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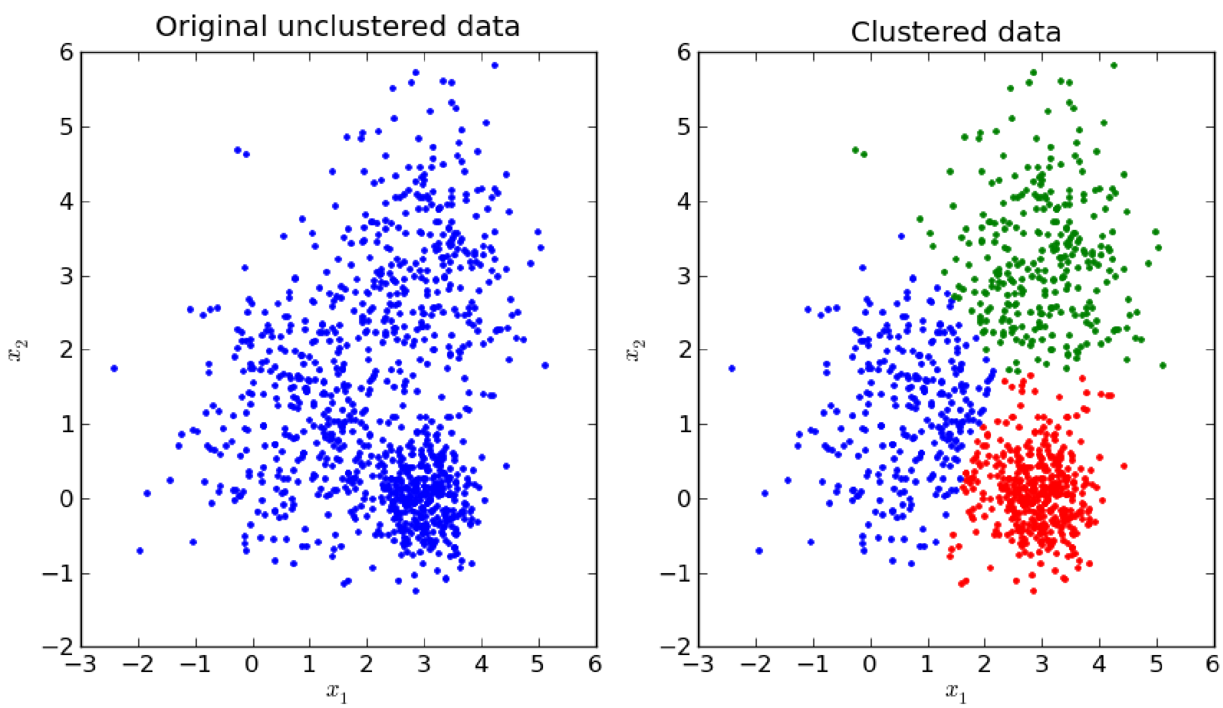
# K-Means Clustering in Python

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

K-Means is widely used for many applications.

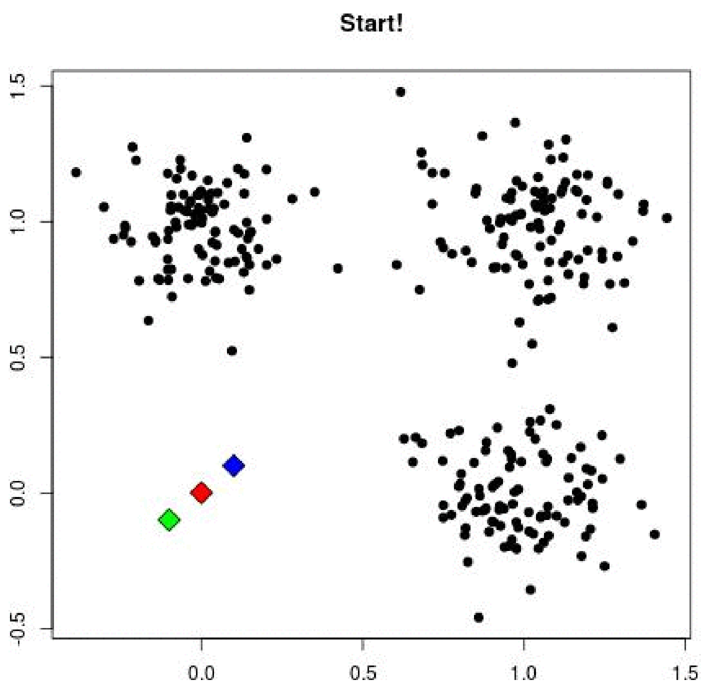
- Image Segmentation
- Clustering Gene Segementation Data
- News Article Clustering
- Clustering Languages
- Species Clustering

- Anomaly Detection

## Algorithm

Our algorithm works as follows, assuming we have inputs $x_1, x_2, x_3, ..., x_n$ 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.

### Step 1

We randomly pick K cluster centers(centroids). Let's assume these are $c_1, c_2, ..., c_k$, and we can say that;

$$C = c_1, c_2, ..., c_k$$

$C$ 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.

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

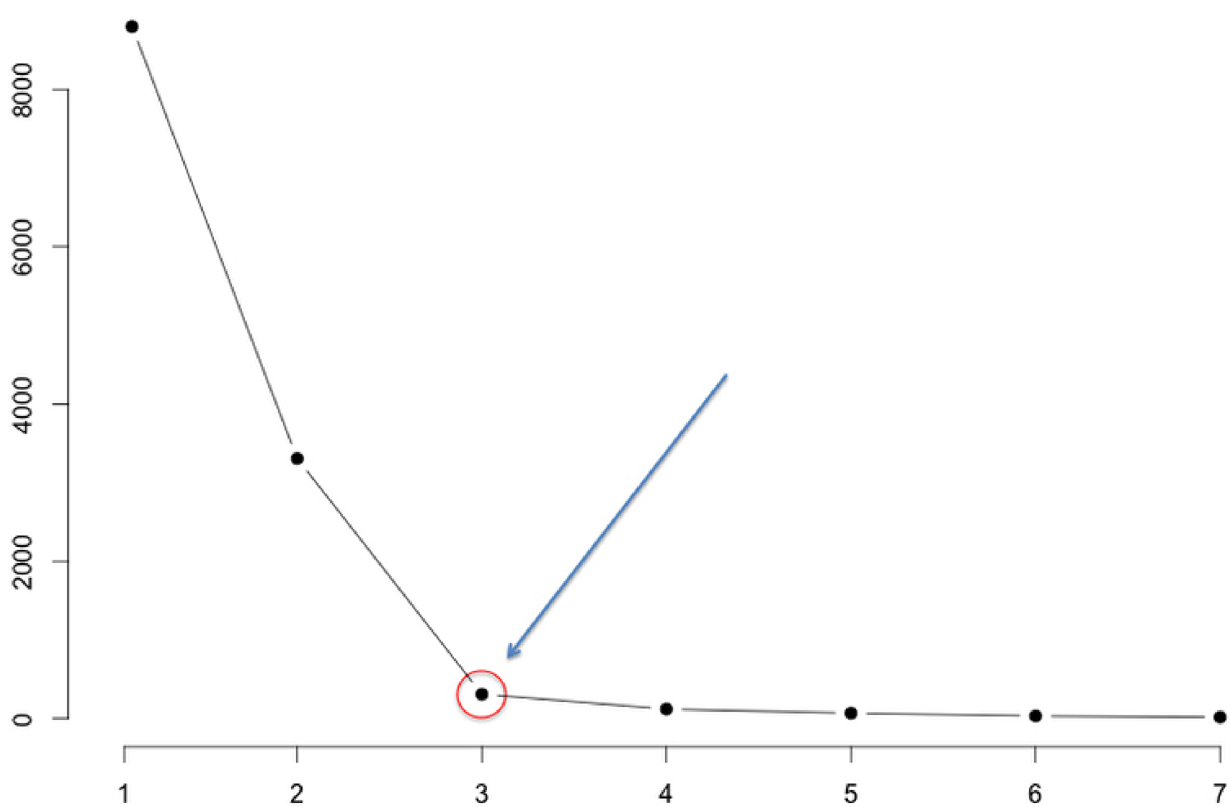
$S_i$ is the set of all points assigned to the $i^{\text{th}}$ cluster.

### Step 4

In this step, we repeat step 2 and 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.



We run the algorithm for different values of K(say K = 10 to 1) and plot the K values against SSE(Sum of Squared Errors). And select the value of K for the elbow 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.

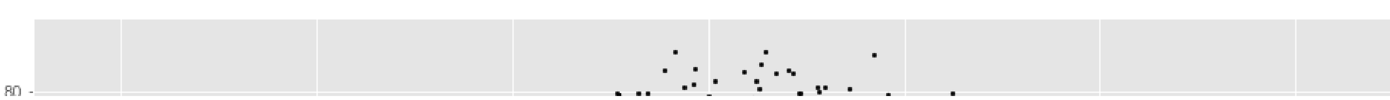
```
%matplotlib inline
from copy import deepcopy
import numpy as np
import pandas as pd
from matplotlib import pyplot as plt
plt.rcParams['figure.figsize'] = (16, 9)
plt.style.use('ggplot')
```

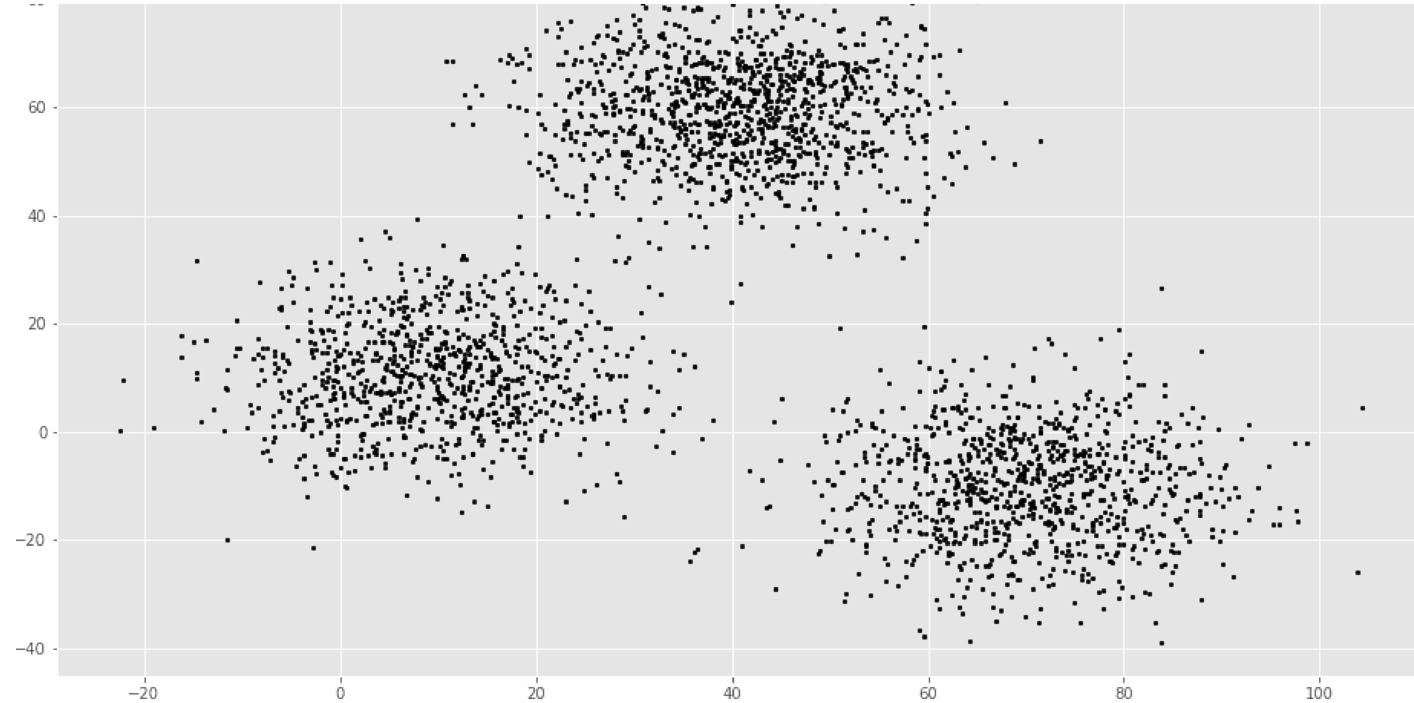
```
# Importing the dataset
data = pd.read_csv('xclara.csv')
print(data.shape)
data.head()
```

```
(3000, 2)
```

| | 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)
```



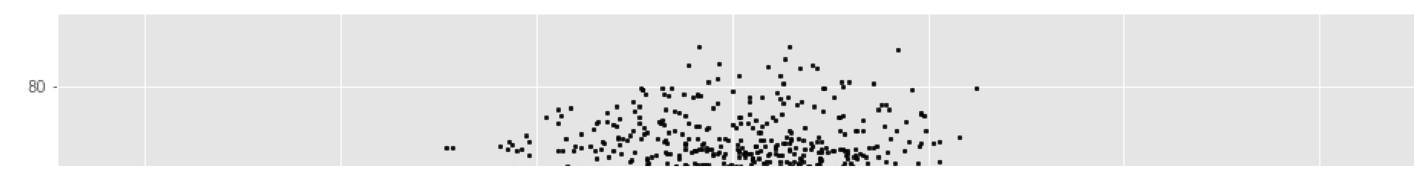


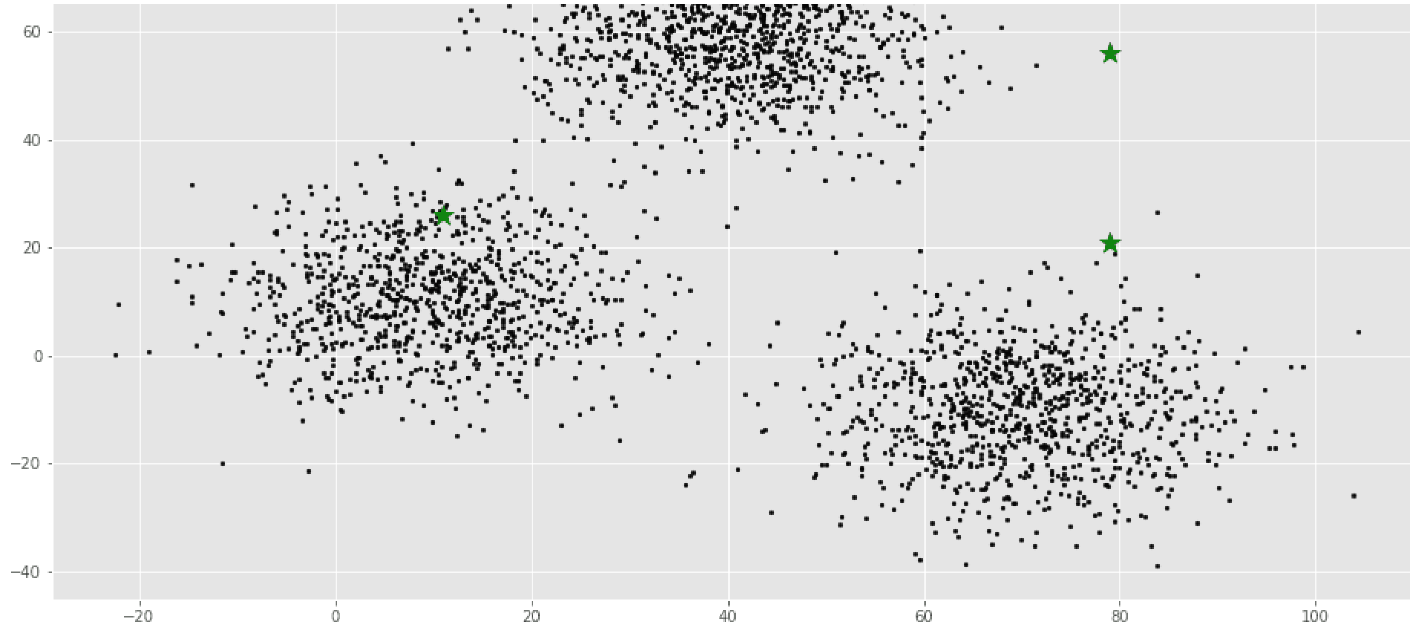
```
# Euclidean Distance Caculator
def dist(a, b, ax=1):
    return np.linalg.norm(a - b, axis=ax)
```

```
# 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)
print(C)
```

```
[[ 11.  26.]
 [ 79.  56.]
 [ 79.  21.]]
```

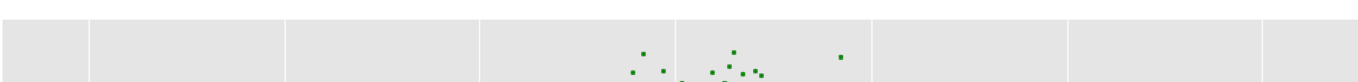
```
# Plotting along with the Centroids
plt.scatter(f1, f2, c='#050505', s=7)
plt.scatter(C_x, C_y, marker='*', s=200, c='g')
```

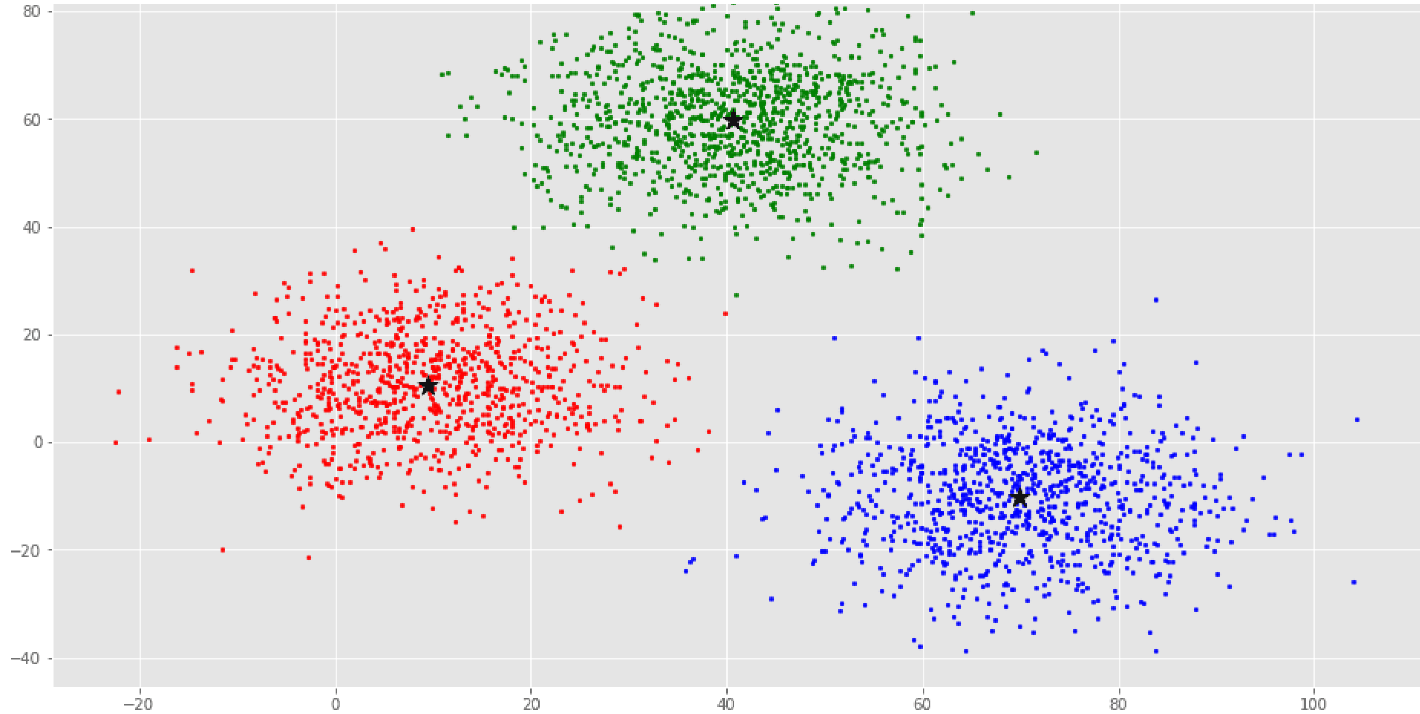





```
# To store the value of centroids when it updates
C_old = np.zeros(C.shape)
# Cluster Lables(0, 1, 2)
clusters = np.zeros(len(X))
# Error func. - Distance between new centroids and old centroids
error = dist(C, C_old, None)
# Loop will run till the error becomes zero
while error != 0:
    # Assigning 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)
```

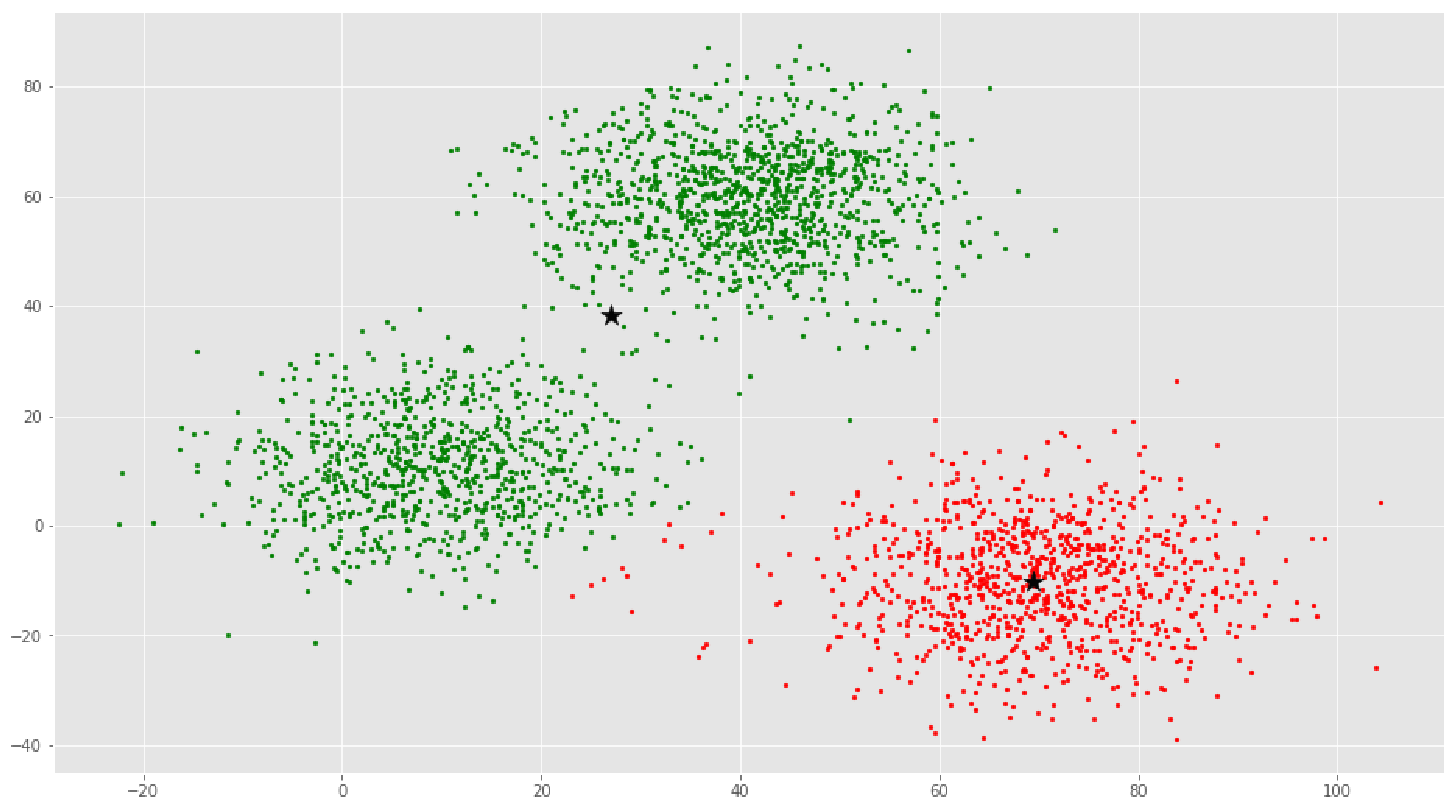
```
colors = ['r', 'g', 'b', 'y', 'c', 'm']
fig, ax = plt.subplots()
for i in range(k):
        points = np.array([X[j] for j in range(len(X)) if clusters[j] == i])
        ax.scatter(points[:, 0], points[:, 1], s=7, c=colors[i])
ax.scatter(C[:, 0], C[:, 1], marker='*', s=200, c='#050505')
```

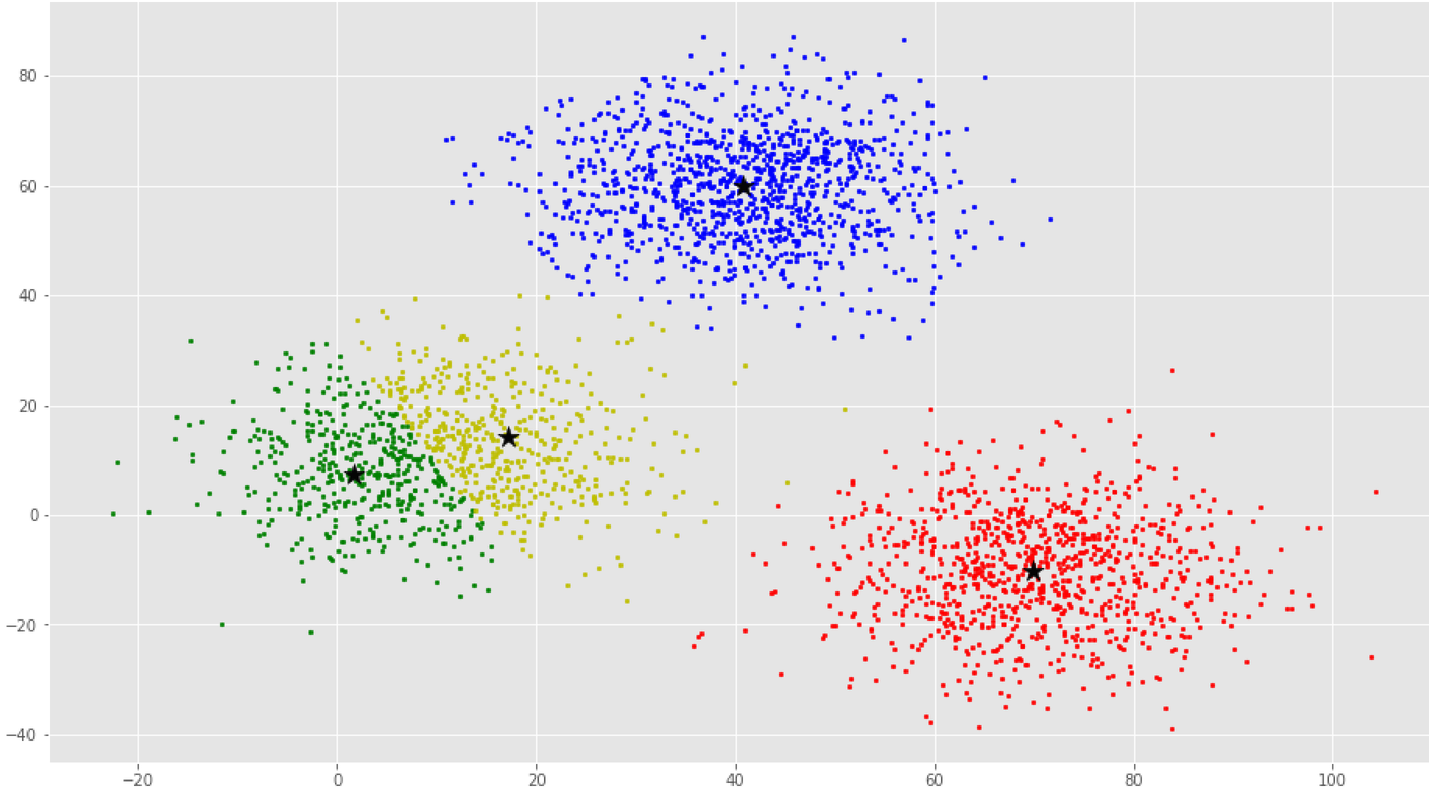


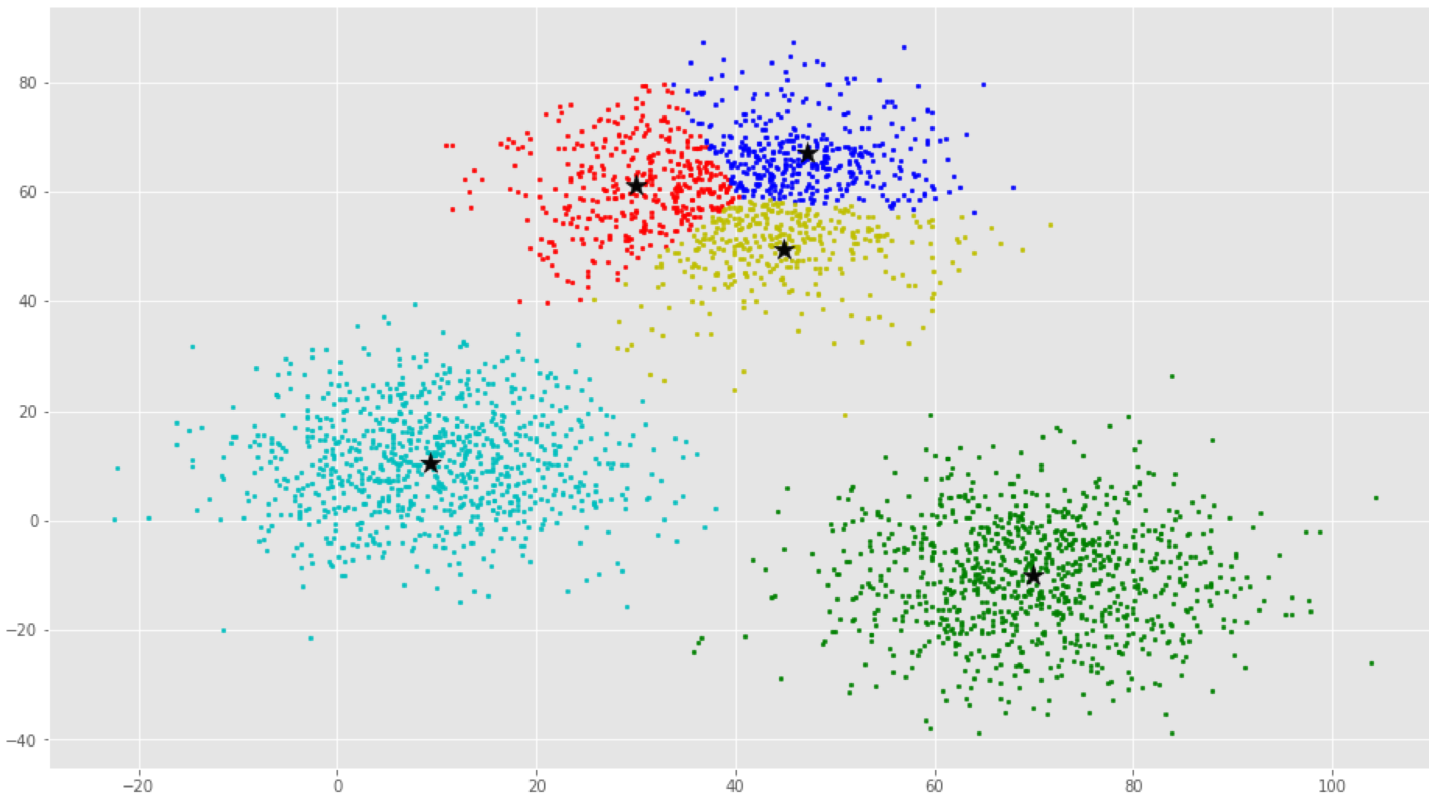



From this visualization it is clear that there are 3 clusters with black stars as their centroid.

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


80
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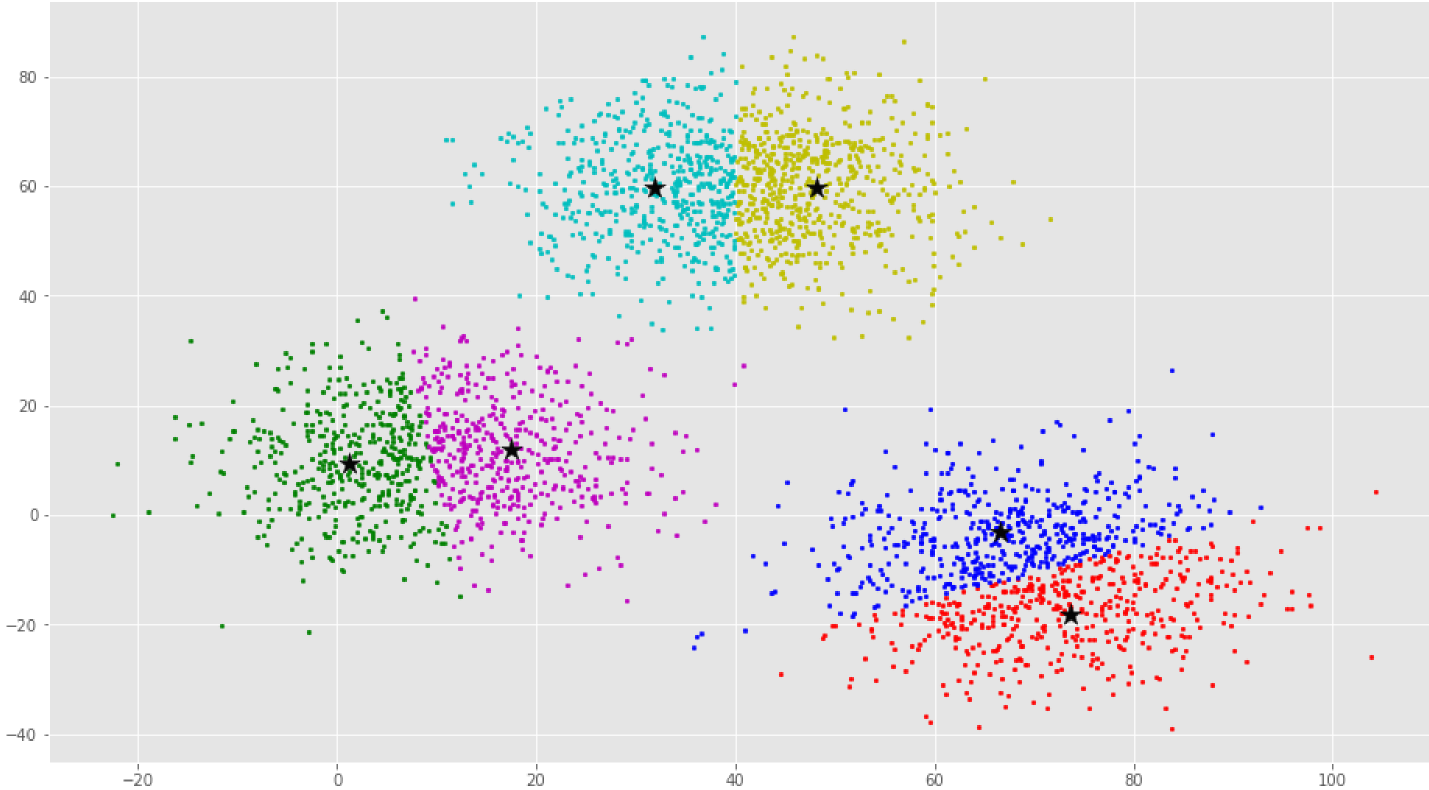
0
20
40
60
80
100




Now we will see how to implement K-Means Clustering using scikit-learn

## The scikit-learn approach

### 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
```

```
[[  9.47804546  10.68605232]
 [ 40.68362808  59.71589279]
 [ 69.92418671 -10.1196413 ]]
[[  9.4780459   10.686052  ]
 [ 69.92418447 -10.11964119]
 [ 40.68362784  59.71589274]]
```

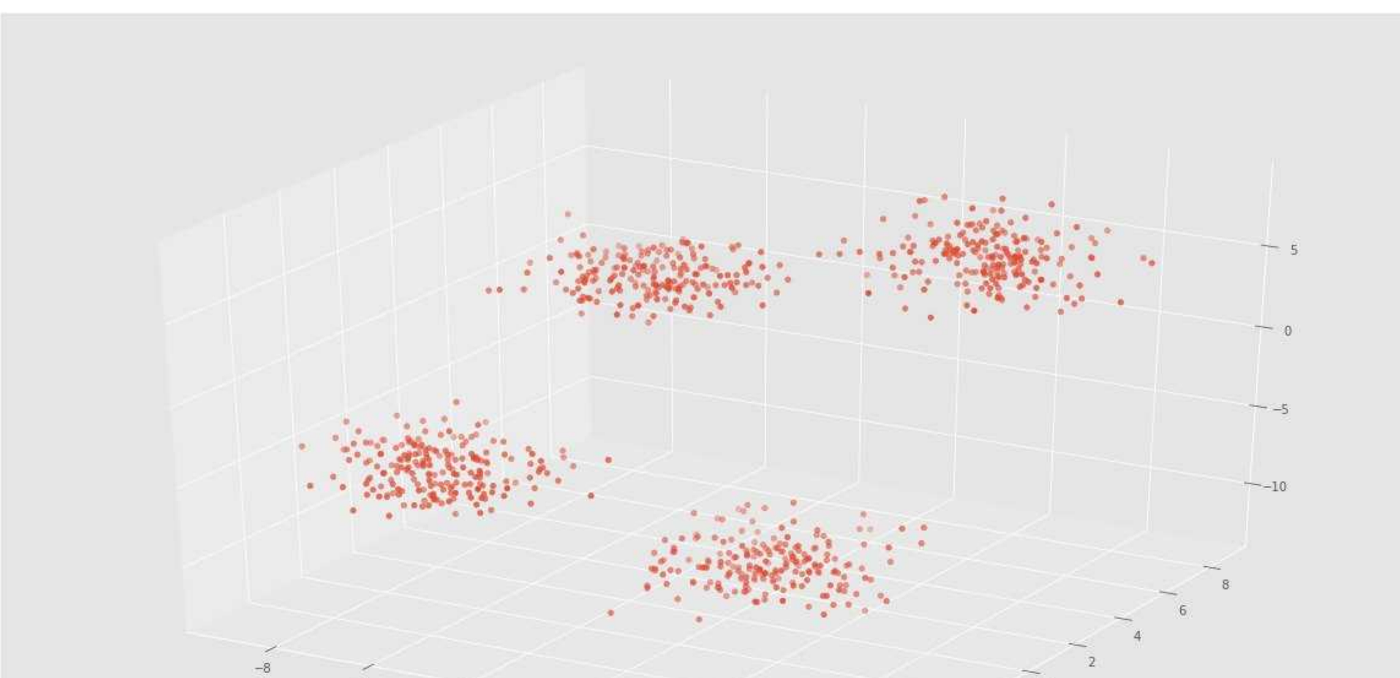
You can see that the centroid values are equal, but in different order.

### Example 2

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

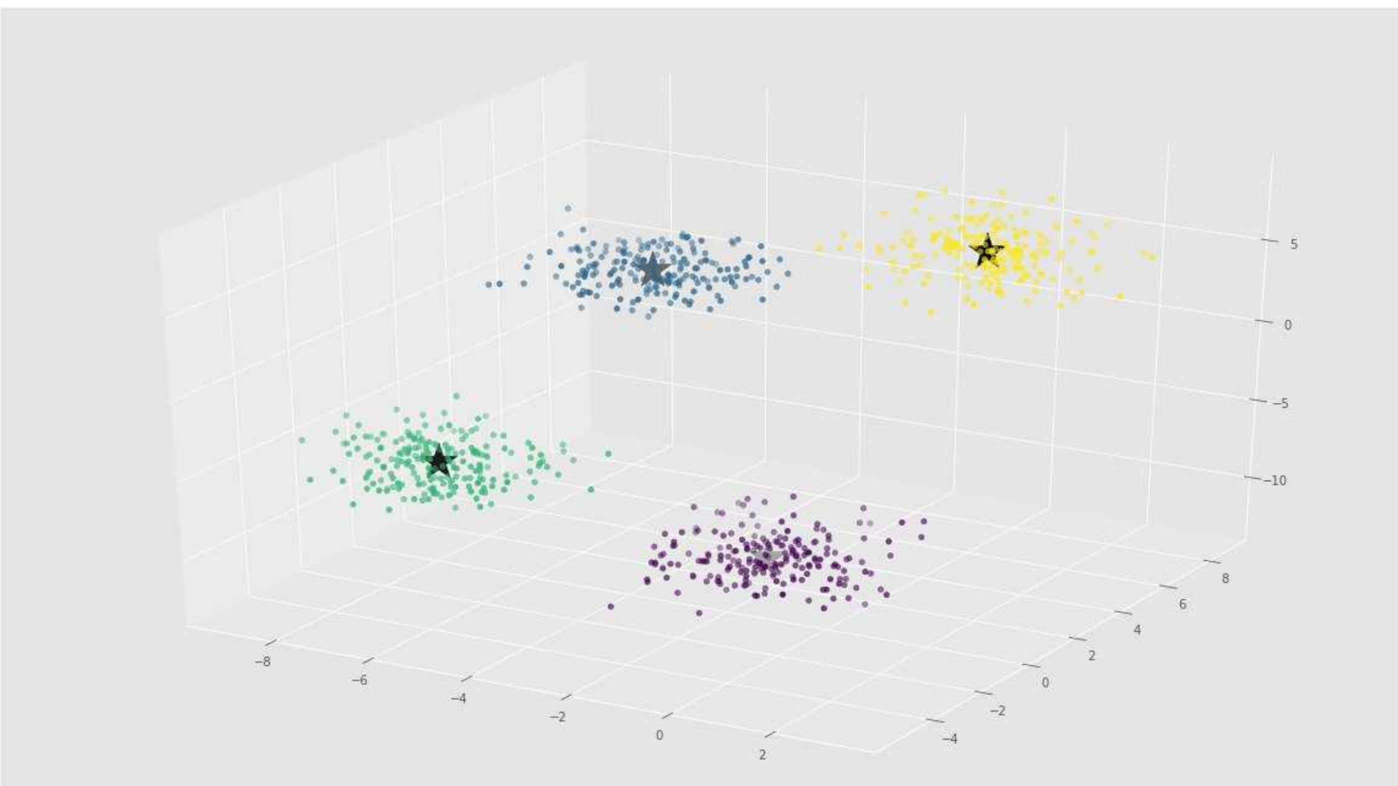
```python
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.cluster import KMeans
from sklearn.datasets import make_blobs

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)
```

```python
fig = plt.figure()
ax = Axes3D(fig)
ax.scatter(X[:, 0], X[:, 1], X[:, 2])
```




```
# Initializing KMeans
kmeans = KMeans(n_clusters=4)
# Fitting with inputs
kmeans = kmeans.fit(X)
# 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.

## Conclusion

Even though it works very well, K-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

Name

**Ashi Singh** • 3 months ago

RuntimeWarning: overflow encountered in square

# 100000 Iterations
newB, cost_history = gradient_descent(X, Y, B, alpha, 100000)

# New Values of B
print(newB)

# Final Cost of new B
print(cost_history[-1])

OUTPUT;\::
RuntimeWarning: overflow encountered in square
This is separate from the ipykernel package so we can avoid doing imports until
RuntimeWarning: invalid value encountered in subtract
del sys.path[0]
[nan nan nan]
nan

6 • Reply • Share ›

**Anderson Ribeiro** • a month ago

What metod return distance for each centroid?

Reply • Share ›

**Rahul Raj** • 3 months ago

Thanks buddy

Reply • Share ›

**Ibrahim Khatkhatay** • 3 months ago

in your make_blobs second scatter plot: why do you use "c=y" instead of "c=labels"? Alternatively, why find the labels if you don't use them?

Reply • Share ›