COMPSCI 762 2022 S1 Week 12 Solutions

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June 7, 2022

Question 1 – Clustering

Figure 1: A data set has 8 instances, from A1 to A8. The Euclidean distances between every two instances are given as the following:

	A1	A2	A3	A4	A5	A6	A7	A8
A1	0	$\sqrt{45}$	$\sqrt{63}$	$\sqrt{57}$	$\sqrt{41}$	$\sqrt{28}$	$\sqrt{95}$	$\sqrt{6}$
A2		0	$\sqrt{55}$	$\sqrt{49}$	$\sqrt{35}$	$\sqrt{11}$	$\sqrt{5}$	$\sqrt{25}$
A3			0	$\sqrt{11}$	$\sqrt{23}$	$\sqrt{54}$	$\sqrt{47}$	$\sqrt{65}$
A4				0	$\sqrt{2}$	$\sqrt{7}$	$\sqrt{26}$	$\sqrt{5}$
A5					0	$\sqrt{5}$	$\sqrt{21}$	$\sqrt{35}$
A6						0	$\sqrt{13}$	$\sqrt{27}$
A7							0	$\sqrt{53}$
A8								0

Use the data in Figure 1 to answer the questions below:

1.1

Suppose that the initial seeds (centers of each cluster) are **A1**, **A4** and **A7**. Run the k-means algorithm for 1 epoch only. At the end of this epoch show the new clusters (i.e. the examples belonging to each cluster)
Answer:

C1 is centred at **A1**, **C2** is centred at **A4**, and **C3** is centred at **A7**.
For each point:

- **A1** $\rightarrow$ **C1**

Item	Centroid	Dist
A2	A1	$\sqrt{45}$
A2	A4	$\sqrt{49}$
A2	A7	$\sqrt{5}$

- **A2** $\rightarrow$ **C3**

Item	Centroid	Dist
A3	A1	$\sqrt{63}$
A3	A4	$\sqrt{11}$
A3	A7	$\sqrt{47}$

- **A3 $\rightarrow$ C2**
- **A4 $\rightarrow$ C2**

Item	Centroid	Dist
A5	A1	$\sqrt{41}$
A5	A4	$\sqrt{2}$
A5	A7	$\sqrt{21}$

- **A5 $\rightarrow$ C2**

Item	Centroid	Dist
A6	A1	$\sqrt{28}$
A6	A4	$\sqrt{7}$
A6	A7	$\sqrt{13}$

- **A6 $\rightarrow$ C2**
- **A7 $\rightarrow$ C3**

Item	Centroid	Dist
A8	A1	$\sqrt{6}$
A8	A4	$\sqrt{5}$
A8	A7	$\sqrt{53}$

- **A8 $\rightarrow$ C2**

The new clusters: $C1 = \{A1\}, C2 = \{A3, A4, A5, A6, A8\}, C3 = \{A2, A7\}$

1.2

Use single-linkage (MIN) agglomerative clustering to group the data. Show the dendrogram.
Answer:

Table 1: Step 1

	A1	A2	A3	A4	A5	A6	A7	A8
A1	0	$\sqrt{45}$	$\sqrt{63}$	$\sqrt{57}$	$\sqrt{41}$	$\sqrt{28}$	$\sqrt{95}$	$\sqrt{6}$
A2		0	$\sqrt{55}$	$\sqrt{49}$	$\sqrt{35}$	$\sqrt{11}$	$\sqrt{5}$	$\sqrt{25}$
A3			0	$\sqrt{11}$	$\sqrt{23}$	$\sqrt{54}$	$\sqrt{47}$	$\sqrt{65}$
A4				0	$\sqrt{2}$	$\sqrt{7}$	$\sqrt{26}$	$\sqrt{5}$
A5					0	$\sqrt{5}$	$\sqrt{21}$	$\sqrt{35}$
A6						0	$\sqrt{13}$	$\sqrt{27}$
A7							0	$\sqrt{53}$
A8								0

Step 3:
Step 4:

Table 2: Step 1 – Clusters

Level	# Clusters	Clusters
0	8	$\{A1\},\{A2\},\{A3\},\{A4\},\{A5\},\{A6\},\{A7\},\{A8\}$
1	7	$\{A1\},\{A2\},\{A3\},\{A4,A5\},\{A6\},\{A7\},\{A8\}$

Table 3: Step 2

	A1	A2	A3	A4	A5	A6	A7	A8
A1	0	$\sqrt{45}$	$\sqrt{63}$	$\sqrt{57}$	$\sqrt{41}$	$\sqrt{28}$	$\sqrt{95}$	$\sqrt{6}$
A2		0	$\sqrt{55}$	$\sqrt{49}$	$\sqrt{35}$	$\sqrt{11}$	$\sqrt{5}$	$\sqrt{25}$
A3			0	$\sqrt{11}$	$\sqrt{23}$	$\sqrt{54}$	$\sqrt{47}$	$\sqrt{65}$
A4				0	$\sqrt{2}$	$\sqrt{7}$	$\sqrt{26}$	$\sqrt{5}$
A5					0	$\sqrt{5}$	$\sqrt{21}$	$\sqrt{35}$
A6						0	$\sqrt{13}$	$\sqrt{27}$
A7							0	$\sqrt{53}$
A8								0

Table 4: Step 2 – Clusters

Level	# Clusters	Clusters
0	8	$\{A1\},\{A2\},\{A3\},\{A4\},\{A5\},\{A6\},\{A7\},\{A8\}$
1	7	$\{A1\},\{A2\},\{A3\},\{A4,A5\},\{A6\},\{A7\},\{A8\}$
2	4	$\{A1\},\{A2,A7\},\{A3\},\{A4,A5,A6,A8\}$

Table 5: Step 3

	A1	A2	A3	A4	A5	A6	A7	A8
A1	0	$\sqrt{45}$	$\sqrt{63}$	$\sqrt{57}$	$\sqrt{41}$	$\sqrt{28}$	$\sqrt{95}$	$\sqrt{6}$
A2		0	$\sqrt{55}$	$\sqrt{49}$	$\sqrt{35}$	$\sqrt{11}$	$\sqrt{5}$	$\sqrt{25}$
A3			0	$\sqrt{11}$	$\sqrt{23}$	$\sqrt{54}$	$\sqrt{47}$	$\sqrt{65}$
A4				0	$\sqrt{2}$	$\sqrt{7}$	$\sqrt{26}$	$\sqrt{5}$
A5					0	$\sqrt{5}$	$\sqrt{21}$	$\sqrt{35}$
A6						0	$\sqrt{13}$	$\sqrt{27}$
A7							0	$\sqrt{53}$
A8								0

Table 6: Step 3 – Clusters

Level	# Clusters	Clusters
0	8	$\{A1\},\{A2\},\{A3\},\{A4\},\{A5\},\{A6\},\{A7\},\{A8\}$
1	7	$\{A1\},\{A2\},\{A3\},\{A4,A5\},\{A6\},\{A7\},\{A8\}$
2	4	$\{A1\},\{A2,A7\},\{A3\},\{A4,A5,A6,A8\}$
3	3	$\{A1,A4,A5,A6,A8\},\{A2,A7\},\{A3\}$

Table 7: Step 4

	A1	A2	A3	A4	A5	A6	A7	A8
A1	0	$\sqrt{45}$	$\sqrt{63}$	$\sqrt{57}$	$\sqrt{41}$	$\sqrt{28}$	$\sqrt{95}$	$\sqrt{6}$
A2		0	$\sqrt{55}$	$\sqrt{49}$	$\sqrt{35}$	$\sqrt{11}$	$\sqrt{5}$	$\sqrt{25}$
A3			0	$\sqrt{11}$	$\sqrt{23}$	$\sqrt{54}$	$\sqrt{47}$	$\sqrt{65}$
A4				0	$\sqrt{2}$	$\sqrt{7}$	$\sqrt{26}$	$\sqrt{5}$
A5					0	$\sqrt{5}$	$\sqrt{21}$	$\sqrt{35}$
A6						0	$\sqrt{13}$	$\sqrt{27}$
A7							0	$\sqrt{53}$
A8								0

Table 8: Step 4 – Clusters. Note that A4 and A6 are already in one cluster.

Level	# Clusters	Clusters
0	8	$\{A1\},\{A2\},\{A3\},\{A4\},\{A5\},\{A6\},\{A7\},\{A8\}$
1	7	$\{A1\},\{A2\},\{A3\},\{A4,A5\},\{A6\},\{A7\},\{A8\}$
2	4	$\{A1\},\{A2,A7\},\{A3\},\{A4,A5,A6,A8\}$
3	3	$\{A1,A4,A5,A6,A8\},\{A2,A7\},\{A3\}$
4	1	$\{A1,A2,A3,A4,A5,A6,A7,A8\}$

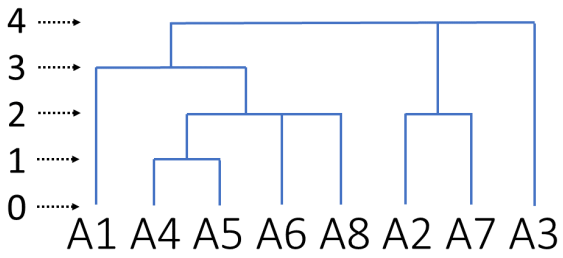


Figure 2: Step 5 – Dendrogram: Make sure you choose the correct order to start with. Use the sequence from the second last level;

Question 2 – Ooutlier/Anomaly Detection

2.1

What are the three types of anomaly? Give an example for each type.
Answer:

- **Global outlier (Point anomaly):** deviates significantly from the rest of the data set. The simplest type of outliers.
- **Contextual outlier (Conditional outlier):** deviates significantly with respect to a specific context of the object.
  - **Contextual attributes:** define the object's context.
  - **Behavioral attributes:** define the object's characteristics, and are used to evaluate whether the object is an outlier in the context.
    For example:
    A temperature sensor measures 4°C in May. It is a perfectly normal reading in Wellington, but it might be an outlier if the location is New York. The location and the date are **contextual attributes**, and the temperature is a **behavioral attribute**.
- **Collective outliers:** the objects as a whole deviate significantly from the entire data set.

Examples:

- Fig. 3 left: Global outliers
- Fig. 3 middle: Contextual outliers – Given the dataset has two clusters, each one has a moon shape.
- Fig. 3 rright: Blue points are collective outliers because the density of those points is much higher than the rest.

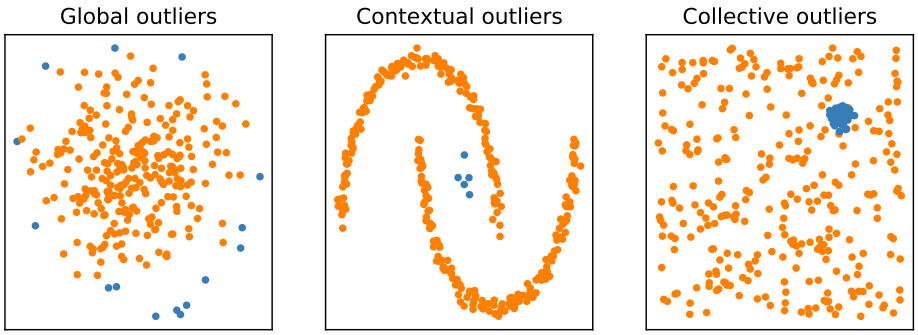


Figure 3: Types of outliers

2.2

You are given the following list of 2D data points:

$$[1;1];[1;2];[2;2];[2;1];[3;3];[2;5];[2;3]$$

If you had to select one point to be anomalous, how to use Manhattan distance to determine the outlier. Explain the anomaly detection technique.

Answer:

There are multiple ways to solve this problem. Let's use **distance-based outlier detection**.

	1,1	**1,2**	**2,2**	**2,1**	**3,3**	**2,5**	**2,3**
1,1	0	1	2	1	4	5	3
1,2	1	0	1	2	3	4	2
2,2	2	1	0	1	2	3	1
2,1	1	2	1	0	3	4	2
3,3	4	3	2	3	0	3	1
2,5	5	4	3	4	3	0	2
2,3	3	2	1	2	1	2	0

Table 9: Manhattan Distance Matrix

$$\frac{|\{o'|\text{dist}(o,o') \leq r\}|}{|D|} \leq \pi$$

where $|D|$ is the *cardinality* of the set D.

We need to define the hyperparameters: r and π.

The number of data points, $|D|$, is 7.

Let $r = 2$,

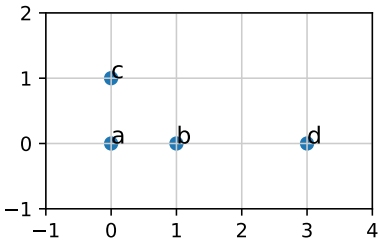
	# of objects within r	**Divide by $|D|$**
1,1	3	0.43
1,2	4	0.57
2,2	5	0.71
2,1	4	0.57
3,3	2	0.29
2,5	1	0.14
2,3	5	0.71

Table 10: The # of neighbours within r

If we select only one point as an outlier, we can set π to any value between 0.14 and 0.29, e.g. 0.15. Therefore, we identify $[2;5]$ is an outlier.

2.3

Consider a set of points (0,0), (1,0), (0,1), (3,0). Calculate the *Local Outlier Factor* (LOF) score for the points using Manhattan distance and k is 2.
Answer:



	a (0,0)	**b (1,0)**	**c (0,1)**	**d (3,0)**
a (0,0)	0	1	1	3
b (1,0)	1	0	2	2
c (0,1)	1	2	0	4
d (3,0)	3	2	4	0

Table 11: Manhattan distance matrix

	$\text{dist}_2(o)$	$N_2(o)$
a (0,0)	1	2
b (1,0)	2	3
c (0,1)	2	2
d (3,0)	3	2

Table 12: Distance between data point o and its k-th nearest neighbour ($k = 2$)

We denote the set of k-nearest neighbours as $N_k(o)$:

$$N_k(o) = \{o' | o' \in D, \text{dist}(o, o') \leq \text{dist}_k(o)\}$$

Note: $|N_k(o)|$ may contain more than k objects, because objects may have same distance.

Let o' be a neighbour of o, to avoid $\text{dist}(o, o')$ is too small, we compute the reachability distance from o to o':

$$\text{reachdist}_k(o' \leftarrow o) = \max\{\text{dist}_k(o), \text{dist}(o, o')\}$$

Note that reachability distance is not symmetric, thus

$$\text{reachdist}_k(o \leftarrow o') \neq \text{reachdist}_k(o' \leftarrow o)$$

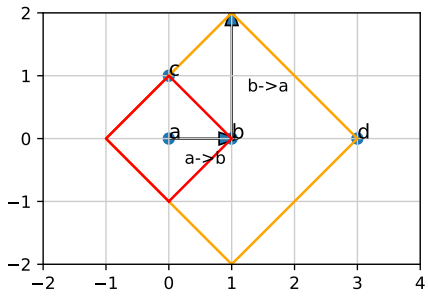


Figure 4: $\text{reachdist}_2(b \leftarrow a) \neq \text{reachdist}_2(a \leftarrow b)$

$$
\begin{array}{lll}
\text{reachdist}_2(b \leftarrow a) & = \max\{\text{dist}_2(a), \text{dist}(a,b)\} & = \max\{1,1\} = 1 \\
\text{reachdist}_2(c \leftarrow a) & = \max\{\text{dist}_2(a), \text{dist}(a,c)\} & = \max\{1,1\} = 1 \\
\text{reachdist}_2(d \leftarrow a) & = \max\{\text{dist}_2(a), \text{dist}(a,d)\} & = \max\{1,3\} = 3 \\
\text{reachdist}_2(a \leftarrow b) & = \max\{\text{dist}_2(b), \text{dist}(b,a)\} & = \max\{2,1\} = 2 \\
\text{reachdist}_2(c \leftarrow b) & = \max\{\text{dist}_2(b), \text{dist}(b,c)\} & = \max\{2,2\} = 2 \\
\text{reachdist}_2(d \leftarrow b) & = \max\{\text{dist}_2(b), \text{dist}(b,d)\} & = \max\{2,2\} = 2 \\
\text{reachdist}_2(a \leftarrow c) & = \max\{\text{dist}_2(c), \text{dist}(c,a)\} & = \max\{2,1\} = 2 \\
\text{reachdist}_2(b \leftarrow c) & = \max\{\text{dist}_2(c), \text{dist}(c,b)\} & = \max\{2,2\} = 2 \\
\text{reachdist}_2(d \leftarrow c) & = \max\{\text{dist}_2(c), \text{dist}(c,d)\} & = \max\{2,4\} = 4 \\
\text{reachdist}_2(a \leftarrow d) & = \max\{\text{dist}_2(d), \text{dist}(d,a)\} & = \max\{3,3\} = 3 \\
\text{reachdist}_2(b \leftarrow d) & = \max\{\text{dist}_2(d), \text{dist}(d,b)\} & = \max\{3,2\} = 3 \\
\text{reachdist}_2(c \leftarrow d) & = \max\{\text{dist}_2(d), \text{dist}(d,c)\} & = \max\{3,4\} = 4
\end{array}
$$

Note that,

$$\text{reachdist}_k(o \leftarrow o') \neq \text{reachdist}_k(o' \leftarrow o)$$

The *Local Reachability Density* (LRD) of an object o is defined as

$$\text{lrd}_k(o) = \frac{|N_k(o)|}{\sum_{o' \in N_k(o)} \text{reachdist}_k(o \leftarrow o')}$$

$$
\begin{array}{lll}
\text{lrd}_2(a) & = |N_2(a)|/(\text{reachdist}_2(a \leftarrow b) + \text{reachdist}_2(a \leftarrow c)) & = 2/(2+2) = 0.5 \\
\text{lrd}_2(b) & = |N_2(b)|/(\text{reachdist}_2(b \leftarrow a) + \text{reachdist}_2(b \leftarrow c) + \text{reachdist}_2(b \leftarrow d)) & = 3/(1+2+3) = 0.5 \\
\text{lrd}_2(c) & = |N_2(c)|/(\text{reachdist}_2(c \leftarrow a) + \text{reachdist}_2(c \leftarrow b)) & = 2/(1+2) = 0.667 \\
\text{lrd}_2(d) & = |N_2(d)|/(\text{reachdist}_2(d \leftarrow a) + \text{reachdist}_2(d \leftarrow b)) & = 2/(3+2) = 0.4
\end{array}
$$

The *Local Outlier Factor* (LOF) of an object o is

$$\text{LOF}_k(o) = \frac{\sum_{o' \in N_k(o)} \frac{\text{lrd}_k(o')}{\text{lrd}_k(o)}}{|N_k(o)|} = \frac{\sum_{o' \in N_k(o)} \text{lrd}_k(o')}{|N_k(o)| \cdot \text{lrd}_k(o)}$$

$$
\begin{array}{lll}
\text{LOF}_2(a) & = (\text{lrd}_2(b) + \text{lrd}_2(c))/(|N_2(a)| \cdot \text{lrd}_2(a)) & = (0.5+0.667)/(2 \times 0.5) = 1.167 \\
\text{LOF}_2(b) & = (\text{lrd}_2(a) + \text{lrd}_2(c) + \text{lrd}_2(d))/(|N_2(b)| \cdot \text{lrd}_2(b)) & = (0.5+0.667+0.4)/(3 \times 0.5) \approx 1.045 \\
\text{LOF}_2(c) & = (\text{lrd}_2(a) + \text{lrd}_2(b))/(|N_2(c)| \cdot \text{lrd}_2(c)) & = (0.5+0.5)/(2 \times 0.667) \approx 0.750 \\
\text{LOF}_2(d) & = (\text{lrd}_2(a) + \text{lrd}_2(b))/(|N_2(d)| \cdot \text{lrd}_2(d)) & = (0.5+0.5)/(2 \times 0.4) = 1.25
\end{array}
$$

LOF is a relative value. We should not compare a LOF from one dataset with other reading from different datasets.

The question does not ask for outlier. There is only 4 data points. If we remove 1 point, we will remove 25% of the data. I do not determine the outlier here.