k-Means Clustering

In this notebook, you will implement the k-means clustering algorithm.

Packages

Following packages is all you need. Do not import any additional packages!

In case you are not familiar with Numpy library, it provides support for large multi-dimensional arrays and matrices, along with functions to operate on these. Matplotlib is a plotting library.

In [ ]:
```
import numpy as np
%matplotlib inline
from matplotlib import pyplot as plt
```

Function

A function for plotting that we are going to use later on.

In [ ]:
```
def plot_clusters(data, centroids):
    """
    Shows a scatter plot with the data points clustered according to the centroids.
    """
    # Assigning the data points to clusters/centroids.
    clusters = [[] for _ in range(centroids.shape[0])]
    for i in range(data.shape[0]):
        distances = np.linalg.norm(data[i] - centroids, axis=1)
        clusters[np.argmin(distances)].append(data[i])

    # Plotting clusters and centroids.
    fig, ax = plt.subplots()
    for c in range(centroids.shape[0]):
        if len(clusters[c]) > 0:
            cluster = np.array(clusters[c])
            ax.scatter(cluster[:, 0], cluster[:, 1], s=7)
    ax.scatter(centroids[:, 0], centroids[:, 1], marker='x', s=200, c='red')
```

Data

Let us generate a dataset you are going to play with. We will stay in the Euclidean space because it is easy to plot.

In [ ]:
```
# We would like to have some control over the randomly generated data.
# This is just for development purposes.
np.random.seed(0)

# Euclidean space.
DIMENSIONS = 2
```

```
# We will generate clusters.
CLUSTERS = [
    {
        'mean': (50, 50),
        'std': (5, 10),
        'size': 300
    },
    {
        'mean': (10, 85),
        'std': (10, 3),
        'size': 100
    },
    {
        'mean': (10, 10),
        'std': (6, 6),
        'size': 200
    },
    {
        'mean': (10, 75),
        'std': (10, 5),
        'size': 200
    },
    {
        'mean': (80, 20),
        'std': (5, 5),
        'size': 100
    }
]

# Initializing the dataset with zeros.
synthetic_data = np.zeros((np.sum([c['size'] for c in CLUSTERS]), DIMENSIONS))

# Generating the clusters.
start = 0
for c in CLUSTERS:
    for d in range(DIMENSIONS):
        synthetic_data[start:start + c['size'], d] = np.random.normal(c['mean'][d], c['
    start += c['size']
print(synthetic_data)
```

```
[[58.82026173 36.93473148]
 [52.00078604 66.5813068 ]
 [54.89368992 48.81835955]
 ...
 [80.85621773 20.91725127]
 [80.19454353 17.64628751]
 [83.13282125 21.36398195]]
```

In [ ]:

```
print('shape (size, dimensions) =', synthetic_data.shape)
```

```
shape (size, dimensions) = (900, 2)
```

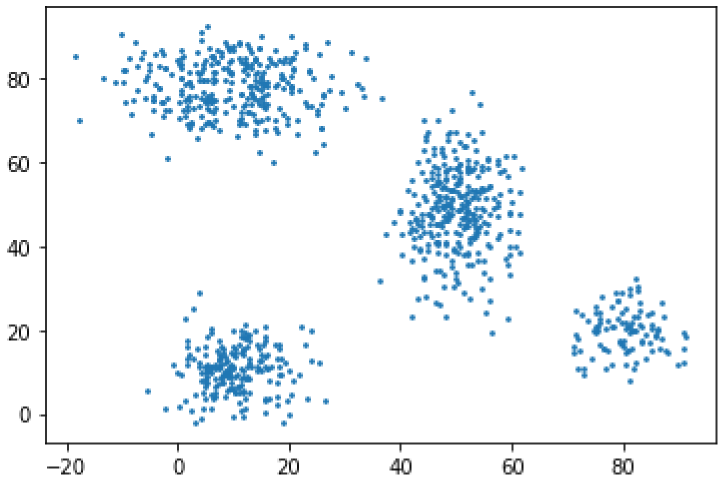
And this is how our data look like when plotted.

In [ ]:

```
plt.figure()
plt.scatter(synthetic_data[:, 0], synthetic_data[:, 1], s=3)
```

```
<matplotlib.collections.PathCollection at 0x7f9b9f606910>
```

Out[ ]:



Implementation

A human can with an ease find five distinct clusters just by watching the plot. A computer, however, needs to be told how to find the clusters.

Exercise:

Implement the k-means clustering algorithm.

- Use the Euclidean (L_2) distance.
- It is sufficient to use the basic Python constructs in your implementation, even though we heavily rely on Numpy throughout this assignment.

In [ ]:

```
def euchlidean_l2(a, b):
    return np.sum(np.sqrt(np.square(a - b)), axis=1)

def kmeans(data, centroids):
    """
    Function implementing the k-means clustering.

    :param data
        data
    :param centroids
        initial centroids
    :return
        final centroids
    """
    ### START CODE HERE ###
    euch_dist = np.zeros((data.shape[0], centroids.shape[0]))
    old_centroids = centroids.copy()

    while True:
        next_iteration_centroids = old_centroids.copy()
        for i in range(next_iteration_centroids.shape[0]):
            euch_dist[:, i] = euchlidean_l2(data, next_iteration_centroids[i])
            # euch_dist[:, i] = np.linalg.norm((data - next_iteration_centroids[i]), ax
        cluster_points = np.zeros((data.shape[0], next_iteration_centroids.shape[0]))
        min_dist = np.amin(euch_dist, axis=1)
```

```
        for i in range(next_iteration_centroids.shape[0]):
            cluster_points[:, i] = euch_dist[:, i] == min_dist

        for i in range(next_iteration_centroids.shape[0]):
            next_iteration_centroids[i] = np.mean(data[cluster_points[:, i] == 1], axis

        if np.all(old_centroids - next_iteration_centroids) == 0:
            centroids = next_iteration_centroids
            break

        old_centroids = next_iteration_centroids.copy()



    ### END CODE HERE ###
    return centroids
```

We have prepared for you a small piece of code, so that you can test that the function works according the expectations.

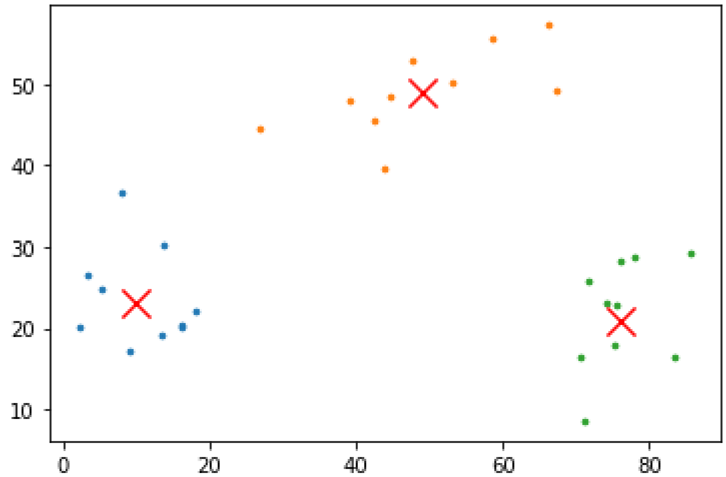
In [ ]:

```
test_data = np.array([
    [66.24345364, 57.31053969],
    [43.88243586, 39.69929645],
    [44.71828248, 48.38791398],
    [39.27031378, 48.07972823],
    [58.65407629, 55.66884721],
    [26.98461303, 44.50054366],
    [67.44811764, 49.13785896],
    [42.38793099, 45.61070791],
    [53.19039096, 50.21106873],
    [47.50629625, 52.91407607],
    [2.29566576, 20.15837474],
    [18.01306597, 22.22272531],
    [16.31113504, 20.1897911],
    [13.51746037, 19.08356051],
    [16.30599164, 20.30127708],
    [5.21390499, 24.91134781],
    [9.13976842, 17.17882756],
    [3.44961396, 26.64090988],
    [8.12478344, 36.61861524],
    [13.71248827, 30.19430912],
    [74.04082224, 23.0017032],
    [70.56185518, 16.47750154],
    [71.26420853, 8.57481802],
    [83.46227301, 16.50657278],
    [75.25403877, 17.91105767],
    [71.81502177, 25.86623191],
    [75.95457742, 28.38983414],
    [85.50127568, 29.31102081],
    [75.60079476, 22.85587325],
    [78.08601555, 28.85141164]
])
test_centroids = np.array([
    [25, 50],
    [50, 50],
    [75, 50]
])
```

```
test_centroids = kmeans(test_data, test_centroids)

print('c0 =', test_centroids[0])
print('c1 =', test_centroids[1])
print('c2 =', test_centroids[2])
plot_clusters(test_data, test_centroids)
```

```
c0 = [10 23]
c1 = [49 49]
c2 = [76 21]
```



We expect the output to be similar to following.

```
c0 = [ 9 25]
c1 = [50 50]
c2 = [75 20]
```

If it is not the case, review your implementation, debug your algorithm, try it on paper, ...

Clustering

Ready to run your implementation of k-means clustering on the dataset? Let's do it...

First, we need to initialize the centroids. We will go for a random initialization eventhough there are some disadvantages of doing so (see the Introduction to Data Mining from Tan et al.).

In [ ]:

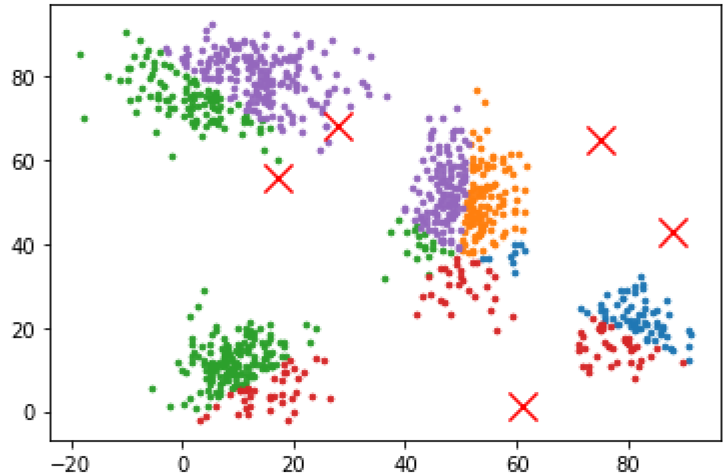
```
# Number of clusters.
K = 5

# Boundaries of our data.
x_min = np.min(synthetic_data[:, 0])
x_max = np.max(synthetic_data[:, 0])
y_min = np.min(synthetic_data[:, 1])
y_max = np.max(synthetic_data[:, 1])

# Generating random centroids within the data boundaries.
centroids = np.zeros((K, synthetic_data.shape[1]))
centroids[:, 0] = np.random.randint(x_min, x_max, size=K)
centroids[:, 1] = np.random.randint(y_min, y_max, size=K)
```

```python
for i in range(len(centroids)):
    print('c%d =' % i, centroids[i])
plot_clusters(synthetic_data, centroids)
```

```
c0 = [88. 43.]
c1 = [75. 65.]
c2 = [17. 56.]
c3 = [61.  1.]
c4 = [28. 68.]
```



Finally, we run the `kmeans()` function you have implemented.

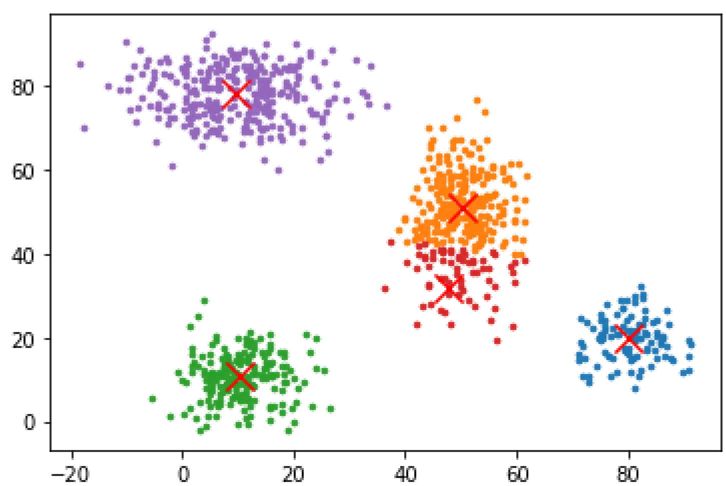
In [ ]:

```python
centroids = kmeans(synthetic_data, centroids)

# plt.scatter(data[:, 0], data[:, 1], s=3)
# plt.scatter(centroids[:, 0], centroids[:, 1], marker='x', s=200, c='red')

for i in range(len(centroids)):
    print('c%d =' % i, centroids[i])
plot_clusters(synthetic_data, centroids)
```

```
c0 = [80.11686062 19.69811265]
c1 = [50.4164693 50.9436439]
c2 = [10.40705505 10.57646643]
c3 = [47.77429001 31.88522513]
c4 = [ 9.55339231 78.22785577]
```



Congratulations! At this point, hopefully, you have found all five distinct clusters with the centroids aligned in their centers.

Evaluation of Clustering

Silhouette Coefficient is an example of a measure for validation of the cluster quality.

Exercise:

Implement a function calculating the mean Silhouette Coefficient of all samples.

- Use the Euclidean (L_2) distance.
- It is sufficient to use the basic Python constructs in your implementation, even though we heavily rely on Numpy throughout this assignment.

In [ ]:
```
def silhouette_score(data, centroids):
    """
    Function implementing the k-means clustering.

    :param data
        data
    :param centroids
        centroids
    :return
        mean Silhouette Coefficient of all samples
    """
    ### START CODE HERE ###
    euch_dist = np.zeros((data.shape[0], centroids.shape[0]))
    silhoutte_scores = np.zeros(data.shape[0])
    for i in range(centroids.shape[0]):
        euch_dist[:, i] = euchlidean_l2(data, centroids[i])

    cluster_points = np.zeros((data.shape[0], centroids.shape[0]))
    min_dist = np.amin(euch_dist, axis=1)

    for i in range(centroids.shape[0]):
        cluster_points[:, i] = euch_dist[:, i] == min_dist

    for i in range(centroids.shape[0]):
        this_cluster_points = data[cluster_points[:, i] == 1]
        avg_this_cluster_point_dist = np.zeros(this_cluster_points.shape[0])
        for point in range(this_cluster_points.shape[0]):
            avg_this_cluster_point_dist[point] = np.mean(euchlidean_l2(this_cluster_poi

        dist_to_other_cluster_points = np.zeros(this_cluster_points.shape[0])
        for point in range(this_cluster_points.shape[0]):
            dist_to_other_cluster_points[point] = float("inf")
            for j in range(centroids.shape[0]):
                if(i == j):
                    continue
                other_cluster_points = data[cluster_points[:, j] == 1]
                dist_to_other_cluster = np.mean(euchlidean_l2(this_cluster_points[point
                if dist_to_other_cluster < dist_to_other_cluster_points[point]:
                    dist_to_other_cluster_points[point] = dist_to_other_cluster

        a = avg_this_cluster_point_dist
```

```
        b = dist_to_other_cluster_points
        silhoutte_scores[cluster_points[:, i] == 1] = (b - a)/np.maximum(a, b)

    score = np.mean(silhoutte_scores)



    ### END CODE HERE ###
    return score
```

First, let's see if the algorithm executes on the test data.

In [ ]:

```
silhouette_score(test_data, test_centroids)
```

Out[ ]:

```
0.7249437983722198
```

We expect the output to be around `0.675` .

Finally, let's cluster again our synthetic data and calculate the Silhouette Coefficient.

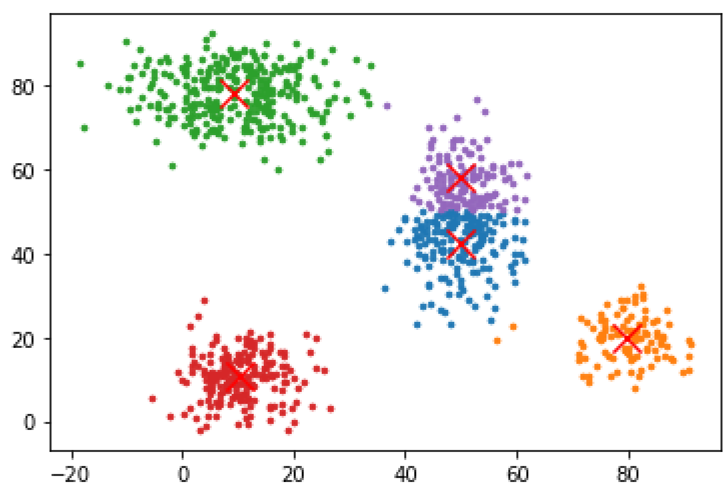
In [ ]:

```
centroids = np.zeros((K, synthetic_data.shape[1]))
centroids[:, 0] = np.random.randint(x_min, x_max, size=K)
centroids[:, 1] = np.random.randint(y_min, y_max, size=K)

centroids = kmeans(synthetic_data, centroids)
silhouette_coefficient = silhouette_score(synthetic_data, centroids)

print('silhouette_coefficient =', silhouette_coefficient)
plot_clusters(synthetic_data, centroids)
```

```
silhouette_coefficient = 0.6288985346520989
```



Exercise:

- Run the clustering multiple times and pay attention to the results.
- In the *Discussion* below, describe your observations and discuss reasons for the possibly strong or weak performance of the algorithm. If you identify any weaknesses, suggest a possible solution.

Discussion

Multiple executions reveal the varying clustering quality. This is due to the randomly initialized centroids and the sensitivity of the k-means algorithm to it. I.e. the cluster quality depends highly on the initial centroids.

Comments

Our k-means clustering implementation can be characterized as a naive. This is for following reasons:

- We are evaluating only one `k` value instead of trying multiple.
- We are initializing the centroids randomly instead of using some heuristic.
- We are initializing and evaluating only one set of centroids instead of initializing multiple sets and analyzing their SSE (Sum of Squared Errors) or Silhouette Coefficient.

✌️

In [ ]:

```
```