K means Clustering – Introduction

K-Means Clustering is an Unsupervised Machine Learning algorithm, which groups the unlabeled dataset into different clusters.

K means Clustering

Unsupervised Machine Learning is the process of teaching a computer to use unlabeled, unclassified data and enabling the algorithm to operate on that data without supervision. Without any previous data training, the machine's job in this case is to organize unsorted data according to parallels, patterns, and variations.

The goal of clustering is to divide the population or set of data points into a number of groups so that the data points within each group are more comparable to one another and different from the data points within the other groups. It is essentially a grouping of things based on how similar and different they are to one another.

We are given a data set of items, with certain features, and values for these features (like a vector). The task is to categorize those items into groups. To achieve this, we will use the K-means algorithm; an unsupervised learning algorithm. 'K' in the name of the algorithm represents the number of groups/clusters we want to classify our items into.

(It will help if you think of items as points in an n-dimensional space). The algorithm will categorize the items into k groups or clusters of similarity. To calculate that similarity, we will use the Euclidean distance as a measurement.

The algorithm works as follows:

1. First, we randomly initialize k points, called means or cluster centroids.
2. We categorize each item to its closest mean and we update the mean's coordinates, which are the averages of the items categorized in that cluster so far.
3. We repeat the process for a given number of iterations and at the end, we have our clusters.

The “points” mentioned above are called means because they are the mean values of the items categorized in them. To initialize these means, we have a lot of options. An intuitive method is to initialize the means at random items in the data set. Another method is to initialize the means at random values between the boundaries of the data set (if for a feature *x,* the items have values in [0,3], we will initialize the means with values for *x* at [0,3]).

The above algorithm in pseudocode is as follows:

```
Initialize k means with random values

--> For a given number of iterations:

    --> Iterate through items:

        --> Find the mean closest to the item by calculating
        the euclidean distance of the item with each of the means

        --> Assign item to mean

        --> Update mean by shifting it to the average of the items in that clus
```

Import the necessary Libraries:

We are importing Numpy for statistical computations, Matplotlib to plot the graph, and make_blobs from sklearn.datasets.

Python3

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.datasets import make_blobs
```

Create the custom dataset with make_blobs and plot it

Python3

```
X,y = make_blobs(n_samples = 500,n_features = 2,centers = 3,

fig = plt.figure(0)
plt.grid(True)
plt.scatter(X[:,0],X[:,1])
plt.show()
```

Output:

Clustering dataset

Initialize the random centroids

Python3

```
k = 3

clusters = {}
np.random.seed(23)

for idx in range(k):
    center = 2*(2*np.random.random((X.shape[1],))-1)
    points = []
    cluster = {
        'center' : center,
        'points' : []
    }

    clusters[idx] = cluster

clusters
```

Output:

```
{0: {'center': array([0.06919154, 1.78785042]), 'points': []},
 1: {'center': array([ 1.06183904, -0.87041662]), 'points': []},
 2: {'center': array([-1.11581855,  0.74488834]), 'points': []}}
```

Plot the random initialize center with data points

Python3

```
plt.scatter(X[:,0],X[:,1])
plt.grid(True)
for i in clusters:
    center = clusters[i]['center']
    plt.scatter(center[0],center[1],marker = '*',c = 'red')
plt.show()
```

Output:

Data points with random center

Define euclidean distance

Python3

```
def distance(p1,p2):
    return np.sqrt(np.sum((p1-p2)**2))
```

Create the function to Assign and Update the cluster center

Python3

```
#Implementing E step
def assign_clusters(X, clusters):
    for idx in range(X.shape[0]):
        dist = []

        curr_x = X[idx]

        for i in range(k):
            dis = distance(curr_x,clusters[i]['center'])
            dist.append(dis)
        curr_cluster = np.argmin(dist)
        clusters[curr_cluster]['points'].append(curr_x)
    return clusters

#Implementing the M-Step
def update_clusters(X, clusters):
    for i in range(k):
        points = np.array(clusters[i]['points'])
        if points.shape[0] > 0:
            new_center = points.mean(axis =0)
            clusters[i]['center'] = new_center

            clusters[i]['points'] = []
    return clusters
```

Create the function to Predict the cluster for the datapoints

Python3

```
def pred_cluster(X, clusters):
    pred = []
    for i in range(X.shape[0]):
        dist = []
        for j in range(k):
            dist.append(distance(X[i],clusters[j]['center'])
        pred.append(np.argmin(dist))
    return pred
```

Assign, Update, and predict the cluster center

Python3

```
clusters = assign_clusters(X,clusters)
clusters = update_clusters(X,clusters)
pred = pred_cluster(X,clusters)
```

Plot the data points with their predicted cluster center

Python3

```
plt.scatter(X[:,0],X[:,1],c = pred)
for i in clusters:
    center = clusters[i]['center']
    plt.scatter(center[0],center[1],marker = '^',c = 'red')
plt.show()
```

Output:

Example 2:

Import the necessary libraries

Python3

```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
import matplotlib.cm as cm
from sklearn.datasets import load_iris
from sklearn.cluster import KMeans
```

Load the Dataset

Python3

```
X, y = load_iris(return_X_y=True)
```

Elbow Method

Finding the ideal number of groups to divide the data into is a basic stage in any unsupervised algorithm. One of the most common techniques for figuring out this ideal value of k is the elbow approach.

Python3

```
#Find optimum number of cluster
sse = [] #SUM OF SQUARED ERROR
for k in range(1,11):
    km = KMeans(n_clusters=k, random_state=2)
    km.fit(X)
    sse.append(km.inertia_)
```

Plot the Elbow graph to find the optimum number of cluster

Python3

```
sns.set_style("whitegrid")
g=sns.lineplot(x=range(1,11), y=sse)
g.set(xlabel ="Number of cluster (k)",
      ylabel = "Sum Squared Error",
      title ='Elbow Method')
plt.show()
```

Output:

Elbow Method

From the above graph, we can observe that at k=2 and k=3 elbow-like situation. So, we are considering K=3

Build the Kmeans clustering model

Python3

```
kmeans = KMeans(n_clusters = 3, random_state = 2)
kmeans.fit(X)
```

Output:

```
KMeans

KMeans(n_clusters=3, random_state=2)
```

Find the cluster center

Python3

```
kmeans.cluster_centers_
```

Output:

```
array([[5.006     , 3.428     , 1.462     , 0.246     ],
       [5.9016129 , 2.7483871 , 4.39354839, 1.43387097],
       [6.85      , 3.07368421, 5.74210526, 2.07105263]])
```

Predict the cluster group:

Python3

```
pred = kmeans.fit_predict(X)
pred
```

Output:

```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 2, 2, 2, 2, 1, 2, 2, 2,
       2, 2, 2, 1, 1, 2, 2, 2, 2, 1, 2, 1, 2, 1, 2, 2, 1, 1, 2, 2, 2, 2,
       2, 1, 2, 2, 2, 2, 1, 2, 2, 2, 1, 2, 2, 2, 1, 2, 2, 1], dtype=int32)
```

Plot the cluster center with data points

Python3

```
plt.figure(figsize=(12,5))
plt.subplot(1,2,1)
plt.scatter(X[:,0],X[:,1],c = pred, cmap=cm.Accent)
plt.grid(True)
for center in kmeans.cluster_centers_:
    center = center[:2]
    plt.scatter(center[0],center[1],marker = '^',c = 'red')
plt.xlabel("petal length (cm)")
plt.ylabel("petal width (cm)")

plt.subplot(1,2,2)
plt.scatter(X[:,2],X[:,3],c = pred, cmap=cm.Accent)
plt.grid(True)
for center in kmeans.cluster_centers_:
    center = center[2:4]
    plt.scatter(center[0],center[1],marker = '^',c = 'red')
plt.xlabel("sepal length (cm)")
plt.ylabel("sepal width (cm)")
plt.show()
```

Output:

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