

#### 4. Clustering

**Update centroid.** We define a function to update the centroid after the group assignment, returning a new list of group centroids.

```
In [ ]: def update_centroid(data, grouping, centroids):
    new_centroids = []
    for i in range(len(centroids)):
        cent = np.zeros(len(data[0]))
        count = 0
        for j in range(len(data)):
            if grouping[j] == (i+1):
                cent = cent+data[j]
                count += 1
        group_average = cent/count
        new_centroids.append(group_average)
    return new_centroids
```

**Clustering objective.** Given the group assignment and the centroids with the data, we can compute the clustering objective as the square of the RMS value of the vector of distances.

```
In [ ]: def clustering_objective(data, grouping, centroids):
    J_obj = 0
    for i in range(len(data)):
        for j in range(len(centroids)):
            if grouping[i] == (j+1):
                J_obj += np.linalg.norm(data[i] - centroids[j])**2
    J_obj = J_obj/len(data)
    return J_obj
```

### 4.3. The $k$ -means algorithm

We can define another function `Kmeans_alg` that uses the three functions defined in the above subsection iteratively.

```
In [ ]: def Kmeans_alg(data, centroids):
    iteration = 0
    J_obj_vector = []
    Stop = False
    while Stop == False:
        grouping = group_assignment(data, centroids)
```

```

new_centroids = update_centroid(data, grouping, centroids)
J_obj = clustering_objective(data, grouping,
    ↪ new_centroids)
J_obj_vector.append(J_obj)
iteration += 1
if np.linalg.norm(np.array(new_centroids) -
    ↪ np.array(centroids)) < 1e-6:
    Stop = True
else:
    centroids = new_centroids
return new_centroids, grouping, J_obj_vector, iteration

```

**Convergence.** Here we use a `while` loop, which executes the statements inside the loop as long as the condition `Stop == False` is true. We terminate the algorithm when the improvement in the clustering objective becomes very small ( $1e-6$ ).

Alternatively, we can use the `Kmeans` function in the `cluster` module of the `sklearn` package.

```

In [ ]: from sklearn.cluster import KMeans
import numpy as np
kmeans = KMeans(n_clusters=4, random_state=0).fit(data)
labels = kmeans.labels_
group_representative = kmeans.cluster_centers_
J_clust = kmeans.inertia_

```

Here we try to apply the  $k$ -means algorithm on `data`, clustering the vectors into 4 groups. Note that the `sklearn.cluster.KMeans` function initialize the algorithms with random centroids and thus the initial values of centroids are not required as an argument but the random state to draw the random initialization is.

## 4.4. Examples

We apply the algorithm on a randomly generated set of  $N = 300$  points, shown in Figure 4.1. These points were generated as follows.

```

In [ ]: import matplotlib.pyplot as plt
plt.ion()

```