01 - Unsupervised Learning - Clustering - K-Means(Solution)_st122097_thantham

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1 Programming for Data Science and Artificial Intelligence

1.1 Unsupervised Learning - Clustering - K-Means

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1.3.1 ===Task===

Your work: Let's modify the above scratch code: - Modify so it **print out the total within-cluster variation**.
- Then try to **run several k and identify which k is best.** - Since k-means can be slow due to its pairwise computations, let's implement a **mini-batch k-means** in which the cluster is create using only partial subset of samples. - Put everything into a class

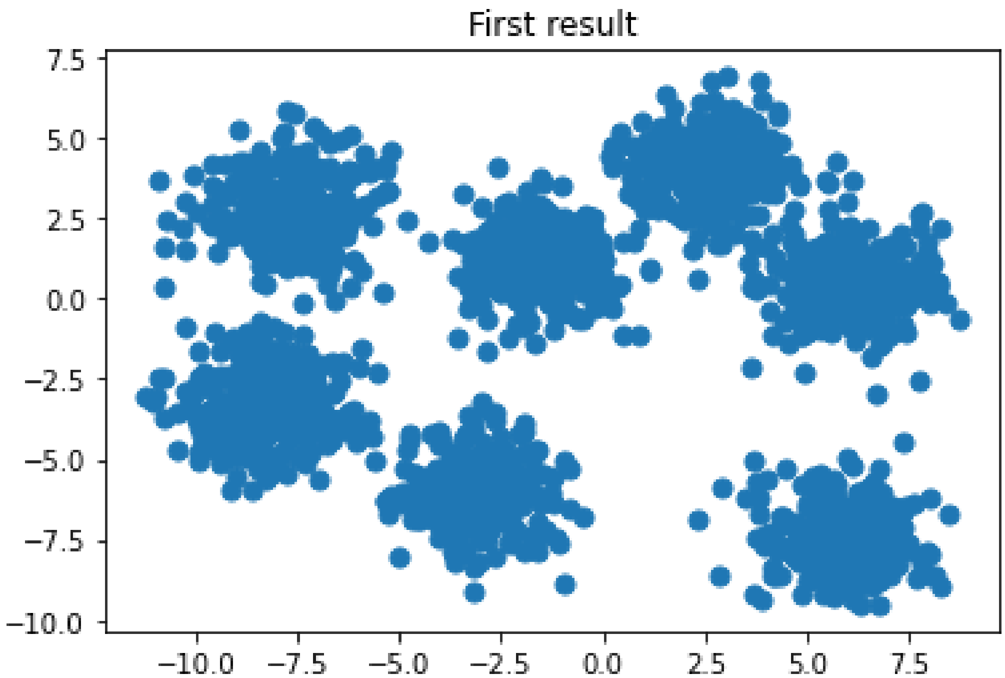
First of all, lets import neccessary and library, then make some clusters sample data for illustrate how Kmean clustering result.

[1]:
```
import numpy as np
#Implement K-means from scratch
from sklearn.datasets import make_blobs
from sklearn.metrics import pairwise_distances_argmin
from time import time
import matplotlib.pyplot as plt

X, y_true = make_blobs(n_samples=2000, centers=7,
                       cluster_std=1.0, random_state=999)

plt.figure()
plt.scatter(X[:, 0], X[:, 1], s=50)
plt.title("First result")
```

[1]:
```
Text(0.5, 1.0, 'First result')
```



From tutorial, this lab work increase more challage to make 7 clusters with 2000 samples (for mini-batching purpose) and more std upto 1.0. But define random state ar 999 because it produced very beautiful clusters

1.4 Task: KMean clustering class

[2]:
```
import numpy as np
from sklearn.metrics import pairwise_distances_argmin
import time

class Kmeans:

    def __init__ (self, n_clusters=4, tol=1e-2, random_state=None,␣
 ↪max_iters=100, batch_size=None):

        self.n_clusters = n_clusters
        self.rtol = tol
        self.max_iters = max_iters
        self.random_state = random_state

        if not isinstance(batch_size, int) and not isinstance(batch_size,␣
 ↪float) and batch_size is not None:
            raise ValueError('batch_size should be float or int')
```

```
        self.batch_size = batch_size



    def fit(self, X):

        # Initialize Training params␣
↪-----------------------------------------------------------------------------
        m,n = X.shape

        rng = np.random.RandomState(self.random_state) # define random state

        idx_rand_centroids = rng.permutation(m)[:self.n_clusters] # random idx␣
↪from X points as initial centroids

        previous_centroids = X[idx_rand_centroids] # define initial centroids

        iteration = 0 # start loop counter

        # ------------------ Check if batch_size is not define (batch) or␣
↪define (int as sampling, float as ratio)
        if self.batch_size is None: # if batch_size is None

            self.batch_size = m # this is full batch

        elif isinstance(self.batch_size, float): # if batch_size is float␣
↪(ratio)

            self.batch_size = int(self.batch_size * m) # calc number define for␣
↪ratio

        start_time = time.time()

        # Traing the␣
↪centers------------------------------------------------------------------------------
        while iteration < self.max_iters: # While iters not reach maximum

            idx_start_batch = 0 if self.batch_size == m else rng.randint(m-self.
↪batch_size) # define idx of batch

            X_batch = X[idx_start_batch:idx_start_batch+self.batch_size] #␣
↪define batch set

            labels = pairwise_distances_argmin(X_batch, previous_centroids) #␣
↪get nearest centers for each X point
```

```python
            new_centroids = np.asarray([X_batch[labels == i].mean(axis=0) for i in range(self.n_clusters)])

            # Check wheter new cluster and old cluster are nearby together under defined tolerance
            if(np.allclose(previous_centroids, new_centroids, rtol=self.rtol)):
                # if closed -> break
                break

            previous_centroids = new_centroids

            iteration+=1

        # ------------- After training ------------------------------------------------------------------

        self.centroids = previous_centroids # save current centroids

        sum_var_score = 0 # init total variation

        X_clusters_labels = pairwise_distances_argmin(X, self.centroids) # use all X for check variation

        for cluster_i in range(self.n_clusters): # each cluster

            cluster_i_mean = X[X_clusters_labels==cluster_i].mean(axis=0) # get idx within cluster i

            #calc total sumsquare for current class
            sum_var_score += ((X[X_clusters_labels==cluster_i] - cluster_i_mean)** 2).sum()

        self.total_variance_score = sum_var_score

        # -------------------------------- Just imform wheter reach max iteration or not
        if iteration == self.max_iters:
            print(f"!!! Reached max iteration! ({iteration}) within {round(time.time()-start_time,5)} seconds")
        else:
            print(f"Done in {iteration} iterations within {round(time.time()-start_time,5)} seconds")

    def predict(self, X):
```

```
        return pairwise_distances_argmin(X, self.centroids) # Simply calculate␣
↪distance and get nearest centroid label
```

Code may be unreadable for some reason because it was relied on my perspective to build them.

1.5 Task: Test the model with printing out Total cluster variation

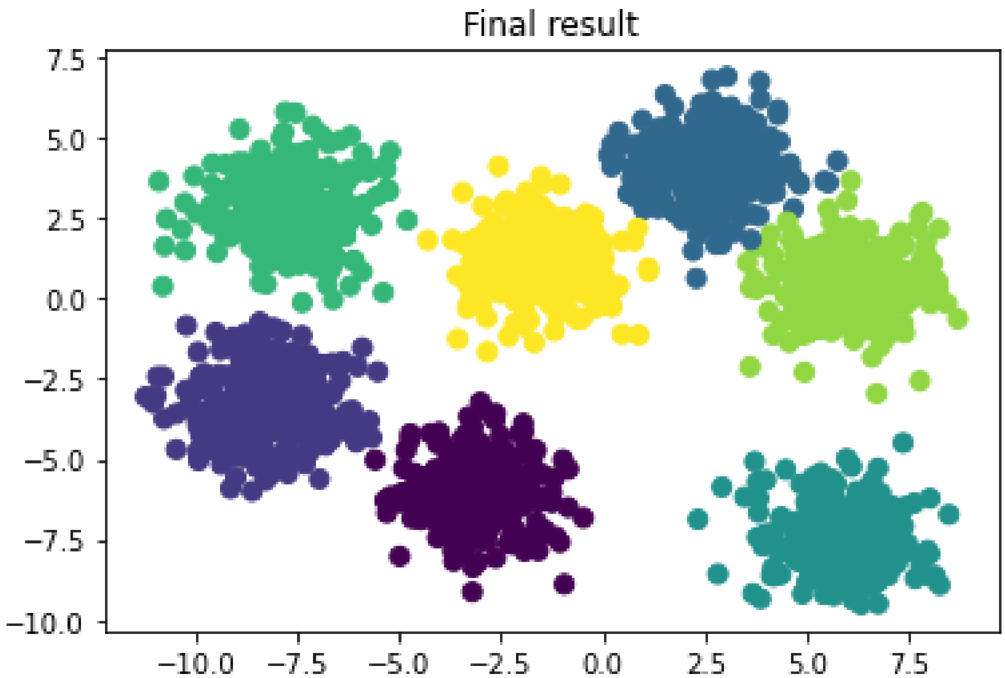
before that, this step is just simply do clustering with simple model parameters. I also defined max iterations in case the model couldnot found optimal centriods. tolerance will be used in np.allclose method. For Mini-Batch purpose, just define some integer or fraction floating number to activate batch size ratio, otherwise, False option will automatically activate Batch mode (train all samples). Fianlly, I just fix random state to stabilize the result

[3]:
```
model = Kmeans(n_clusters=7, max_iters=10000, tol=1e-12, batch_size=None,␣
↪random_state=1)
model.fit(X)
preds = model.predict(X)
print(f'Total variation score: {model.total_variance_score}')
```

```
Done in 3 iterations within 0.00997 seconds
Total variation score: 4040.0734142610786
```

[4]:
```
plt.figure()
plt.scatter(X[:, 0], X[:, 1], c=preds, s=50)
plt.title("Final result")
```

[4]:
```
Text(0.5, 1.0, 'Final result')
```



The result should be exactly prefect because we know certain number of clusters.

1.6 Task: Iterative training by Range of K With Mini-Batch Implementation

Nevertheless, What if we dont know K (unknown domain knowledge). We should eun several k and occupie them to plot total cluster variation each k trained

[5]:
```
pred_list = []
centroids_list = []
variation_list = []

for i in range(2, 13):

    model_i = Kmeans(n_clusters=i, tol=1e-5, max_iters=10000, batch_size=0.2,␣
 ↪random_state=1)
    model_i.fit(X)
    print(f'At K = {i} got total variation score: {round(model_i.
 ↪total_variance_score,3)}')

    pred_list.append(model_i.predict(X))
    centroids_list.append(model_i.centroids)
    variation_list.append(model_i.total_variance_score)

    print()
```

```
Done in 3636 iterations within 1.52399 seconds
At K = 2 got total variation score: 49047.223

Done in 1249 iterations within 0.54565 seconds
At K = 3 got total variation score: 29391.771

!!! Reached max iteration! (10000) within 4.91952 seconds
At K = 4 got total variation score: 17939.927

Done in 4427 iterations within 2.42301 seconds
At K = 5 got total variation score: 13241.602

Done in 1249 iterations within 0.85273 seconds
At K = 6 got total variation score: 7378.126

Done in 1249 iterations within 1.3715 seconds
At K = 7 got total variation score: 4040.212

Done in 2512 iterations within 2.07822 seconds
At K = 8 got total variation score: 3829.059

!!! Reached max iteration! (10000) within 6.52754 seconds
At K = 9 got total variation score: 3675.18

!!! Reached max iteration! (10000) within 6.18651 seconds
At K = 10 got total variation score: 3459.872

!!! Reached max iteration! (10000) within 6.28161 seconds
At K = 11 got total variation score: 3254.261

!!! Reached max iteration! (10000) within 6.90404 seconds
At K = 12 got total variation score: 3070.427
```

After training, we predict the class of each clusters

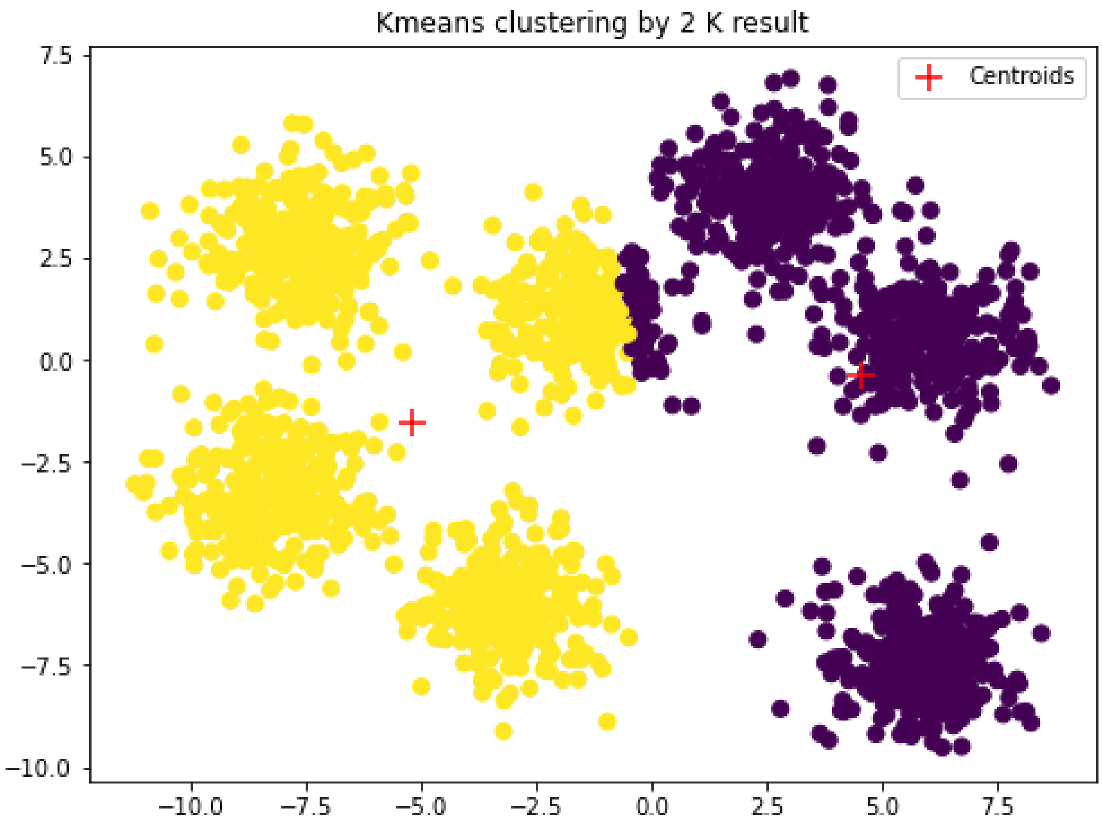
[6]:
```python
pred_list = np.asarray(pred_list)
```

Now, we can plot the scatter points with each centroid separating each k

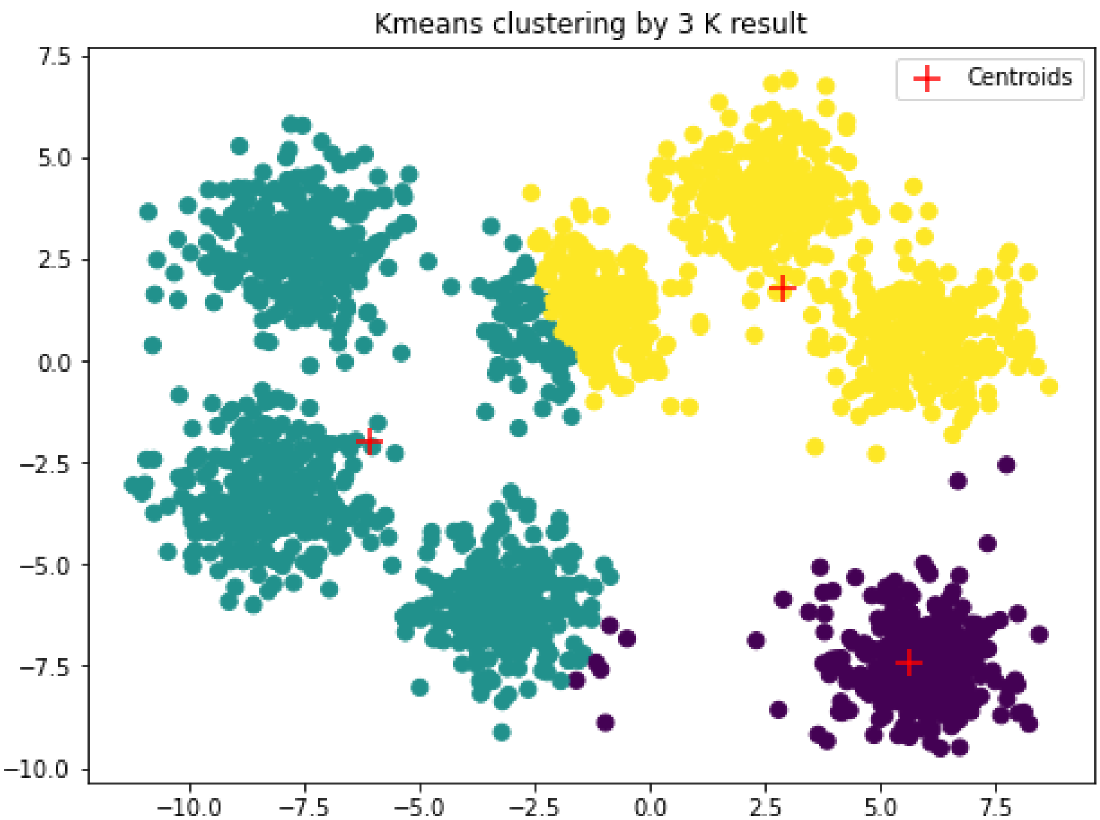
[7]:
```python
for i in range(len(pred_list)):

    plt.figure(figsize=(8,6))
    plt.scatter(X[:, 0], X[:, 1], c=pred_list[i], s=50)
    plt.scatter(centroids_list[i][:,0], centroids_list[i][:,1], c='red',s=150,␣
 ↪marker='+', label='Centroids')
    plt.legend()
    plt.title(f"Kmeans clustering by {i+2} K result")
```

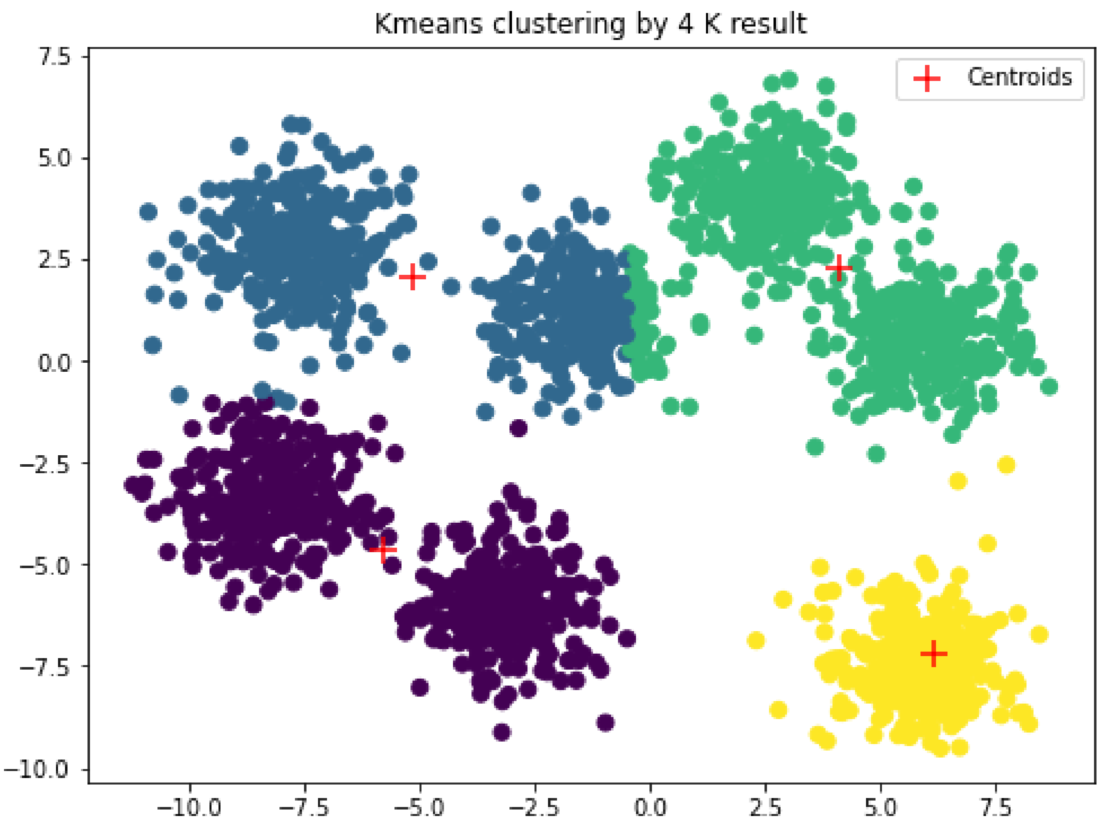
```
plt.show()
```



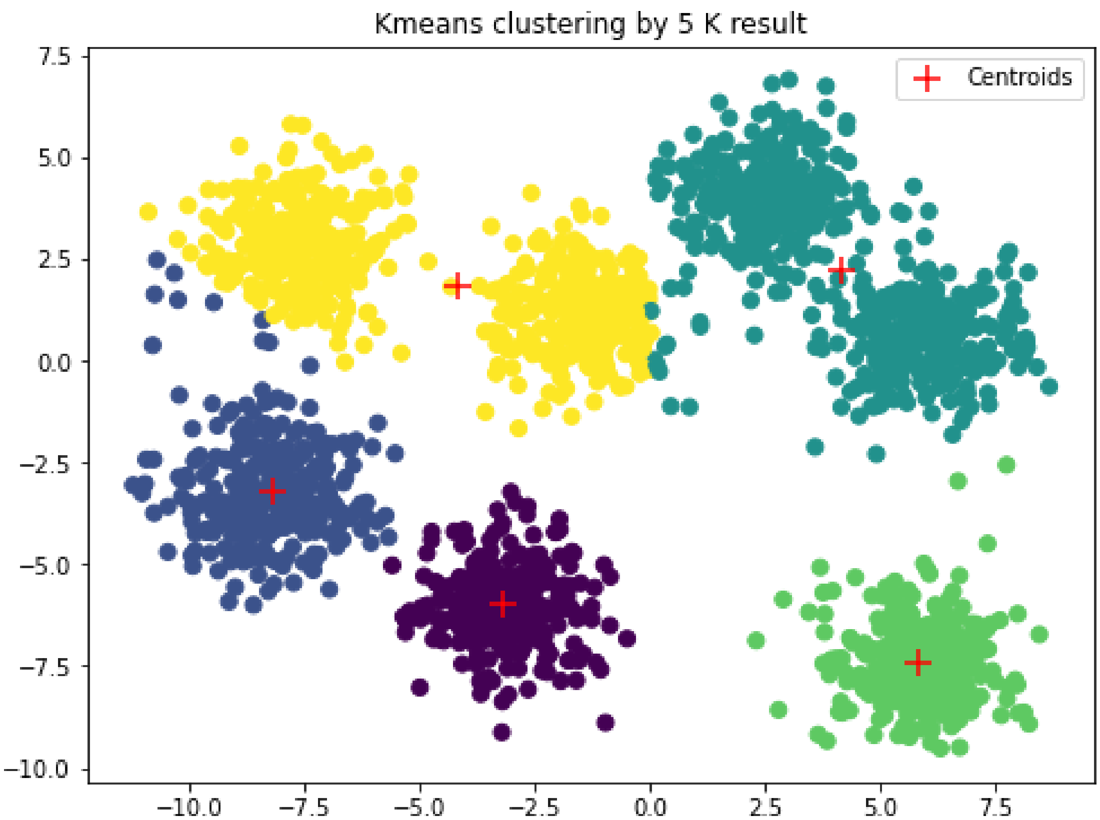
Kmeans clustering by 2 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5



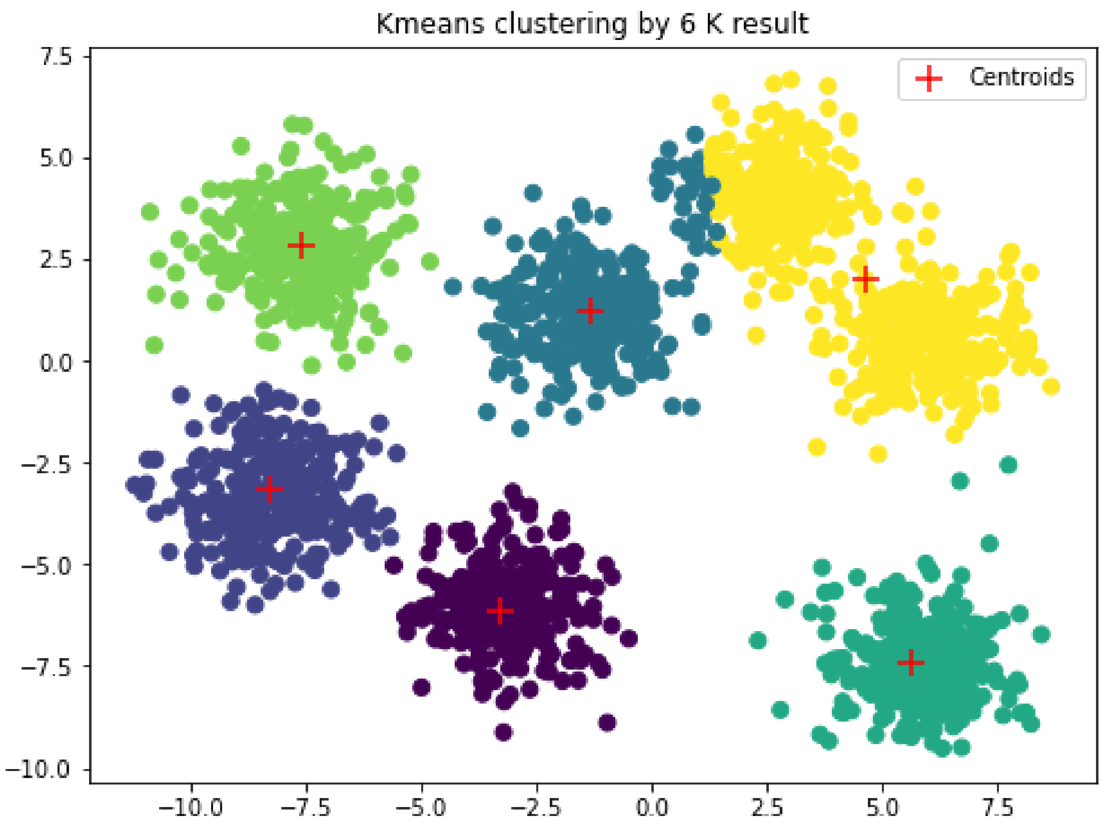
Kmeans clustering by 3 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5

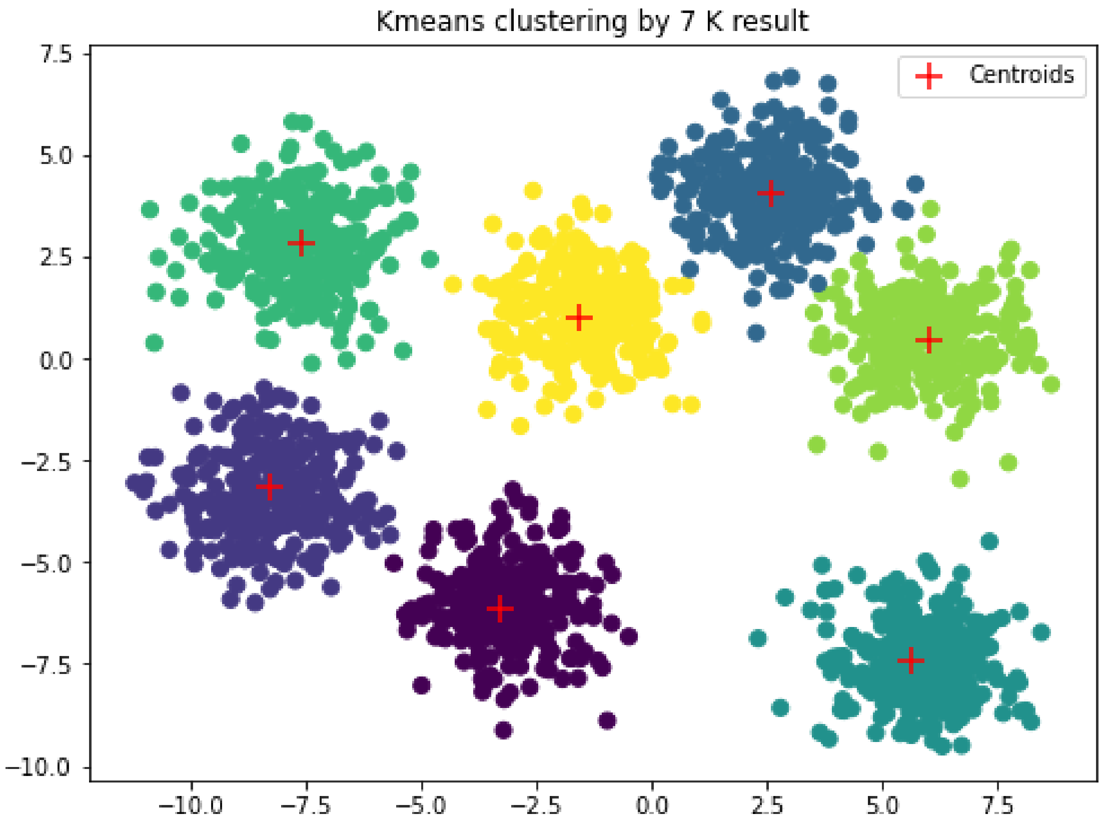


Kmeans clustering by 4 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5

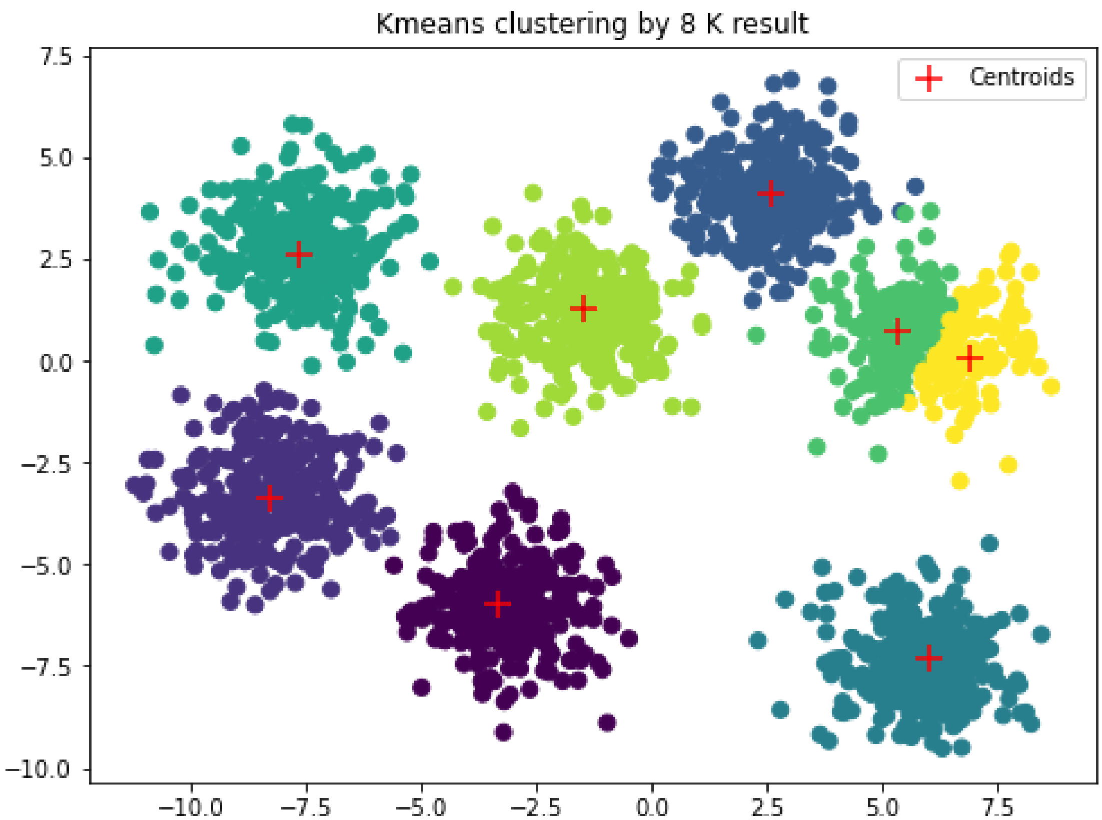


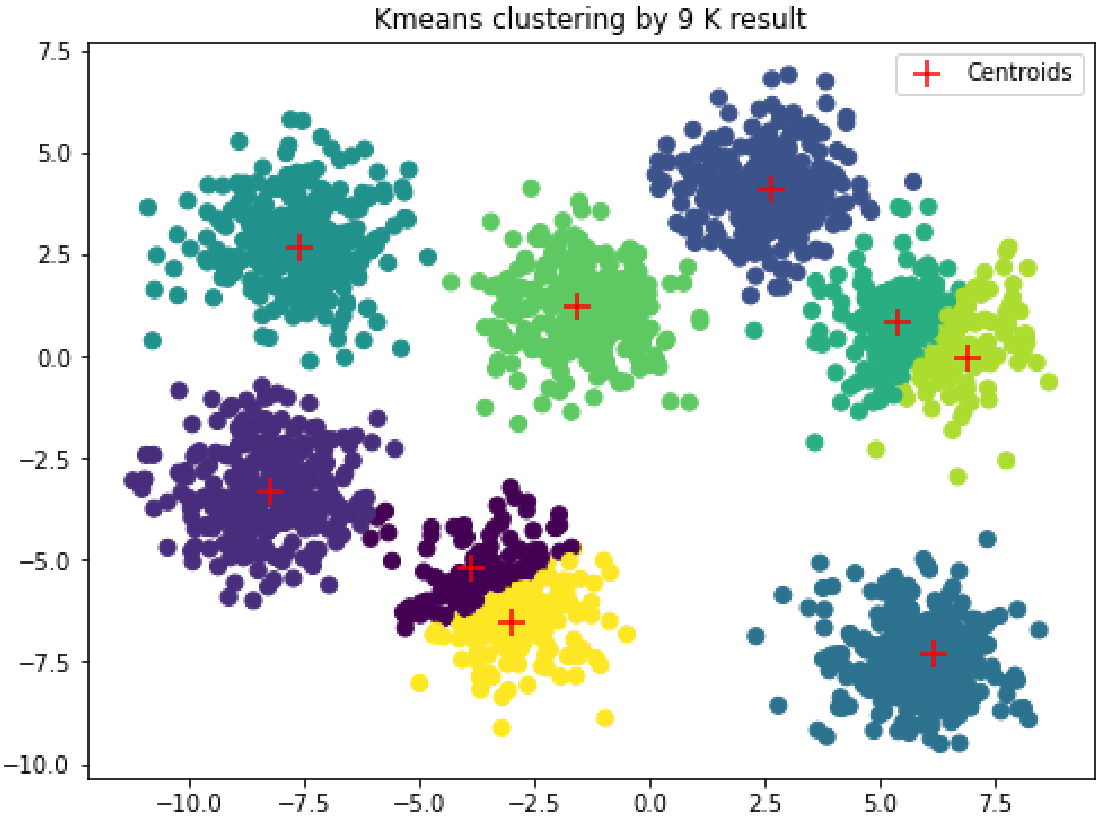
Kmeans clustering by 5 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5


Kmeans clustering by 6 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5

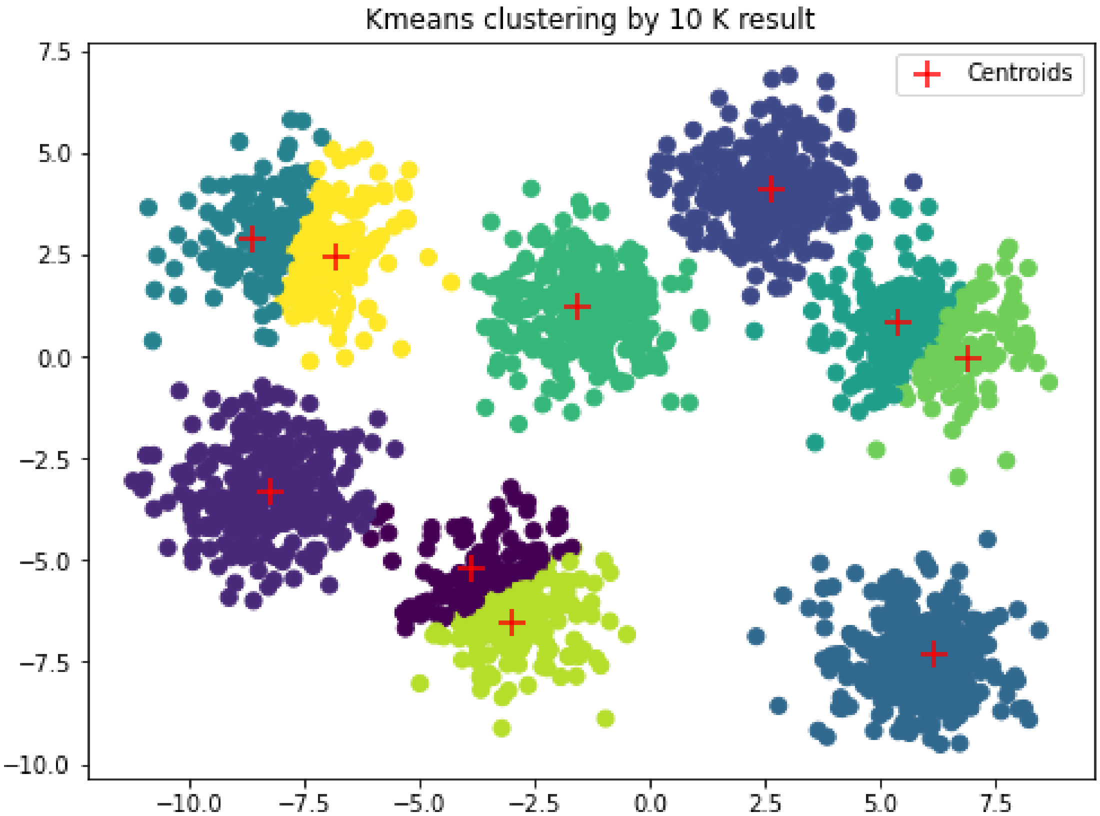


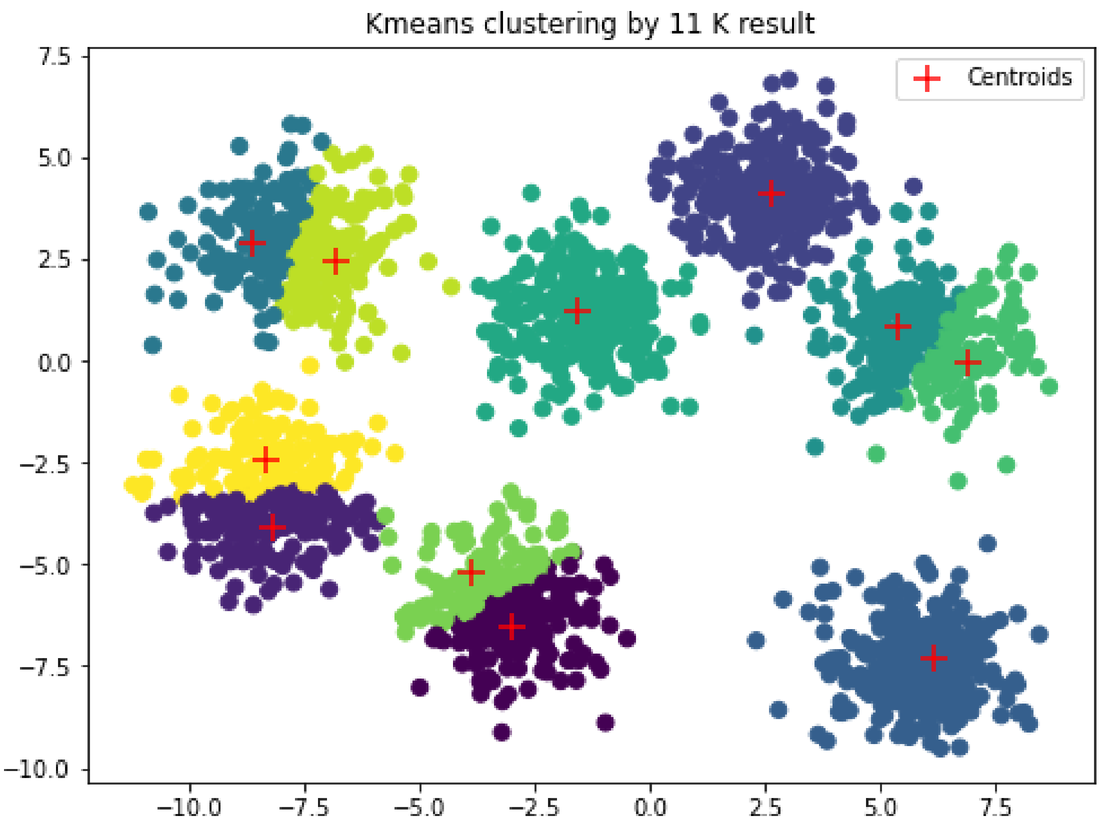
Kmeans clustering by 7 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5

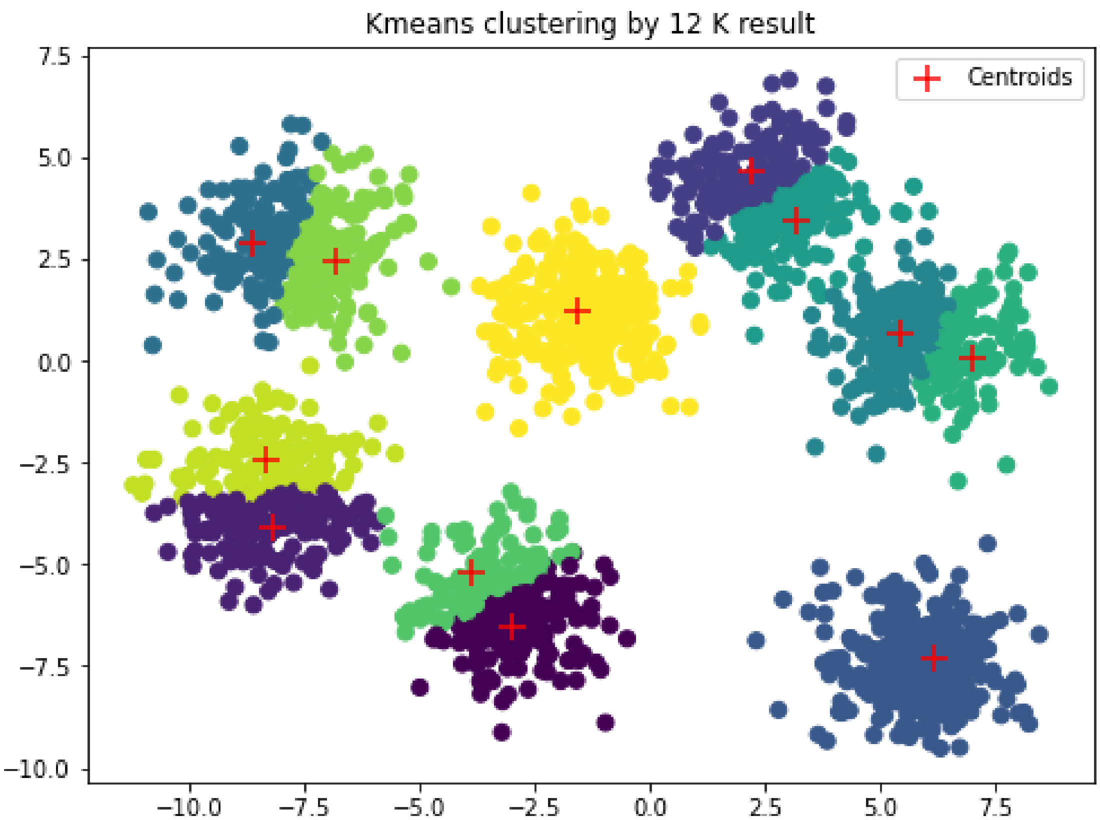

Kmeans clustering by 8 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5



Kmeans clustering by 9 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5

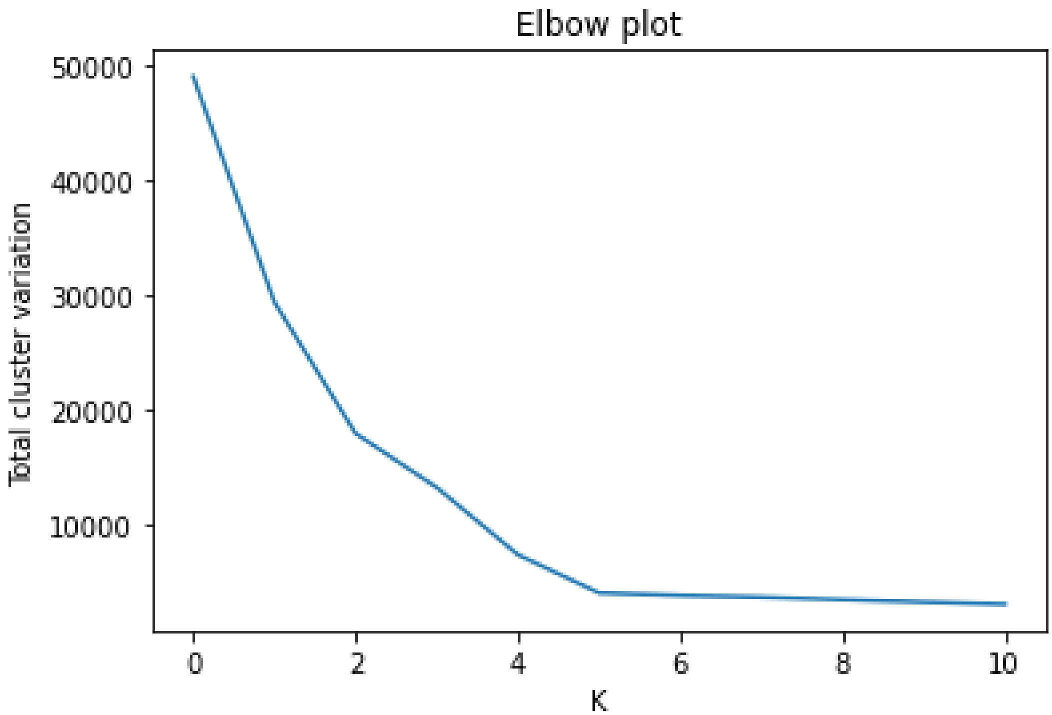

Kmeans clustering by 10 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5


Kmeans clustering by 11 K result
Centroids
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5



If we rounghly see the results, it should be exactly that k = 7 should be the best because it discrimated all clusters perfectly. but however, if we plot the **Elbow plot** what will be

[8]:
```
plt.plot(variation_list)
plt.title('Elbow plot')
plt.xlabel('K')
plt.ylabel('Total cluster variation')
plt.show()
```



We will examine that the near-minimum total variation will be around 5 clusters which may not be true! alhtough 7 is correct one.

This is the reason why **Domain Knowledge is important!!** to define suitable number of k implemented in real world project

```
[ ]:
```