Ludwig-Maximilians-Universität München Institut für Informatik Prof. Dr. Thomas Seidl Max Berrendorf, Julian Busch

Knowledge Discovery and Data Mining I WS 2018/19

Exercise 8: Outlier Scores

Exercise 8-1 Monotonicity of Simple Outlier Scores

Proof or give an counterexample for the following claims:

(a) If o is an $D(\epsilon, \pi)$ -outlier, it is also an $D(\epsilon', \pi)$ -outlier for $\epsilon' \leq \epsilon$.

The statement is true. Let o be an $D(\epsilon, \pi)$ -outlier. Then,

$$\pi \left| D \right| \stackrel{\clubsuit}{\geq} \left| \left\{ q \in D \mid dist(o,q) < \epsilon \right\} \right| \stackrel{\heartsuit}{\geq} \left| \left\{ q \in D \mid dist(o,q) < \epsilon' \right\} \right|$$

where \clubsuit is the definition of $D(\epsilon, \pi)$ -outlier, and \heartsuit holds due to the transitivity of < and \leq :

$$dist(o,q) < \epsilon' \land \epsilon' \le \epsilon \implies dist(o,q) < \epsilon$$

(b) If o is an $D(\epsilon, \pi)$ -outlier, it is also an $D(\epsilon, \pi')$ -outlier for $\pi' \ge \pi$.

This statement is also true.

$$\pi'|D| \ge \pi|D| \ge |\{q \in D \mid dist(o,q) < \epsilon\}|$$

- (c) If o is an kNN-outlier for threshold τ , it is also an k'NN-outlier for the same threshold with k' > k.
 - Let nndist(o, k) denote the k-distance of o. As the k-distance is the kth smallest distance to an object in the database, we clearly have $nndist(o, k) \leq nndist(o, k+1)$ (the (k+1)-smallest distance cannot be larger than the k-smallest). Hence,

$$nndist(o, k') \ge nndist(o, k) > \tau,$$

i.e. o is also a k'NN outlier for threshold τ .

(d) If o is an kNN-outlier for threshold τ , it is also an kNN-outlier for threshold $\tau' < \tau$. Let nndist(o, k) denote the k-distance of o. Then,

$$nndist(o,k) > \tau > \tau'$$

i.e. *o* is also a *k*NN outlier for threshold τ' .

(e) The local density is monotonously decreasing in k, i.e. $ld_k(o) \ge ld_{k'}(o)$ for k' > k.

This statement is true. Let nndist(o, k) denote the k-distance of o, i.e. the distance between o and its kth nearest neighbor. Then, we have

$$k' \ge k \implies nndist(o,k') \ge nndist(o,k)$$

i.e. the k-distance is monotonously increasing in k. With this notation, we can note the (*reciprocal*) local density $ld_k(o)$ by

$$(ld_k(o))^{-1} = \frac{1}{k} \sum_{i=1}^k nndist(o,i)$$

Moreover, we can apply the following sequence of equivalence transformations of the inequality of interest

$$\begin{aligned} ld_{k}(o) &\geq ld_{k+1}(o) \\ &\longleftrightarrow (ld_{k}(o))^{-1} \leq (ld_{k+1}(o))^{-1} \\ &\Leftrightarrow \frac{1}{k} \sum_{i=1}^{k} nndist(o,i) \leq \frac{1}{k+1} \sum_{i=1}^{k+1} nndist(o,i) \\ &\Leftrightarrow (k+1) \sum_{i=1}^{k} nndist(o,i) \leq k \sum_{i=1}^{k+1} nndist(o,i) \\ &\Leftrightarrow k \sum_{i=1}^{k} nndist(o,i) + \sum_{i=1}^{k} nndist(o,i) \leq k \sum_{i=1}^{k+1} nndist(o,i) \\ &\Leftrightarrow \sum_{i=1}^{k} nndist(o,i) \leq k \cdot nndist(o,k+1) \end{aligned}$$

The last inequality holds due to

$$\sum_{i=1}^{k} nndist(o,i) \stackrel{\clubsuit}{\leq} \sum_{i=1}^{k} nndist(o,k+1) = k \cdot nndist(o,k+1)$$

where \blacklozenge uses the monotonicity of the k-distance.

Exercise 8-2 Outlier Scores

Given the following 2 dimensional data set:



As distance function, use Manhattan distance $L_1(a, b) := |a_1 - b_1| + |a_2 - b_2|$. The following table summarises the pairwise distances.

∢ -	0	1	1	2	6	10	11	12	13	13	15	17	14	12	13	14	11	12	13	11
а-	1	0	2	1	5	9	10	11	12	12	14	16	13	11	12	13	10	11	12	10
<u></u> -	1	2	0	1	5	9	10	11	12	12	14	16	13	11	12	13	10	11	12	10
Δ-	2	1	1	0	4	8	9	10	11	11	13	15	12	10	11	12	9	10	11	9
ш-	6	5	5	4	0	4	5	6	7	7	9	11	8	6	7	8	7	8	9	9
ш.	10	9	9	8	4	0	1	2	3	3	5	7	10	10	11	12	11	12	13	13
ט -	11	10	10	9	5	1	0	1	2	2	4	8	11	11	12	13	12	13	14	14
т-	12	11	11	10	6	2	1	0	1	1	3	7	10	10	11	12	11	12	13	13
	13	12	12	11	7	3	2	1	0	2	4	8	11	11	12	13	12	13	14	14
<u> </u>	13	12	12	11	7	3	2	1	2	0	2	6	9	9	10	11	10	11	12	12
⊻ -	15	14	14	13	9	5	4	3	4	2	0	4	7	7	8	9	8	9	10	10
<u> </u>	17	16	16	15	11	7	8	7	8	6	4	0	3	5	4	5	6	5	6	6
Σ-	14	13	13	12	8	10	11	10	11	9	7	3	0	2	1	2	3	2	3	3
z -	12	11	11	10	6	10	11	10	11	9	7	5	2	0	1	2	1	2	3	3
0 -	13	12	12	11	7	11	12	11	12	10	8	4	1	1	0	1	2	1	2	2
۹.	14	13	13	12	8	12	13	12	13	11	9	5	2	2	1	0	3	2	1	3
ο-	11	10	10	9	7	11	12	11	12	10	8	6	3	1	2	3	0	1	2	2
∝ -	12	11	11	10	8	12	13	12	13	11	9	5	2	2	1	2	1	0	1	1
<i>S</i> -	13	12	12	11	9	13	14	13	14	12	10	6	3	3	2	1	2	1	0	2
⊢ -	11	10	10	9	9	13	14	13	14	12	10	6	3	3	2	3	2	1	2	0
	Å	B	Ċ	b	Ė	F	Ġ	H	Ì	j	ĸ	Ļ	M	N	ò	P	, Q	R	Ś	Ť

(a) Calculate the $D(\epsilon, \pi)$ -outliers using

- (i) $\epsilon = 2$ with $n\pi = 1$ and $n\pi = 2$.
- (ii) $\epsilon = 4$ with $n\pi = 1$, $n\pi = 3$ and $n\pi = 4$.
- (iii) $\epsilon = 6$ with $n\pi = 4$, $n\pi = 5$ and $n\pi = 6$.

For the $D(\epsilon, \pi)$ outliers we have to check whether at most π percent of all points have a distance less than ϵ . Hence, we count per column how many times the distance is less than ϵ yielding

ϵ	Α	В	С	D	Ε	F	G	Η	Ι	J	K	L	Μ	Ν	0	Р	Q	R	S	Т
2	3	3	3	3	1	2	3	4	2	2	1	1	2	3	5	3	3	5	3	2
4	4	4	4	4	1	5	5	6	5	6	3	2	9	8	8	8	8	8	8	8
6	4	5	5	5	6	7	7	6	6	6	7	7	9	9	9	9	8	9	8	8

Finally, we check if the number divided by the number of objects n = 20 is at most the threshold π . We obtain the following outliers:

(i) For $(\epsilon, n\pi) = (2, 1)$: *EKL*. For $(\epsilon, n\pi) = (2, 2)$: EFIJKLMT.

(ii) For $(\epsilon, n\pi) = (4, 1)$: *E*. For $(\epsilon, n\pi) = (4, 3)$: EKL. For $(\epsilon, n\pi) = (4, 4)$: ABCDEKL.

(iii) For $(\epsilon, n\pi) = (6, 4)$: A. For $(\epsilon, n\pi) = (6, 5)$: ABCD. For $(\epsilon, n\pi) = (6, 6)$: ABCDEHIJ.

(b) Calculate the kNN based outliers for $(k, \tau) = (3, 3)$ and $(k, \tau) = (5, 8)$. The point itself is counted as the 0-nearest neighbour.

k	A	B	С	D	Е	F	G	Н	Ι	J	K	L	М	N	0	Р	Q	R	S	Т
3	2	2	2	2	5	3	2	1	2	2	4	4	2	2	1	2	2	1	2	2
5	10	9	9	8	5	4	4	3	4	3	4	5	3	2	2	2	2	2	2	3

First, we compute the k-distances for each point.

Finally, we obtain the outliers as those points whose k-distance exceeds the threshold τ , i.e. for $(k, \tau) = (3,3)$ we have E, K, L, and for $(k, \tau) = (5,8)$ we have A, B, C.

(c) Given the following curves of the local density ld_k for different values of k.



Can you identify which curve belongs to which point? Explain your mapping. This is the ground truth mapping.



We can observe:

- The dark green line has a ld_k of one up to k = 4. Hence, the inverse average distance to the 4nearest neighbours is 1, and equivalently, the average of distances of the 4-nearest neighbours is one. We can only find two points in the dataset fulfilling this requirement: O and R.
- The dark blue line has a ld_1 of 0.25, i.e. the 1-nearest neighbour has distance 4. This requirement is only fulfilled by E.
- For the light blue line we can observe that ld_k stays one until k = 2, i.e. there are two points with distance 1. This reduces the candidate set to ABCDG. As we observe a sharp drop afterwards, the point is likely to reside in ABCD. All of these points have a quite similar ld_k -line.

• The light green line is also in a region that has a low local density already for small k values. As it is still higher, as the light green line, we might suspect a point that has a slightly smaller 1-distance, such as K, or L. Using $ld_1 = 0.5$, we can conclude that the 1-distance is equal to 2, and hence only K possible.