Kmeans Clustering

Clustering is an unsupervised learning method as we don't have labels for the dataset. We try to find similarity by forming cluster in an n-dimensional space. Points which are "closer" to each other are considered more similar than the ones which are further apart. This "closeness" can be measure in a number of ways like Euclidian distance, cosine similarity etc.

Kmeans is one of the most popular clustering algorithm. Our objective is to find k points in the n-dimensional space such these points sit at the centre of the k dense clusters formed by plotting the dataset in n-dimensional space. The basic implementation of the algorithm is as follows

1) Select k unique random points from the dataset and call them inital centroids

2) For each point in the dataset find the closest centroid and assign that point to the cluster of that centroid

3) For each cluster,calculate the mean of all the points. Mean values will give new centroids

4) Repeat steps 2 and 3 until you get a new set of centroids which is very close to the previous one.

In [1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from PIL import Image
from sklearn.datasets.samples_generator import make_blobs
```

In [2]:
```
def initialize_centroids(X,k):
    """
    randomly picks k unique points from X as the initial centroids

    inputs--
    X: input matrix--> np.ndarray
    k: number of centroids

    outputs--
    array of centroid vectors
    """
    return X[np.random.choice(range(X.shape[0]), k, replace=False)]
```

In [3]:
```
def distance_bw_centroids(old:np.ndarray,new:np.ndarray):
    """returns euclidian distance between old and new centroids"""
    return np.linalg.norm(old.ravel()-new.ravel())
```

```python
In [4]: def assign_buckets(X:np.ndarray, centroids:np.ndarray):
    """
    returns a np.array of bucket indices
    for a given set of points and centroids
    """
    dist_matrix = np.stack([np.linalg.norm(X-c, axis=1) for c in centroids])
    return np.argmin(dist_matrix, axis=0)
```

```python
In [5]: def kmeans(X:np.ndarray, k:int, centroids=None, tolerance=1e-2):
    """
    Inputs :
        X:Dataset array
        k:number of clusters
        centroids: None for random initialization, 'kmeans++' for smart initialization
        tolerance: max tolerable distance between new and old centroids
    Outputs :
        array of centroids (k,X.shape[1])
        array of cluster indices corresponding to each data-point (X.shape[0])
    """
    if centroids=='kmeans++':
        centroids = initialize_centroids_plus(X,k)
    else:
        centroids = initialize_centroids(X,k)

    # for values of k>20, it takes a very long time to converge
    # so we are putting a limit on iterations such that if k increases, number of iterations decrease
    # also we can have more iterations for smaller values of k, which will yield a better set of centroids
    iter_limit = int(800/k)
    iters = 0
    d = 5
    while (d > tolerance) and (iters< iter_limit):
        bucket_idx = assign_buckets(X, centroids)
        new_centroids = [np.mean(X[bucket_idx == i], keepdims = True, axis = 0 ) for i in range(k)]
        new_centroids = np.array(new_centroids).ravel().reshape(k,X.shape[1])
        old_centroids = centroids
        centroids = new_centroids
        d = distance_bw_centroids(old_centroids, new_centroids)
        iters+=1
    return centroids,bucket_idx
```

TOY Dataset with Random Initialization

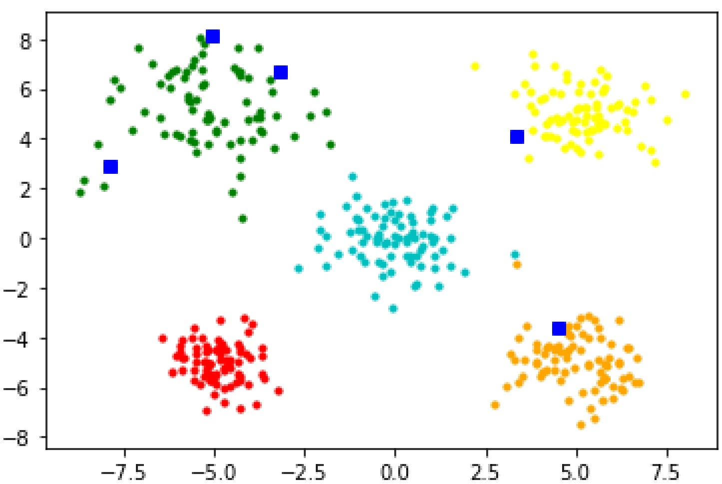
In [17]:
```python
#creating dataset
centers = [(-5, -5), (5, 5), (-5,5),(5,-5), (0,0)]
cluster_std = [0.8, 1, 1.5,1, 1]

X, y = make_blobs(n_samples=400, cluster_std=cluster_std, centers=centers, n_features=4, random_state=1)

#initial centroids
centroids = initialize_centroids(X,5)

plt.scatter(X[y == 0, 0], X[y == 0, 1], color="red", s=10, label="Cluster1")
plt.scatter(X[y == 1, 0], X[y == 1, 1], color="yellow", s=10, label="Cluster2")
plt.scatter(X[y == 2, 0], X[y == 2, 1], color="green", s=10, label="Cluster3")
plt.scatter(X[y == 3, 0], X[y == 3, 1], color="orange", s=10, label="Cluster4")
plt.scatter(X[y == 4, 0], X[y == 4, 1], color="c", s=10, label="Cluster5")
plt.plot(centroids[:,0],centroids[:,1],"bs")
plt.plot()
```

Out[17]: []

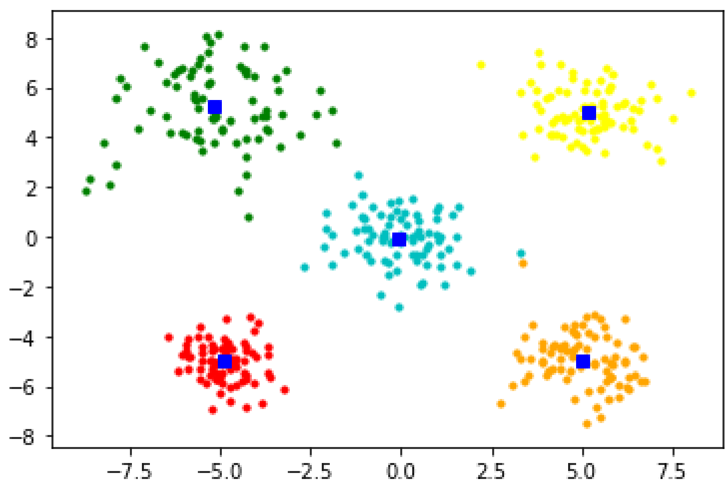


After applying kmeans with Random Initialization

In [18]:
```
center_kmeans, buckets_kmeans  = kmeans(X,k=5)

plt.scatter(X[y == 0, 0], X[y == 0, 1], color="red", s=10, label="Cluster1")
plt.scatter(X[y == 1, 0], X[y == 1, 1], color="yellow", s=10, label="Cluster2")
plt.scatter(X[y == 2, 0], X[y == 2, 1], color="green", s=10, label="Cluster3")
plt.scatter(X[y == 3, 0], X[y == 3, 1], color="orange", s=10, label="Cluster4")
plt.scatter(X[y == 4, 0], X[y == 4, 1], color="c", s=10, label="Cluster5")
plt.plot(center_kmeans[:,0],center_kmeans[:,1],"bs")
```

Out[18]:
```
[<matplotlib.lines.Line2D at 0x7fde005f43d0>]
```



KMEANS++

As you can see when we randomly initialize, points chosen as initial centroids are far from optimal solution. For larger datasets this may result in slower convergence towards the optimal centroids. As a solution to this problem we use "kmeans++"

How does Kmeans++ initialize centroids?

1) Pick a random point from the dataset as the first centroid.

2) Find a point in the dataset which is farthest from this point and make it the second centroid.

3) Now for selecting the third centroid, for each point in the dataset find the minimum distance of that point from the current set of centroids and then select the point for which this "minimum" distance is the maximum(example below)

4) repeat step 3 till we obtain k centroids

Example: Our dataset has 10 points p1,....,p10 we already selected two centroids, c1(lets say p3) and c2(lets say p7) using the above steps Next we are trying to find the third centroid

MAX (min(p1-c1, p1-c2), min(p2-c1, p2-c2), min(p3-c1, p3-c2), min(p4-c1, p4-c2), min(p5-c1, p5-c2), min(p6-c1, p6-c2), min(p7-c1, p7-c2), min(p8-c1, p8-c2), min(p9-c1, p9-c2), min(p10-c1, p10-c2))

Lets assume we get p4-c2 after this operation, then p4 becomes our third centroid

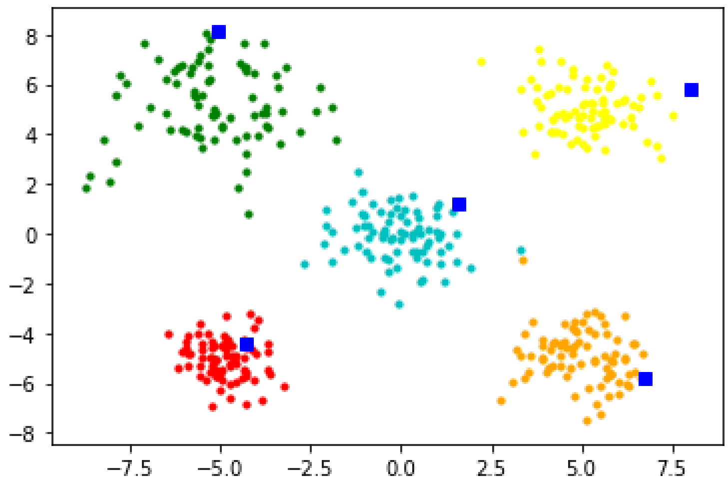
In [8]:
```
def initialize_centroids_plus(X:np.ndarray,k:int):
    """
    implementing kmeans++ initialization
    input : X,k
    output : returns k smartly selected centroids
    """
    centroids = initialize_centroids(X,1)
    for _ in range(k-1):
        dist_matrix = np.stack([np.linalg.norm(X-c, axis=1) for c in cen
troids]) #centroids*X.shape[0]
        min_point_to_centroids = np.min(dist_matrix, axis=0)
        new_centroid_idx = np.argmax(min_point_to_centroids)
        centroids = np.vstack((centroids,X[new_centroid_idx]))
    return centroids
```

TOY dataset the kmeans++ initialization

In [9]:
```
centroids = initialize_centroids_plus(X,5)

plt.scatter(X[y == 0, 0], X[y == 0, 1], color="red", s=10, label="Cluste
r1")
plt.scatter(X[y == 1, 0], X[y == 1, 1], color="yellow", s=10, label="Clu
ster2")
plt.scatter(X[y == 2, 0], X[y == 2, 1], color="green", s=10, label="Clus
ter3")
plt.scatter(X[y == 3, 0], X[y == 3, 1], color="orange", s=10, label="Clu
ster4")
plt.scatter(X[y == 4, 0], X[y == 4, 1], color="c", s=10, label="Cluster
5")
plt.plot(centroids[:,0],centroids[:,1],"bs")
plt.plot()
```

Out[9]: []



Comparing kmeans++ initialization to random initialization, we clearly see that inital locations of the centroids are much closer to their soon to be optimal positions

MODEL EVALUATION

Elbow Plot

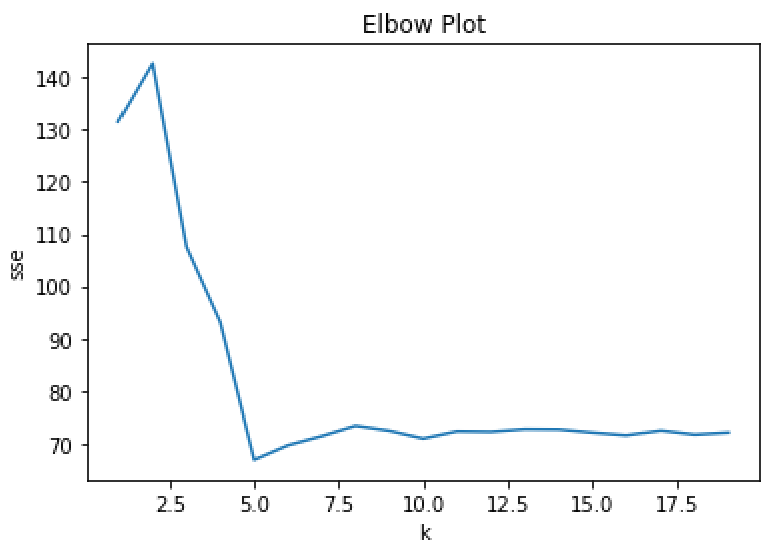
Elbow plot helps us estimte the value of k which will best for the data at hand. We choose the value of k for which either sse is smallest or after which the plot begins to flatten. The intuition is, we want the k for which the error is smallest(lowest point in the graph) or we could go for k beyond which plot begins to flatten, meaning even if we increase the clusters beyond that point, error is not going to decrease. As discussed above, if we go for more clusters this algorithm start to get more expesive.

In [10]:
```
def sse(X, k):
    center_kmeans, buckets_kmeans  = kmeans(X,k,centroids='kmeans++')
    sum_err = 0
    for i in range(k):
        sum_err += np.linalg.norm(X[buckets_kmeans==i]-center_kmeans[i])
    return sum_err
```

In [11]:
```
x_axis, y_axis = [],[]
for k in range(1,20):
    x_axis.append(k)
    y_axis.append(sse(X,k))

plt.plot(x_axis, y_axis)
plt.xlabel("k")
plt.ylabel("sse")
plt.title("Elbow Plot")
```

Out[11]:
```
Text(0.5, 1.0, 'Elbow Plot')
```



We choose k = 5 in this case

IMAGE COMPRESSION

One of the interesting applications of clustering is image compression. We take an image which has all sorts of colors and compress to an image with only a few. How do we go about this?

(Please refer to the ipynb in case pdf is not clear) Intuition: 1) We split the image into three channels (r,g and b) 2) For the below 4X3 coloured image, each pixel has r,g and b intensity values. 12 44 12 12 11 14 22 18 23 56 89 91 22 32 01 02 12 72 92 31 81 92 74 65 42 31 15 29 14 23 46 69 22 33 44 81 3) Next we represent each pixel as a vector (r,g,b) In this case P11 -> (12,11,23) P32 -> (31,23,33) and so on 4) Here we will end up with (3*4, 3) matrix. 5) Kmeans clustering on this dataset will give us a set of centroids. Color associated with each centroid will be the color by which the respective cluster will be identified.

In [12]:
```
def compressor(pic:np.ndarray,k:int):
    """
    inputs :
        pic : original image matrix of the form (h,w,c)
        k   : number of clusters
    output : compressed image
    """
    if len(pic.shape)==2: #greyscale images
        h,w = pic.shape
        c =1
    else:
        h,w,c = pic.shape
    pic = pic.reshape(h*w,c)
    centroids, buckets_idx = kmeans(pic,k=k, centroids='kmeans++')
    new_img_arr = centroids[buckets_idx].astype('uint8')
    if c==1:
        new_img_matrix = new_img_arr.reshape(h,w)
    else:
        new_img_matrix = new_img_arr.reshape(h,w,c)
    return Image.fromarray(new_img_matrix)
```

In [13]:

```
#image import
im = Image.open('messi.jpg')
pic_array = np.asarray(im)
h,w,c = pic_array.shape
uniq_colors = len(np.unique(pic_array.reshape(h*w,c)))
print(f"number of unique colours in this picture is {uniq_colors}")
im
```

```
number of unique colours in this picture is 256
```

Out[13]:

In [14]:
```
#compressed image
compressed_pic = compressor(pic_array,20)
pic_array = np.asarray(compressed_pic)
h,w,c = pic_array.shape
uniq_colors = len(np.unique(pic_array.reshape(h*w,c)))
print(f"number of unique colours in this picture is {uniq_colors}")
compressed_pic
```

```
number of unique colours in this picture is 48
```

Out[14]:

In [15]:

```
#grey scale images
im = Image.open('north-africa-1940s-grey.png')
pic_array = np.asarray(im)
im
```

Out[15]:

In [16]:
```
compressed_pic = compressor(pic_array,4)
compressed_pic
```

Out[16]:

Other applications of kmeans clustering could be in extension to a variety of deep learning algorithms. Once we have the embeddings we can treat them as vectors in n-dimensional space and apply kmeans to get similarity between the data points. This acts as a very important tool to analyse a dataset that we know nothing about.