

K Means

K means is a classification ML algorithm that works as follows:

1. Initialization of k centroids (randomly chosen)
2. Assigning each point in the data set to its closest cluster (via a distance parameter to the centroid such as the euclidean distance)
3. Moving the centroids of the clusters

In K means clustering, we keep iterating through the set until our centroids have no longer changed (i.e they have converged), and every point in the data set is assigned to a certain cluster.

K means is a discriminative method, that hard assigns data points to a given cluster.

```
In [1]: import numpy as np
import math
from matplotlib import pyplot as plt
from copy import deepcopy
from sklearn.datasets.samples_generator import make_blobs
from sklearn.metrics import mean_squared_error
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/utils/deprecation.py:144: FutureWarning: The sklearn.datasets.samples_generator module is deprecated in version 0.22 and will be removed in version 0.24. The corresponding classes / functions should instead be imported from sklearn.datasets. Anything that cannot be imported from sklearn.datasets is now part of the private API.
  warnings.warn(message, FutureWarning)
```

Since we need a distance metric, to measure the distance to the center of the clusters, we can write it down as a helper function pre-hand to aid with calculations, in the implementation below I simply implement the euclidean distance, but many metrics such as the manhattan distance and more distance metrics can be used.

```
In [0]: def eucl_dist(p1, p2):
axis_val = 0
if len(p1.shape) != 1:
axis_val = 1
return np.linalg.norm(np.subtract(p1,p2),axis=axis_val)
```

```

In [0]: def k_means(data,k):
    features = data
    dim1 = features.shape[0]
    dim2 = features.shape[1]
    #we will now generate random centers
    mean = np.mean(features, axis = 0)
    std = np.std(features, axis = 0)
    centroids = np.random.randn(k,dim2)*std + mean
    len_centroids= centroids.shape
    centroids_old= np.zeros((len_centroids))
    centroids_new= deepcopy(centroids)
    diff= np.linalg.norm(np.subtract(centroids_new,centroids_old))
    clusters= np.zeros((len_centroids))
    euclidean_distances= np.zeros((dim1,k))

    while diff!=0:
        for num in range(k):
            euclidean_distances[:,num] = np.linalg.norm(
                np.subtract(features,centroids[num]),axis=1)
            clusters= np.argmin(euclidean_distances, axis = 1)
            centroids_old= deepcopy(centroids_new)
            for num in range(k):
                centroids_new[num]= np.mean(features[clusters==num],axis=0)
            diff= np.linalg.norm(np.subtract(centroids_new,centroids_old))
        labels= np.zeros(len(features))
        colors= [0,1,2,3,4,5,6,7,8,9,10,11]
        for i in range(len(features)):
            dist= np.zeros((len(centroids_new)))
            for c in range(len(centroids_new)):
                dist[c]= np.linalg.norm(np.subtract(features[i],centroids_new[c]),
                    axis=0)

            index=np.argmin(dist)
            labels[i]= colors[index]
    return labels,centroids_new

```

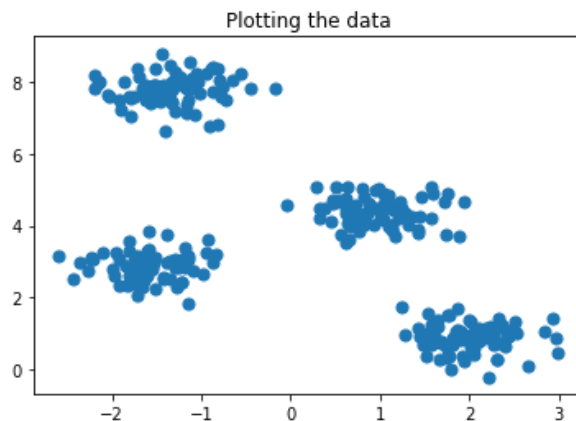
Let us now load an example dataset

```

In [9]: X, y_true = make_blobs(n_samples=300, centers=4,
                                cluster_std=0.4, random_state=0)
plt.scatter(X[:, 0], X[:, 1], s=50)
plt.title("Plotting the data")

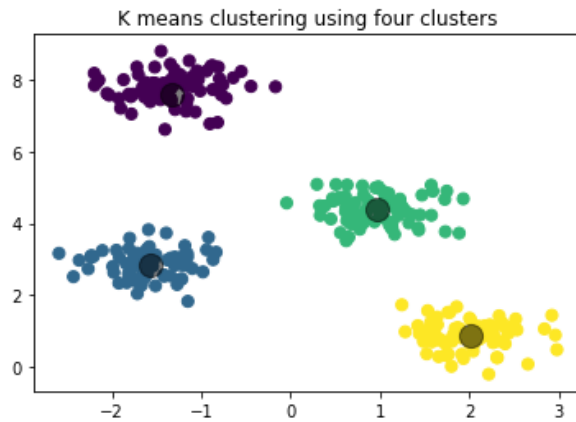
```

Out[9]: Text(0.5, 1.0, 'Plotting the data')



```
In [10]: y_predict, centroids = k_means(X, 4)
plt.scatter(X[:, 0], X[:, 1], c=y_predict, s=50, cmap='viridis')
plt.scatter(centroids[:, 0], centroids[:, 1], c='black', s=200, alpha=0.5)
plt.title("K means clustering using four clusters")
```

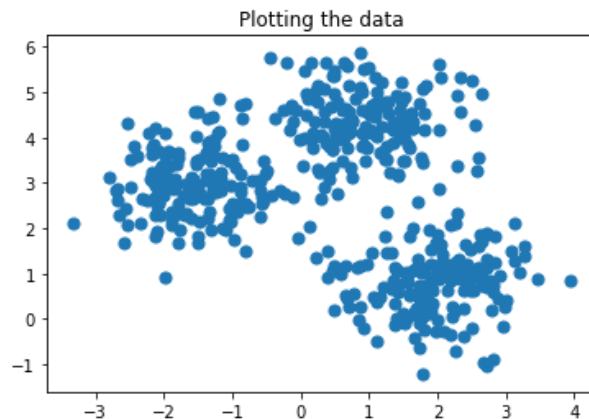
```
Out[10]: Text(0.5, 1.0, 'K means clustering using four clusters')
```



As we can see the algorithm worked! Here since the data was pretty clearly in four clusters, we picked k to be 4, let us now look at a case where the data is more overlapped, and plot a few variations of k , to see which looks best.

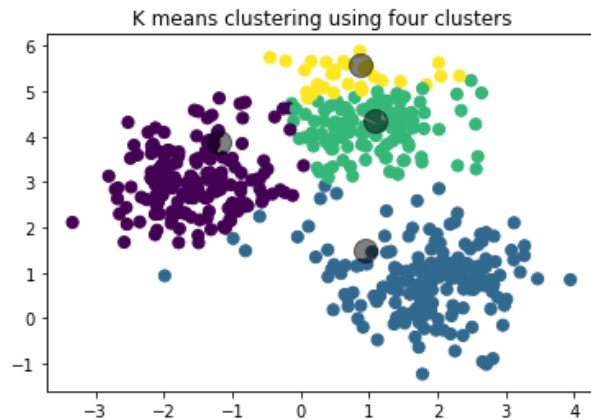
```
In [13]: X_2, y_true_2 = make_blobs(n_samples=500, centers=3,
                                   cluster_std=0.7, random_state=0)
plt.scatter(X_2[:, 0], X_2[:, 1], s=50)
plt.title("Plotting the data")
```

```
Out[13]: Text(0.5, 1.0, 'Plotting the data')
```



```
In [24]: y_predict_2, centroids_2 =k_means(X_2,4)
plt.scatter(X_2[:, 0], X_2[:, 1], c=y_predict_2, s=50, cmap='viridis')
plt.scatter(centroids_2[:, 0], centroids_2[:, 1], c='black', s=200, alpha=0.5)
plt.title("K means clustering using four clusters")
```

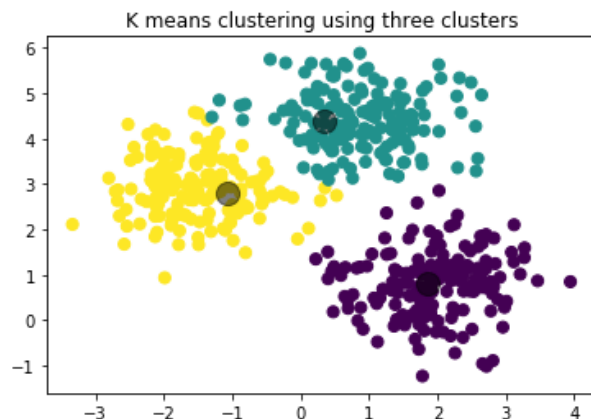
Out[24]: Text(0.5, 1.0, 'K means clustering using four clusters')



As we can see, using a k value of 4 does not work super well in this case, so let us try another value and see what happens

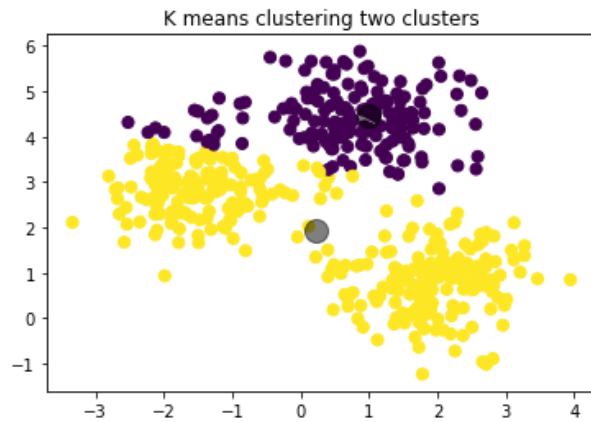
```
In [25]: y_predict_2, centroids_2 =k_means(X_2,3)
plt.scatter(X_2[:, 0], X_2[:, 1], c=y_predict_2, s=50, cmap='viridis')
plt.scatter(centroids_2[:, 0], centroids_2[:, 1], c='black', s=200, alpha=0.5)
plt.title("K means clustering using three clusters")
```

Out[25]: Text(0.5, 1.0, 'K means clustering using three clusters')



```
In [26]: y_predict_2, centroids_2 =k_means(X_2,2)
plt.scatter(X_2[:, 0], X_2[:, 1], c=y_predict_2, s=50, cmap='viridis')
plt.scatter(centroids_2[:, 0], centroids_2[:, 1], c='black', s=200, alpha=0.5)
plt.title("K means clustering two clusters")
```

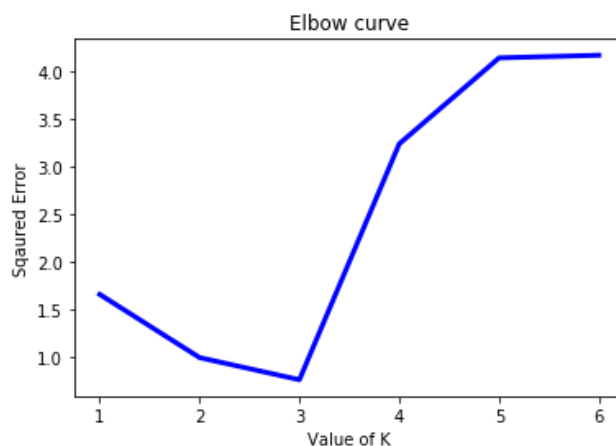
```
Out[26]: Text(0.5, 1.0, 'K means clustering two clusters')
```



Here we see slightly more distinct clusters shapes in the case of k being equal to 3, but too much overlap in the case of k being equal to 2, is there a way to quantitatively analyze this, without depending on a qualitative analysis?

```
In [30]: cost =[]
for i in range(1, 7):
    y_predict_2, centroids_2 =k_means(X_2,i)
    cost.append(mean_squared_error(y_true_2, y_predict_2))

plt.plot(range(1, 7), cost, color='b', linewidth='3')
plt.xlabel("Value of K")
plt.ylabel("Sqaured Error")
plt.title('Elbow curve')
plt.show()
```



What we see above is an elbow curve, a very common metric to determine the k value in k -means, k nearest neighbours, and many other machine learning methods. It helps quantitatively determine the correct value of k , by picking the value of k that forms the elbow. Even though it may look like a toss up between the values of 3 and 4, it is clear from the elbow curve that 3 is the best value for this particular set.