

Outlier Detection: Partitioning Methods

Mining Massive Datasets

Prof. Carlos Castillo

Topic 21

Sources

Liu, F. T., Ting, K. M., & Zhou, Z. H. Isolation forest. ICDM 2008.

(1) Eryk Lewinson: Outlier detection with isolation forest (2018)

(2) Tobias Sterbak: Detecting network attacks with isolation forests (2018)

Partitioning-based method: isolation forest

Isolation forest method

- `tree_build(X)`
 - Pick a random dimension r of dataset X
 - Pick a random point p in $[\min_r(X), \max_r(X)]$
 - Divide the data into two pieces: $x_r < p$ and $x_r \geq p$
 - Recursively process each piece

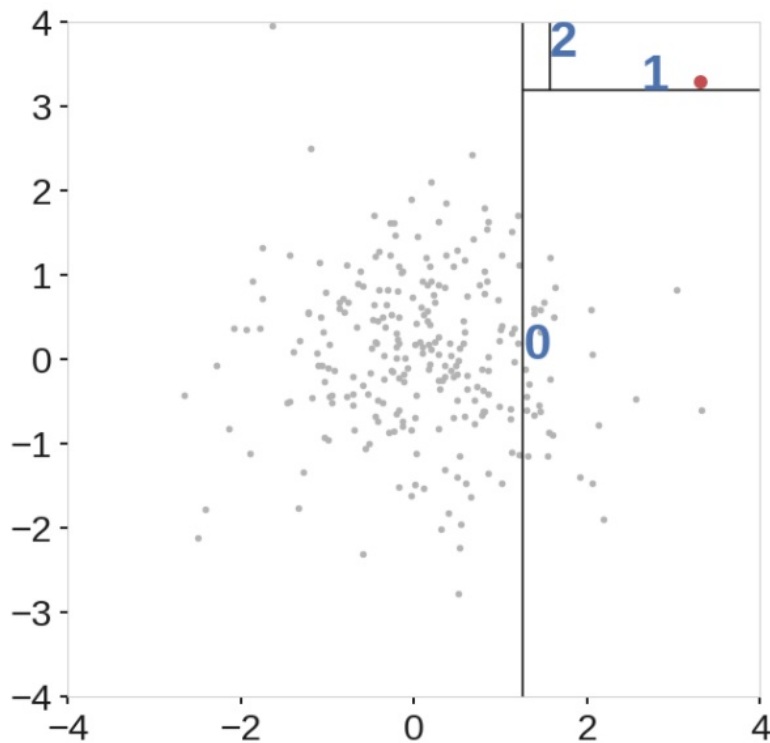
Stopping criteria for recursion

- Stop when a **maximum depth** has been reached

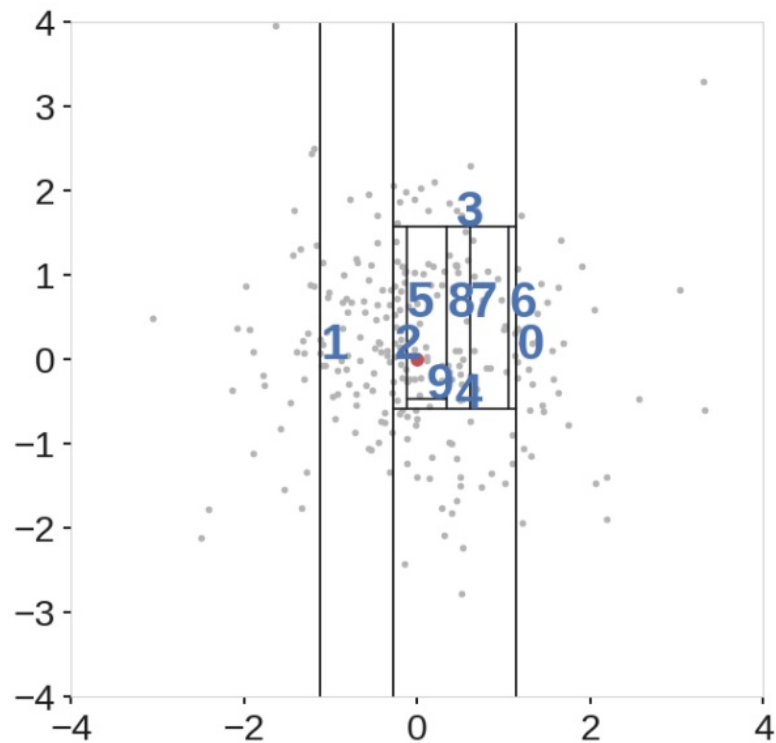
-or-

- Stop when each point is **alone** in one partition

Key: outliers lie at **small depths**



(a) Anomaly point



(b) Nominal point

Outlier score

- Let $c(n)$ be the average path length of an unsuccessful search in a binary tree of n items

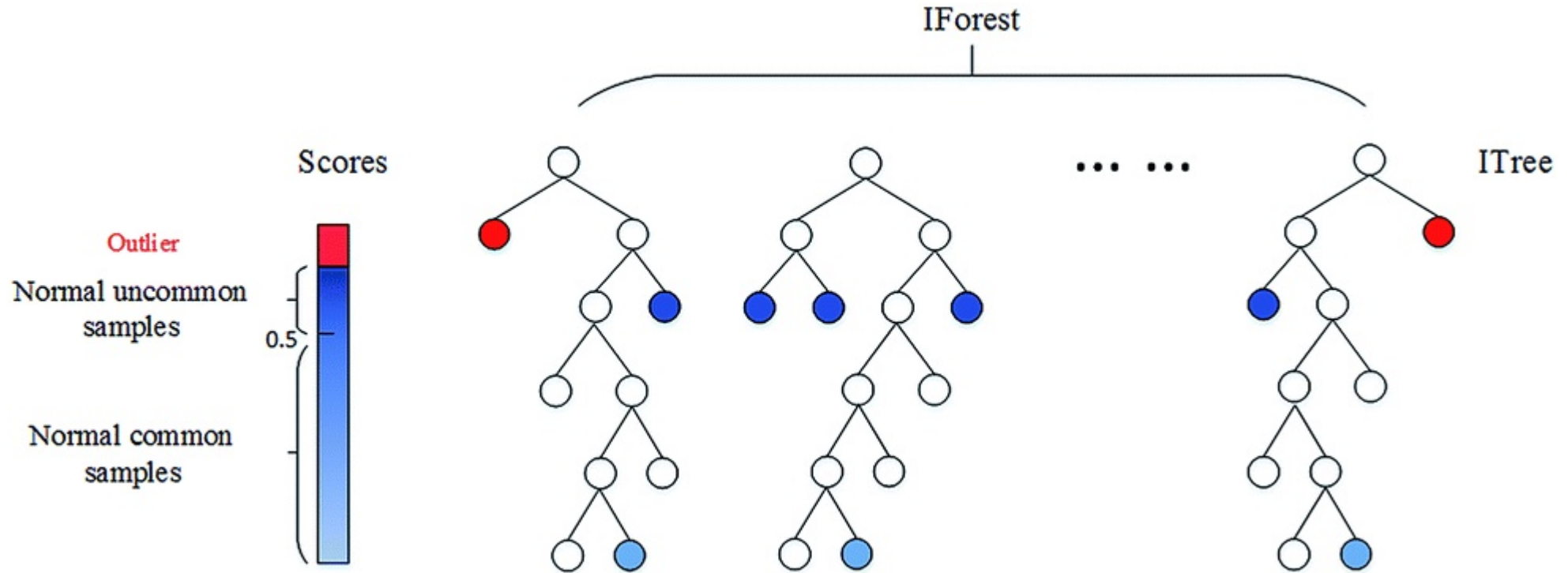
$$c(n) = 2H(n-1) - (2(n-1)/n) \qquad H(n) = \sum_{k=1}^n \frac{1}{k}$$

- $h(x)$ is the depth at which x is found in tree
- Score:

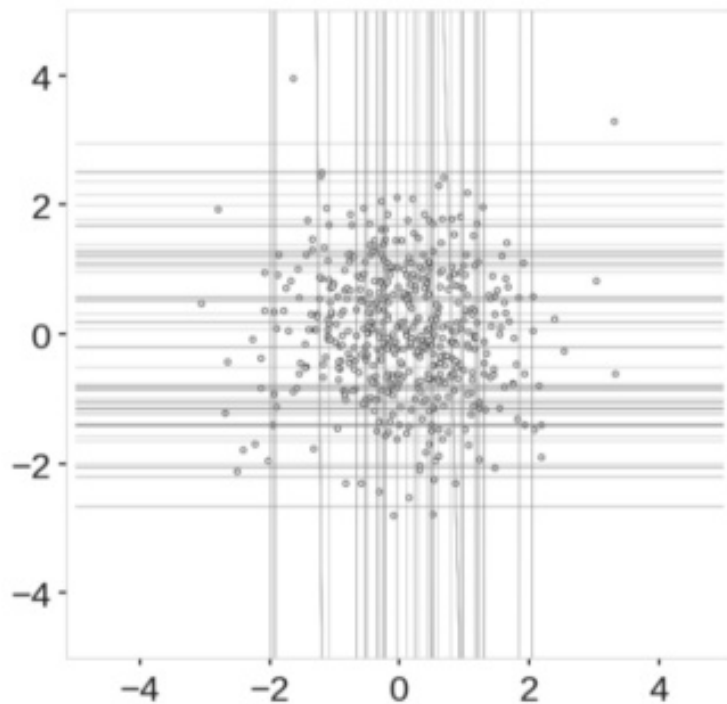
$$\text{outlier}(x, n) = 2^{-\frac{E(h(x))}{c(n)}}$$

Outlier scores in isolation forests

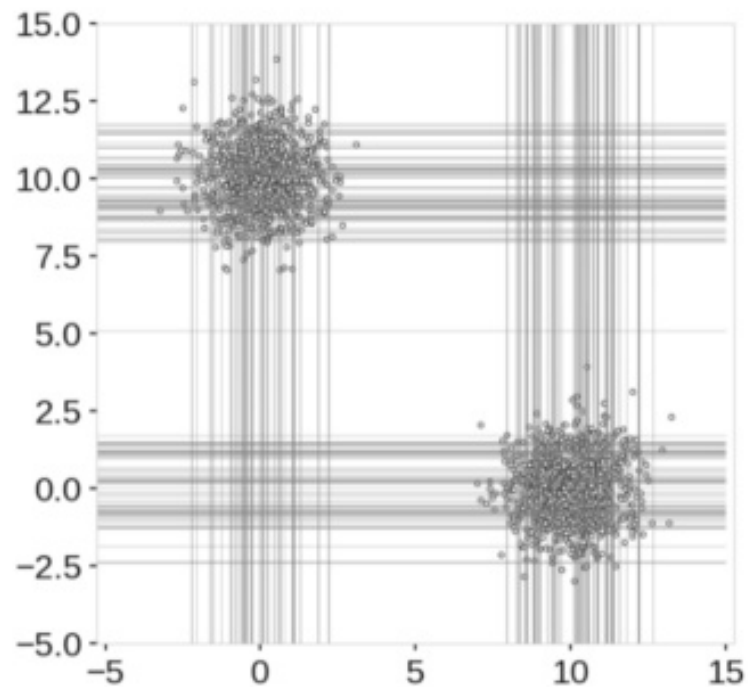
(each tree is built from a sub-sample of original data)



Example



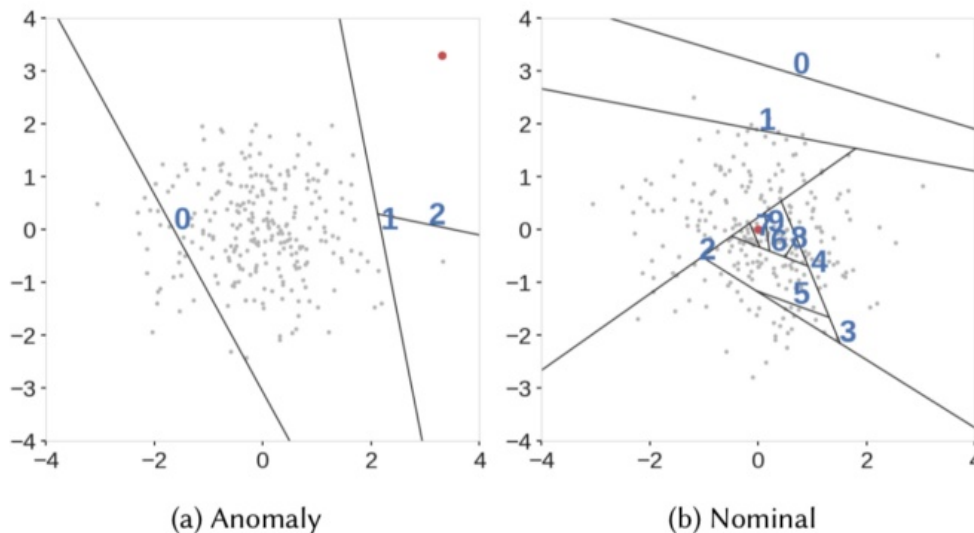
(a) Single blob



(b) Multiple Blobs

Extended Isolation Forest

- More freedom to partitioning by choosing a random slope and a random intercept



Exercise

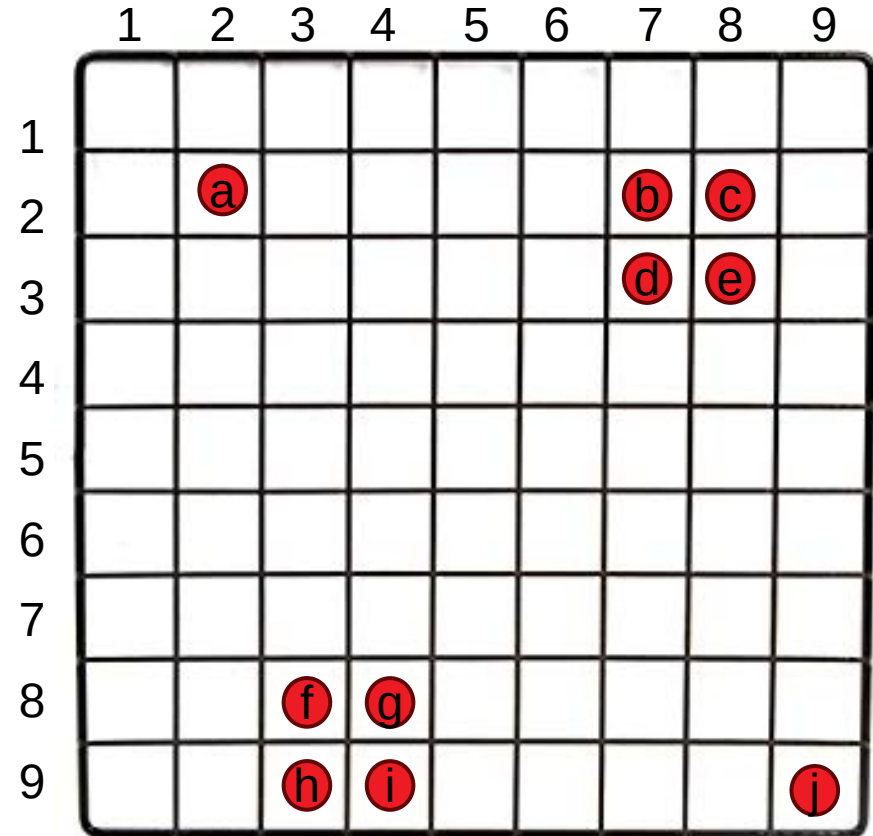
Answer in
Nearpod Draw-it

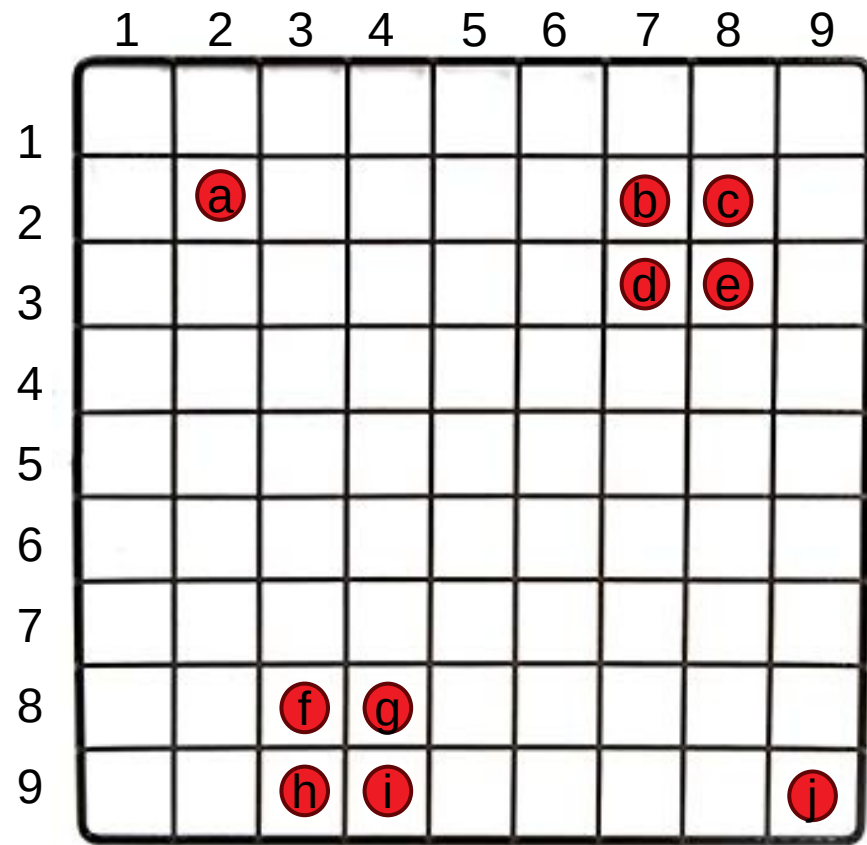
- Create one tree of the isolation forest by repeating 4 times:
 - Picking a sector containing >1 element
 - Picking a random dimension
 - Picking a random cut-off between min and max value along that dimension
- Draw the lines of your cuts
- Label each point with its depth $h(x)$

This is normally repeated several times, in the end:

$$\text{outlier}(x, n) = 2^{-\frac{E(h(x))}{c(n)}}$$

In this case $c(10) = 2 \times H(9) - (2 \times 9/10) \approx 3.857 \approx 4$



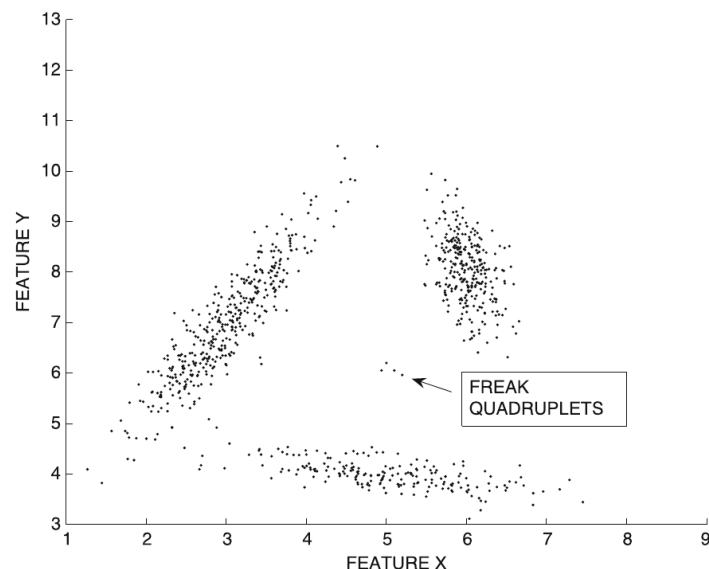


Additional materials

Distance-based methods

Instance-specific definition

- The distance-based outlier score of an object x is **its distance to its k^{th} nearest neighbor**
- In this example of a small group of 4 outliers, we can set $k > 3$

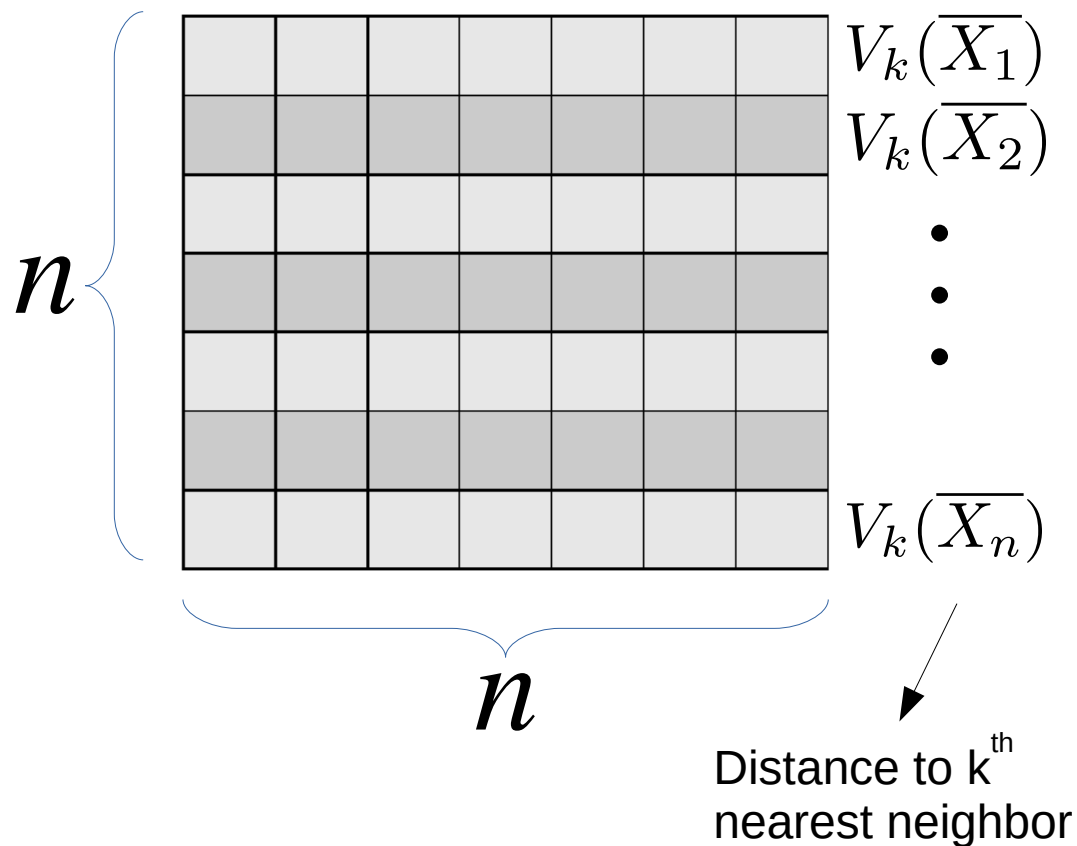


Problem: computational cost

- The distance-based outlier score of an object x is its distance to its k^{th} nearest neighbor
- In principle this requires $O(n^2)$ computations!
 - Index structure:
useful only for cases of low data dimensionality
 - Pruning tricks:
useful when only top- r outliers are needed

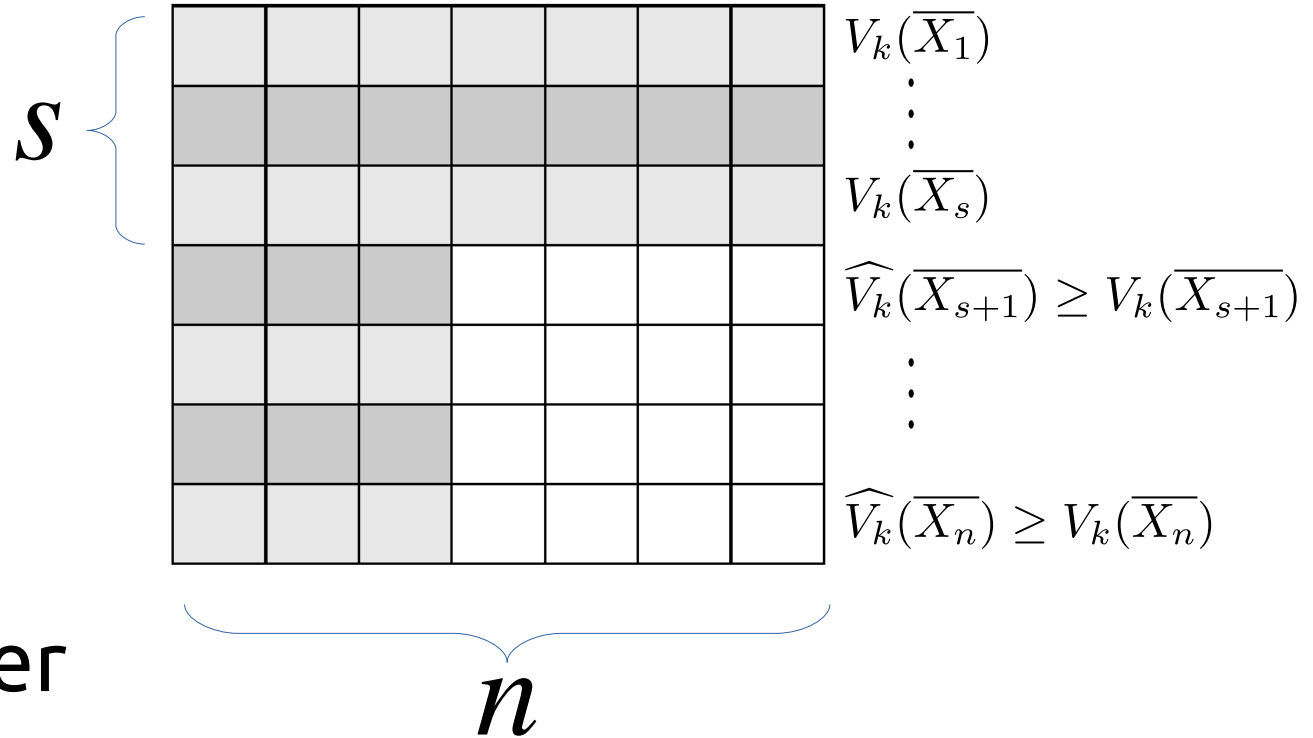
Problem: computational cost

- The distance-based outlier score of an item x is its distance to its k^{th} nearest neighbor
- In principle this requires:
 - $O(n^2)$ computations for evaluating the $n \times n$ distance matrix
 - $O(n^2)$ computations for finding the r smallest values on each row



Pruning method: sampling

- Evaluate $s \times n$ distances
- For points $1 \dots s$ we are OK
- For points $(s+1) \dots n$ we know only upper bounds

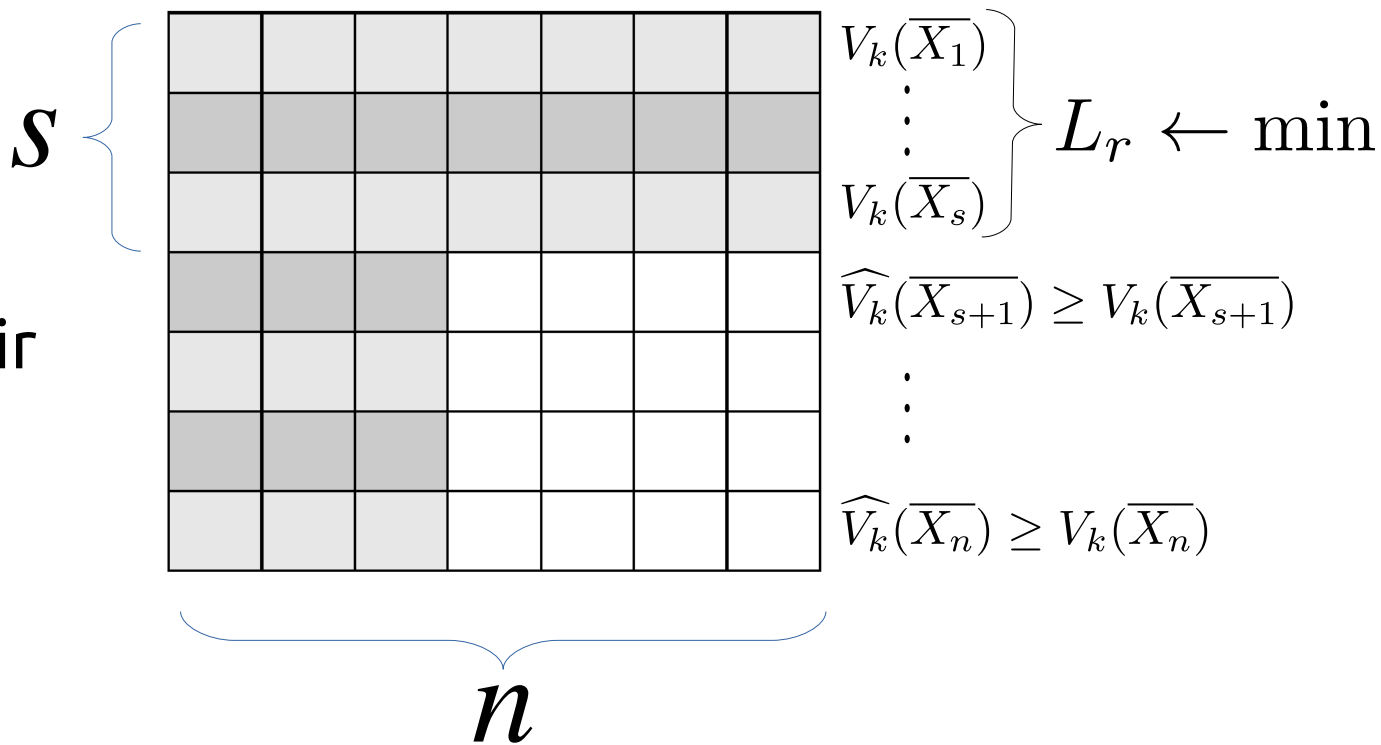


Pruning method: sampling (cont.)

From points
 $1...s$ we already know
 the r “winners”

($r \leq s$ nodes with the
 larger distance to their
 k^{th} nearest neighbor)

Any point having
 $V_k < L_s$ cannot be
 among the top r
 outliers

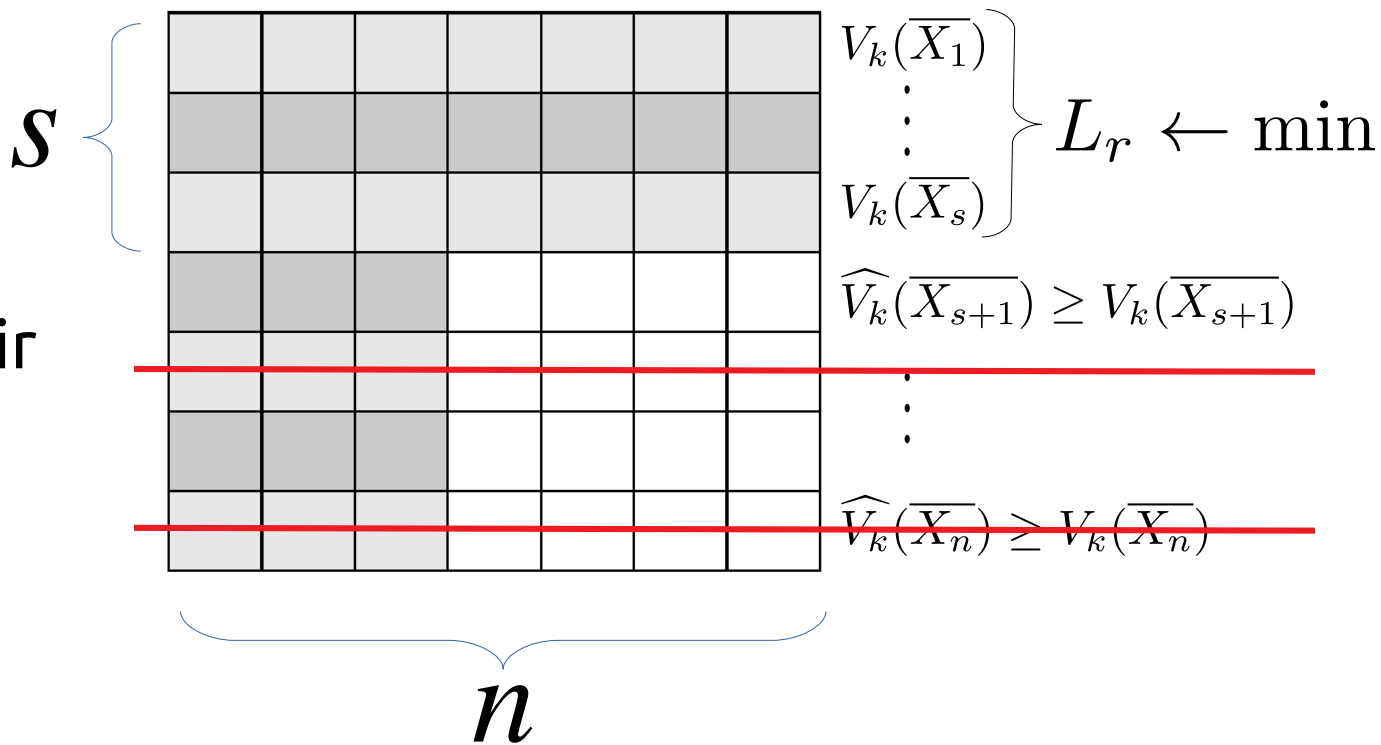


Pruning method: sampling (cont.)

From points $1...s$ we already know the r "winners"

($r \leq s$ nodes with the larger distance to their k^{th} nearest neighbor)

Any point having $V_k < L_s$ cannot be among the top r outliers

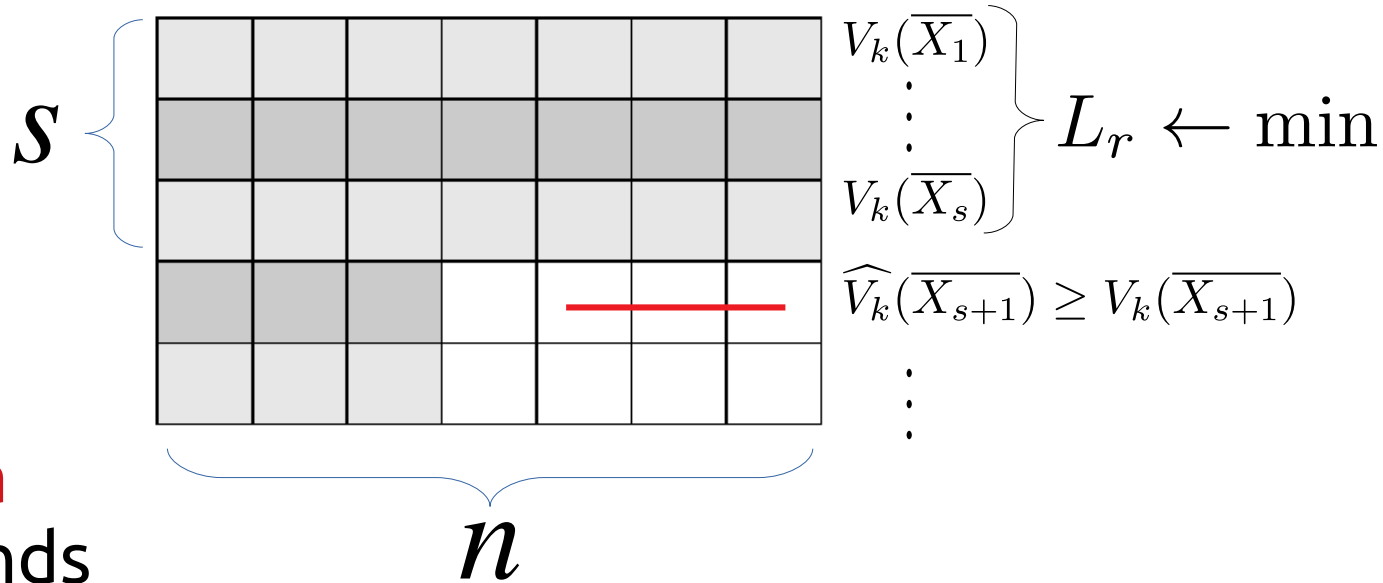


Pruning method: sampling (cont.)

Remove points

having $\widehat{V}_k \leq L_r$

Update L_r keeping
r largest values, and
stop computing for a
row if one already finds
k nearest neighbors in that
row that are all below
distance L_r



Local outlier factor

Local Outlier Factor (LOF)

- Let $V_k(\bar{X})$ be the distance of \bar{X} to its k-nearest neighbor
- Reachability distance

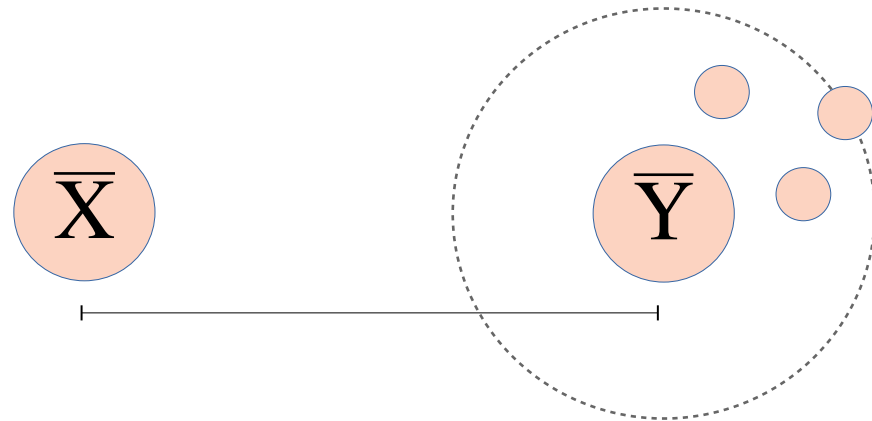
$$R_k(\bar{X}, \bar{Y}) = \max\{\text{Dist}(\bar{X}, \bar{Y}), V_k(\bar{Y})\}$$

Local Outlier Factor (LOF) (cont.)

- $V_k(\bar{X})$: distance of \bar{X} to its k-nearest neighbor
- Reachability distance

$$R_k(\bar{X}, \bar{Y}) = \max\{\text{Dist}(\bar{X}, \bar{Y}), V_k(\bar{Y})\}$$

- Not symmetric
- Equal to simple distance for long distances
- Smoothed by $V_k(\bar{X})$ for short distances



Local Outlier Factor (LOF) (cont.)

- Reachability distance

$$R_k(\bar{X}, \bar{Y}) = \max\{\text{Dist}(\bar{X}, \bar{Y}), V_k(\bar{Y})\}$$

- Average reachability distance

$$AR_k(\bar{X}) = \underset{\bar{Y} \in L_k(\bar{X})}{E} [R_k(\bar{X}, \bar{Y})]$$

$L_k(\bar{X})$ is the set of points within distance $V_k(\bar{X})$ of \bar{X} (might be more than k due to ties)

Local Outlier Factor (LOF) (cont.)

$$R_k(\bar{X}, \bar{Y}) = \max\{\text{Dist}(\bar{X}, \bar{Y}), V_k(\bar{Y})\}$$

$$AR_k(\bar{X}) = \frac{E}{\bar{Y} \in L_k(\bar{X})} [R_k(\bar{X}, \bar{Y})]$$

- Local outlier factor

$$\text{LOF}_k(\bar{X}) = \frac{E}{\bar{Y} \in L_k(\bar{X})} \frac{AR_k(\bar{X})}{AR_k(\bar{Y})}$$

Outlier score

$$\max_k \text{LOF}_k(\bar{X})$$

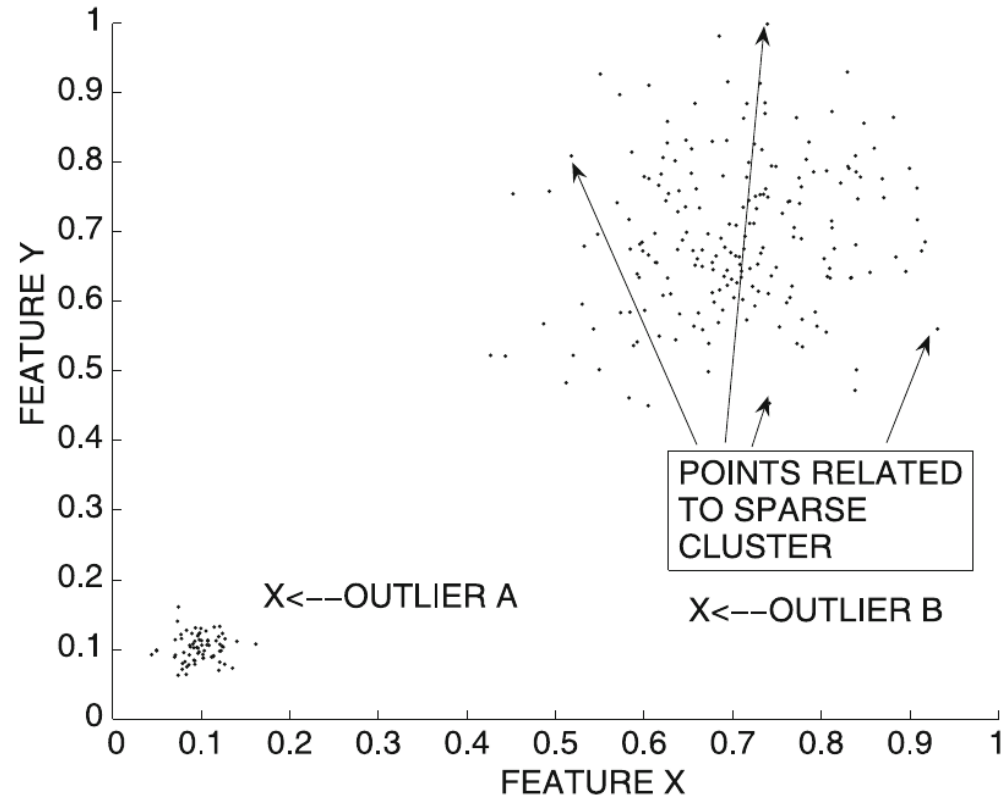
- Large for outliers, close to 1 for others

Local Outlier Factor (LOF) (cont.)

- Local outlier factor

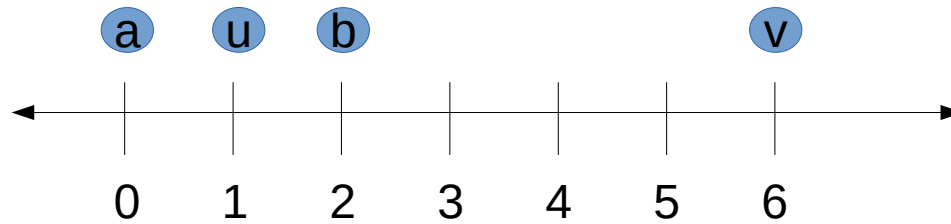
$$\text{LOF}_k(\bar{X}) = \frac{E}{\bar{Y} \in L_k(\bar{X})} \frac{AR_k(\bar{X})}{AR_k(\bar{Y})}$$

- LOF values for points inside a cluster are close to one if cluster is homogeneous
- LOF values much higher for outliers: they are computed in terms of average distances of near-by clusters



Try it!

compare outlier score $\text{LOF}(u)$, $\text{LOF}(v)$



- Let $k=2$
- $\text{LOF}_2(u) = E[\{ \text{AR}_2(u) / \text{AR}_2(a), \text{AR}_2(u) / \text{AR}_2(b) \}] = \underline{\hspace{2cm}}$
- $\text{LOF}_2(v) = E[\{ \text{AR}_2(v) / \text{AR}_2(b), \text{AR}_2(v) / \text{AR}_2(u) \}] = \underline{\hspace{2cm}}$
- $\text{AR}_2(u) = E[\{ R_k(u,a), R_k(u,b) \}] = \underline{\hspace{2cm}}$
- $\text{AR}_2(v) = E[\{ R_k(v,b), R_k(v,u) \}] = \underline{\hspace{2cm}}$
- $\text{AR}_2(a) = E[\{ R_k(a,u), R_k(a,b) \}] = \underline{\hspace{2cm}}$
- $\text{AR}_2(b) = E[\{ R_k(b,u), R_k(b,a) \}] = \underline{\hspace{2cm}}$
- $R_k(a,u) = \underline{\hspace{1cm}}; R_k(a,b) = \underline{\hspace{1cm}}; R_k(b,u) = \underline{\hspace{1cm}}; R_k(b,a) = \underline{\hspace{1cm}}$
- $R_k(u,a) = \underline{\hspace{1cm}}; R_k(u,b) = \underline{\hspace{1cm}}; R_k(v,b) = \underline{\hspace{1cm}}; R_k(v,u) = \underline{\hspace{1cm}}$
- $V_2 = \text{distance to 2}^{\text{nd}} \text{ nearest neighbor: } V_2(u) = \underline{\hspace{1cm}}; V_2(v) = \underline{\hspace{1cm}}; V_2(a) = \underline{\hspace{1cm}}; V_2(b) = \underline{\hspace{1cm}}$

$$\text{LOF}_k(\bar{X}) = E_{\bar{Y} \in L_k(\bar{X})} \frac{\text{AR}_k(\bar{X})}{\text{AR}_k(\bar{Y})}$$

$$\text{AR}_k(\bar{X}) = E_{\bar{Y} \in L_k(\bar{X})} [R_k(\bar{X}, \bar{Y})]$$

$$R_k(\bar{X}, \bar{Y}) = \max\{\text{Dist}(\bar{X}, \bar{Y}), V_k(\bar{Y})\}$$

Summary

Things to remember

- Isolation forest
- Clustering-based methods
- Distance-based methods

Exercises for TT19-TT21

- Data Mining, The Textbook (2015) by Charu Aggarwal
 - Exercises 8.11 → all except 10, 15, 16, 17