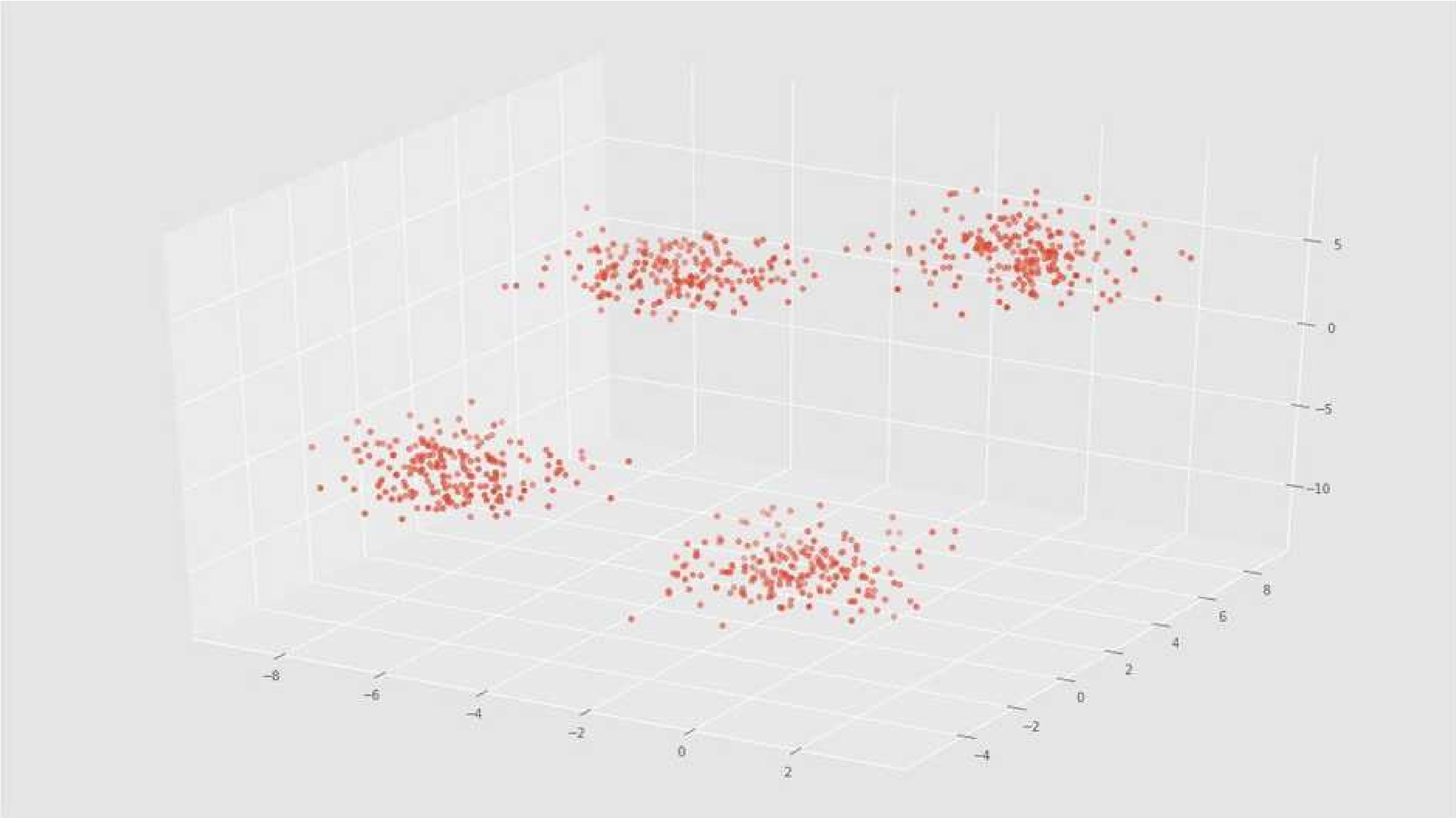
Example 2

We will generate a new dataset using `make_blobs` function.

```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.cluster import KMeans
from sklearn.datasets import make_blobs

plt.rcParams['figure.figsize'] = (16, 9)

# Creating a sample dataset with 4 clusters
X, y = make_blobs(n_samples=800, n_features=3, centers=4)
```



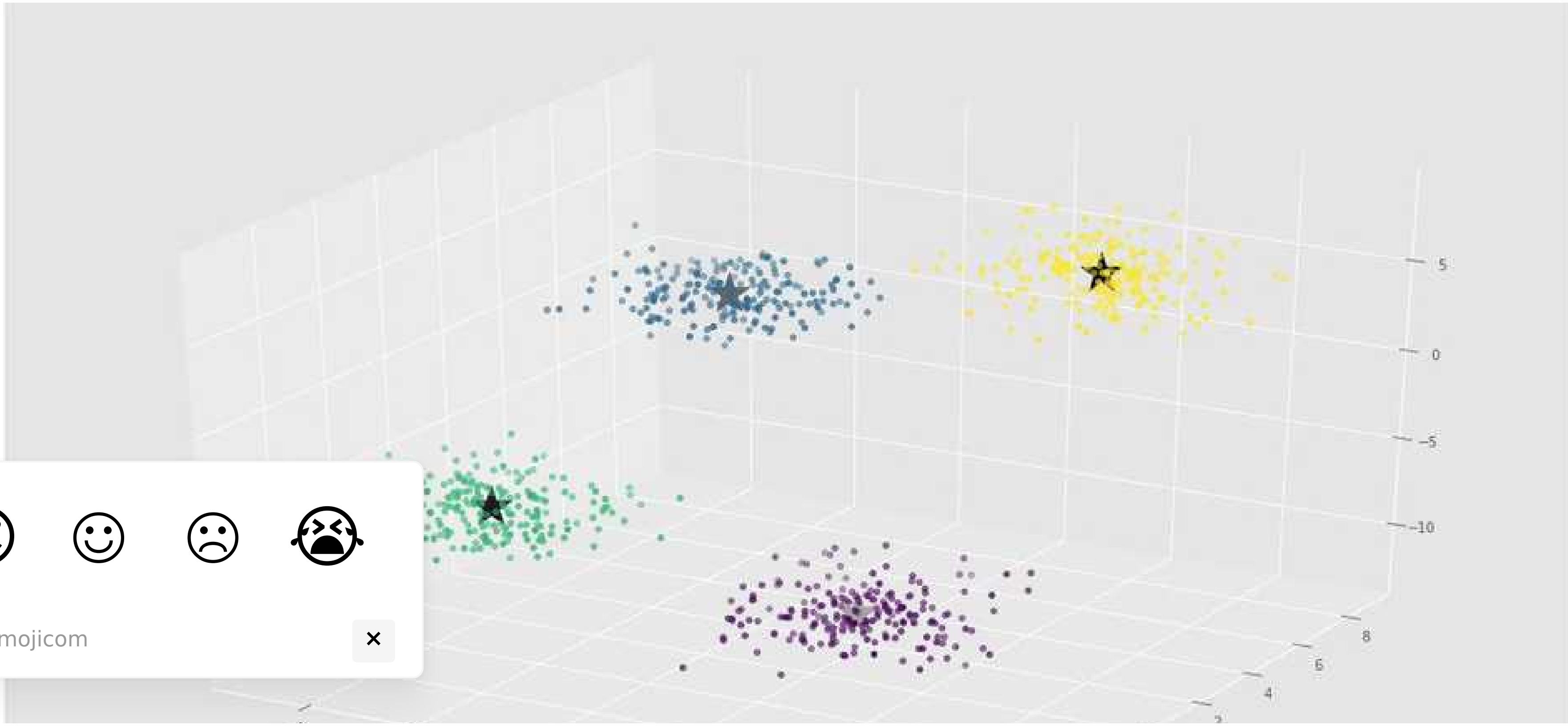
```
1], X[:, 2])
```

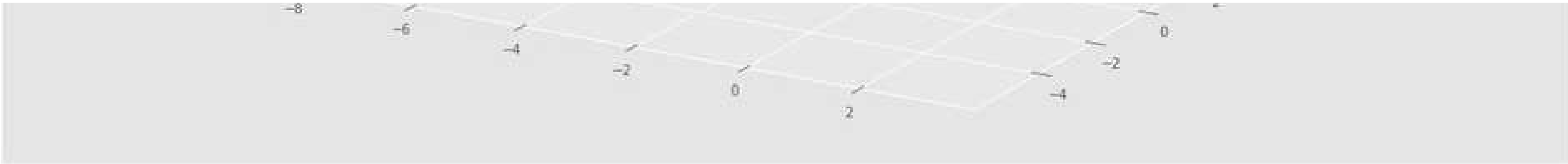



```
ers=4)

# Predicting the clusters
```

```
labels = kmeans.predict(X)
# Getting the cluster centers
C = kmeans.cluster_centers_
```

```
fig = plt.figure()
ax = Axes3D(fig)
ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=y)
ax.scatter(C[:, 0], C[:, 1], C[:, 2], marker='*', c='#050505', s=1000)
```





In the above image, you can see 4 clusters and their centroids as stars. scikit-learn approach is very simple and concise.

More Resources

- K-Means Clustering Video by Siraj Raval
- K-Means Clustering Lecture Notes by Andrew Ng
- K-Means Clustering Slides by David Sontag (New York University)
- Programming Collective Intelligence Chapter 3
- The Elements of Statistical Learning Chapter 14
- Pattern Recognition and Machine Learning Chapter 9

Checkout this Github Repo for full code and dataset.

Means clustering has its own issues. That include:

- If you run K-means on uniform data, you will get clusters.
- Sensitive to scale due to its reliance on Euclidean distance.
- Even on perfect data sets, it can get stuck in a local minimum

Have a look at this [StackOverflow Answer] for detailed explanation.

Let me know if you found any errors and checkout this post on [Hacker News]

Published 1 Oct 2017

Python Tutorial Machine Learning

Everything you can imagine is real

[Mubaris NK on Twitter]

😍 ☺ ☹ 😫

by emojicom ✕