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Business Analytics & Machine Learning
Tutorial sheet 8: Clustering – Solution

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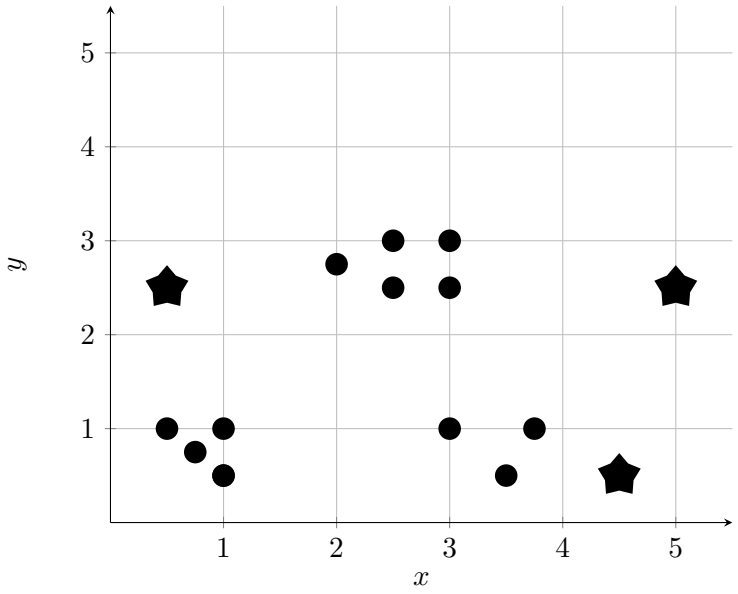
Exercise T8.1 *k-means*

Group the following data into three clusters applying the k-Means algorithm and the Euclidean distance function.



i	x_i	y_i
1	2.5	3
2	3	3
3	2	2.75
4	2.5	2.5
5	3	2.5
6	0.5	1
7	1	1
8	3	1
9	3.75	1
10	0.75	0.75
11	1	0.5
12	3.5	0.5

Table 1 Dataset

i	x_i	y_i
A	0.5	2.5
B	5	2.5
C	4.5	0.5

Table 2 Initial Centroids

Solution

1. Assign instances to the nearest cluster center: see Table 3.

i	x_i	y_i	Assigned Cluster Center
1	2.5	3	A
2	3	3	B
3	2	2.75	A
4	2.5	2.5	A
5	3	2.5	B
6	0.5	1	A
7	1	1	A
8	3	1	C
9	3.75	1	C
10	0.75	0.75	A
11	1	0.5	A
12	3.5	0.5	C

Table 3 Iteration I: Instance Assignments

2. Update cluster centers: see Table 4.

i	x_i	y_i
A	1.46	1.64
B	3.00	2.75
C	3.42	0.83

Table 4 Iteration I: Cluster Centers

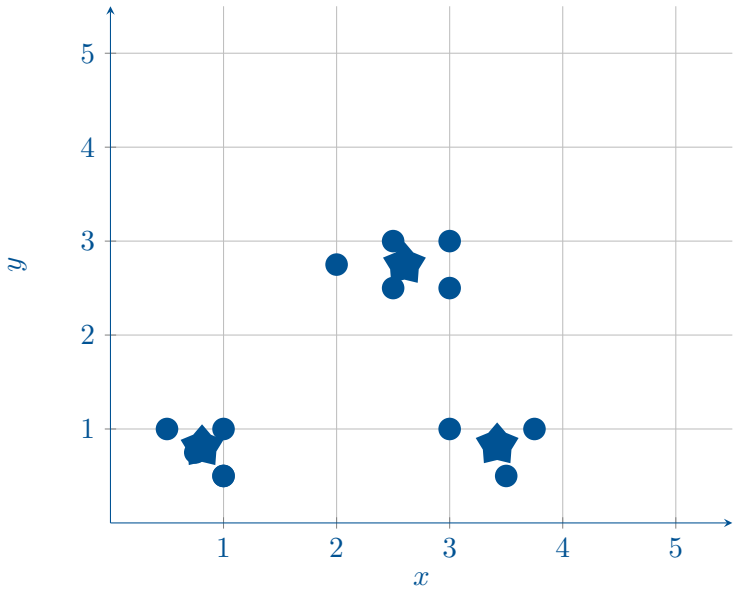
3. Assign instances to the nearest cluster center: see Table 5.
4. Update cluster centers: see Table 6.
5. Assign instances to the nearest cluster center
   No reassignment $\Rightarrow$ termination

i	x_i	y_i	Assigned Cluster Center
1	2.5	3	B
2	3	3	B
3	2	2.75	B
4	2.5	2.5	B
5	3	2.5	B
6	0.5	1	A
7	1	1	A
8	3	1	C
9	3.75	1	C
10	0.75	0.75	A
11	1	0.5	A
12	3.5	0.5	C

Table 5 Iteration II: Instance Assignments

i	x_i	y_i
A	0.81	0.81
B	2.60	2.75
C	3.42	0.83

Table 6 Iteration II: Cluster Centers



Exercise T8.2 *Problems with k-means*

You are given the following small dataset in Table 7:

i	x_i	y_i
0	1	1
1	1	2
2	7	1
3	7	2

Table 7 Small Dataset

(a) Perform 2-means clustering using the L2 norm with initial centroids $A = (4, 1)$ and $B = (4, 2)$ on the data in Table 7. Based on your result, discuss one problem with k-means and name one possible remedy.

(b) Now a fifth point $(3, 20)$ is added to the dataset in Table 7. Perform 2-means clustering using the L2 norm with initial centroids $A = (1, 1)$ and $B = (7, 1)$. Based on your result, discuss another problem with k-means and name one possible remedy.

Solution

(a) k-means terminates after the first iteration. However, this does not result in the "obvious" clusters (0,1) and (2,3). In particular, k-means got "trapped" in a local minimum due to the choice of initial cluster centers. A possible remedy would be multiple iterations of k-means with different random initial centroids.

i	x_i	y_i	Assigned Cluster Center	Distance to Cluster Center
0	1	1	A	3
1	1	2	B	3
2	7	1	A	3
3	7	2	B	3

Table 8 Iteration I: Assignments

i	x_i	y_i
A	4	1
B	4	2

Table 9 Iteration I: Cluster Centers

(b) k-means terminates after the third iteration. However, the cluster centroid of the first cluster now coincides with the outlier and not representative of its observations. In particular, k-means is sensitive to outliers and dependent on the ex-ante chosen number of clusters. A possible remedy would be multiple iterations of k-means with different numbers of clusters k or alternative clustering such as hierarchical or k-medoids.

i	x_i	y_i	Assigned Cluster Center	Distance to Cluster Center
0	1	1	A	0
1	1	2	A	1
2	7	1	B	0
3	7	2	B	1
4	3	20	A	19.10

Table 10 Iteration I: Assignments

i	x_i	y_i
A	3	20
B	4	1.5

Table 11 Iteration III: Cluster Centers

Exercise T8.3 *Hierarchical clustering*

You are given the following dataset:

i	x_i	y_i
0	0	0
1	-1	1
2	3	0
3	-3	5
4	1	2
5	-2	-3
6	0	2
7	4	1
8	-3	-1
9	-2	-2

Table 12 Dataset

You are further given the distance matrix D_1 based on the L1 norm.

$$D_1 = \begin{bmatrix} 0 & 2 & 3 & 8 & 3 & 5 & 2 & 5 & 4 & 4 \\ & 0 & 5 & 6 & 3 & 5 & 2 & 5 & 4 & 4 \\ & & 0 & 11 & 4 & 8 & 5 & 2 & 7 & 7 \\ & & & 0 & 7 & 9 & 6 & 11 & 6 & 8 \\ & & & & 0 & 8 & 1 & 4 & 7 & 7 \\ & & & & & 0 & 7 & 10 & 3 & 1 \\ & & & & & & 0 & 5 & 6 & 6 \\ & & & & & & & 0 & 9 & 9 \\ & & & & & & & & 0 & 2 \\ & & & & & & & & & 0 \end{bmatrix}$$

You want to perform bottom-up hierarchical clustering using the L1 norm. Use single-linkage clustering, i.e., the distance between two sets of observations A, B is defined as $\min_{a \in A, b \in B} d(a, b)$. The first couple of steps have already been conducted and there are currently four clusters:

- Cluster 1: points 0, 1, 4, 6
- Cluster 2: points 2, 7
- Cluster 3: points 5, 8, 9
- Cluster 4: point 3

Complete the remaining steps of the hierarchical clustering.

Solution

We first derive the current distance matrix using single-linkage:

	(0,1,4,6)	(2,7)	(5,8,9)	(3)
(0,1,4,6)	0	3	4	6
(2,7)		0	7	11
(5,8,9)			0	6
(3)				0

The smallest distance is $d((0,1,4,6),(2,7))$ and we merge those two clusters. The updated distance matrix is:

	(0,1,2,4,6,7)	(5,8,9)	(3)
(0,1,2,4,6,7)	0	4	6
(5,8,9)		0	6
(3)			0

The smallest distance is $d((0,1,2,4,6,7),(5,8,9))$ and we merge those two clusters. The updated distance matrix is:

	(0,1,2,4,5,6,7,8,9)	(3)
(0,1,2,4,5,6,7,8,9)	0	6
(3)		0

We merge the remaining two clusters and the hierarchical clustering is complete.

Exercise T8.4 *k-means for image compression*

The goal of this exercise is to use k-means clustering for image compression in Python.

a) Load an image of the famous painting "American Gothic" by Grant Wood and refactor it to an RGB-Image. You can access the painting here. Use the following code:

```
# Load the image
url = #INSERT LINK HERE
img = io.imread(url)
io.imsave("original.png", img)

# notice, that the image has 3 channels (red, green, blue)
print("shape:", img.shape)
```

```
# split the image into the channels (red, green, blue)
r = img[:, :, 0]
g = img[:, :, 1]
b = img[:, :, 2]
)
```

The first two columns in img describe the position of the pixel in the painting. The variables r, g, and b together encode the color of each pixel.

b) How many unique colors does the painting contain?

c) Apply k-means clustering to the pixel colors. Choose $k = 5$ as the number of clusters. Plot the resulting compressed image. The following code snippet may be helpful:

```
km = KMeans(n_clusters=5, init="random", max_iter=300)
km.fit(img)
new_colors = km.cluster_centers_[km.predict(img)]
```

d) Apply k-means clustering for $k = \{1, 2, 3, 5, 10, 20, 50\}$. Plot and save the compressed image in each iteration. Be aware of increased runtimes on personal computers. Observe the size of the image files. Looking at the images, at what point do you notice only minor differences?

e) Determine a reasonable number of clusters using the "elbow criterion". For this purpose, plot the total within-cluster sum of squares (attribute `inertia_` of the `KMeans` object) against the number of clusters, e.g., for $k \in [1, 10]$. Does the elbow point correspond to your visual impression in part d)?

Solution

See file "solution.py".