Outlier Detection:

Density and Partition-Based

Mining Massive Datasets

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Sources

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

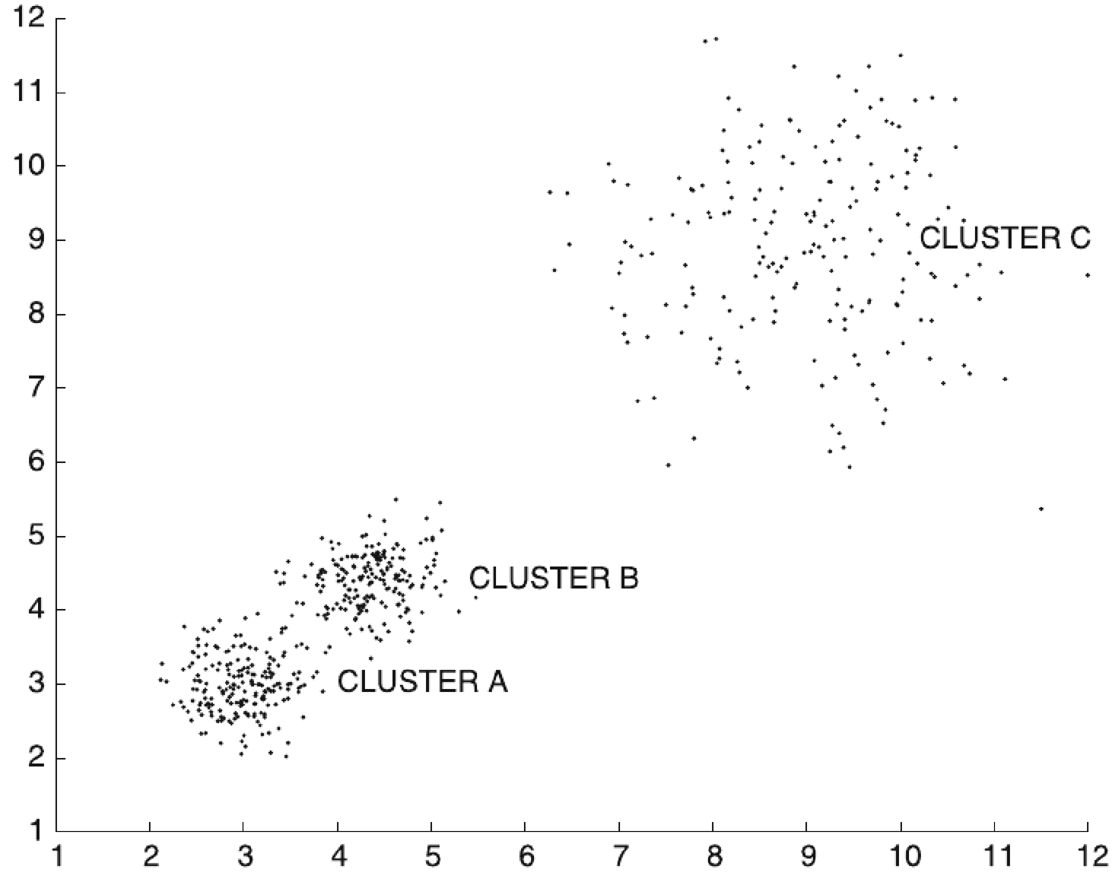
(1) Eryk Lewinson: Outlier detection with isolation forest (2018)

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

Density-based methods

Density-based methods

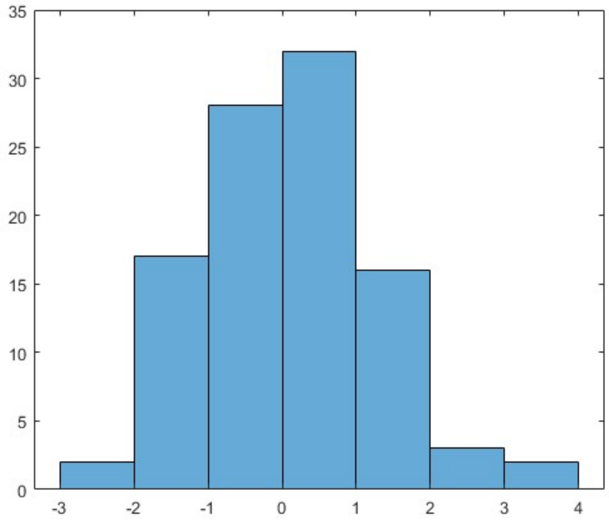
- Key idea:
  find sparse regions in the data
- Limitation:
  cannot handle variations of density



Histogram- and grid-based methods

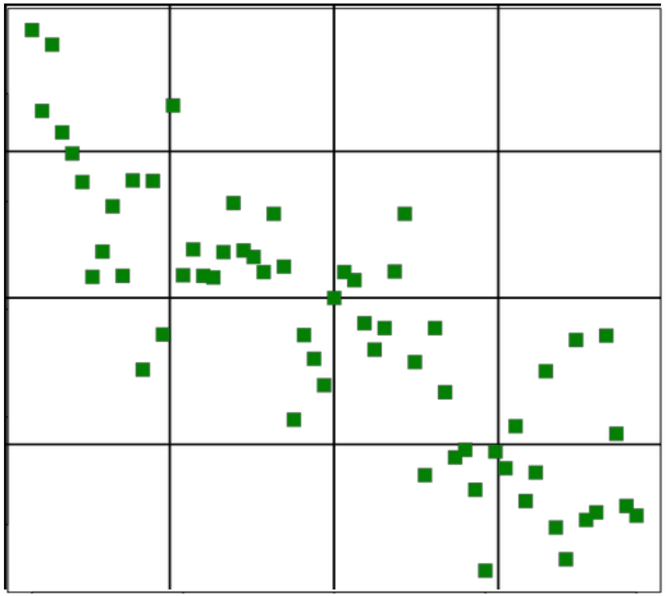
Histogram-based method:

1) Put data into **bins**
2) Outlier score: $num - 1$,
   where *num* is the number of items in the same **bin**



Clear outliers are alone or almost alone in a **bin**

Histogram- and grid-based methods



Grid-based method

1)Put data into a **grid**

2)Outlier score: $num - 1$,
where num is the number of items in the same **cell**

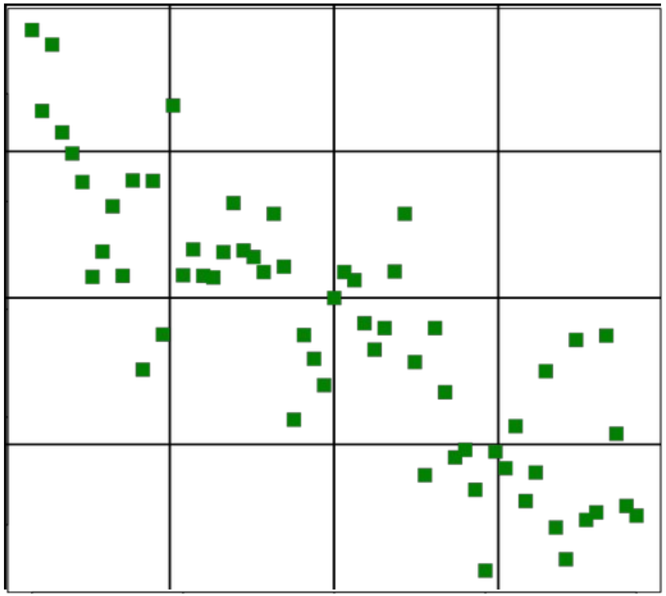
Clear outliers are alone or almost alone in a **cell**

Problems with grid-based methods

How to choose the grid size?

Grid size should be chosen considering data density, but density might vary across regions

If dimensionality is high, then most cells will be empty



Kernel-based methods

- Given n points $\overline{X_1}, \overline{X_2}, \ldots, \overline{X_n}$

$$f(\overline{X}) = \frac{1}{n} \sum_{i=1}^{n} K_h(\overline{X} - \overline{X_i})$$

- K_h is a function peaking at $\overline{X_i}$ with *bandwidth* h

- For instance, a Gaussian kernel:

$$K_h(\overline{X} - \overline{X_i}) = \left(\frac{1}{\sqrt{2\pi} \cdot h} \right)^d \cdot e^{-\|\overline{X} - \overline{X_i}\|^2/(2h^2)}$$

Kernel-based methods (cont.)

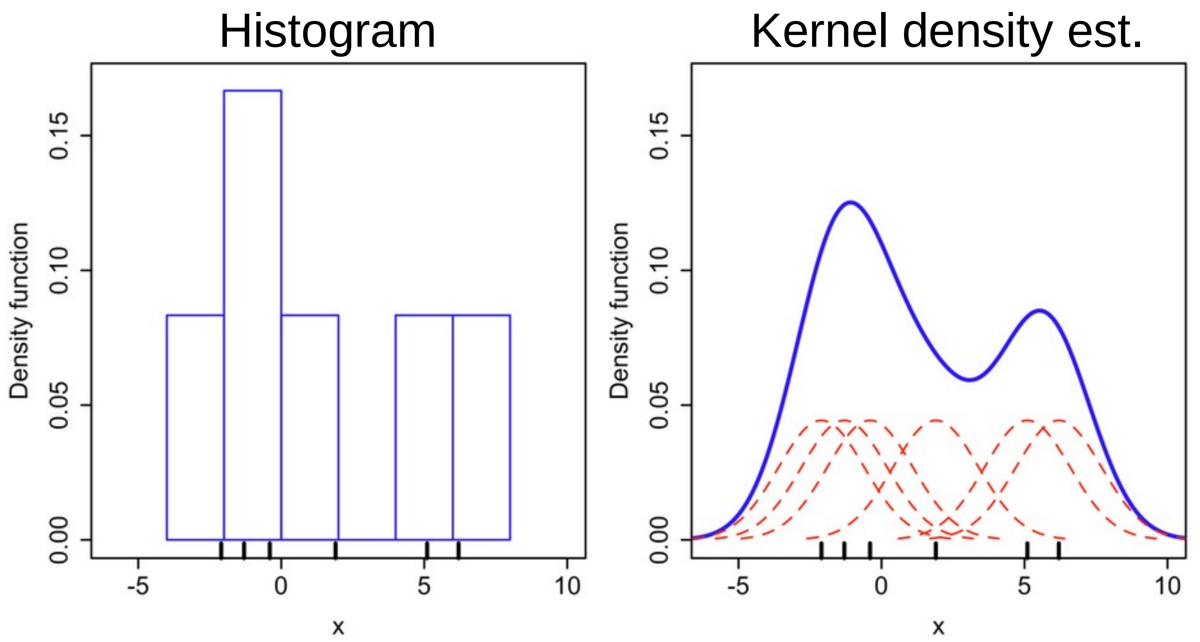
- Example with a Gaussian kernel

$$\overline{X} = < -2.1, -1.3, -0.4, 1.9, 5.1, 6.2 >$$

- Each K_h in red

- f = sum of K_h in blue

$$f(\overline{X}) = \frac{1}{n}\sum_{i=1}^{n} K_h(\overline{X} - \overline{X}_i)$$



[Wikipedia: Kernel density estimation]

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

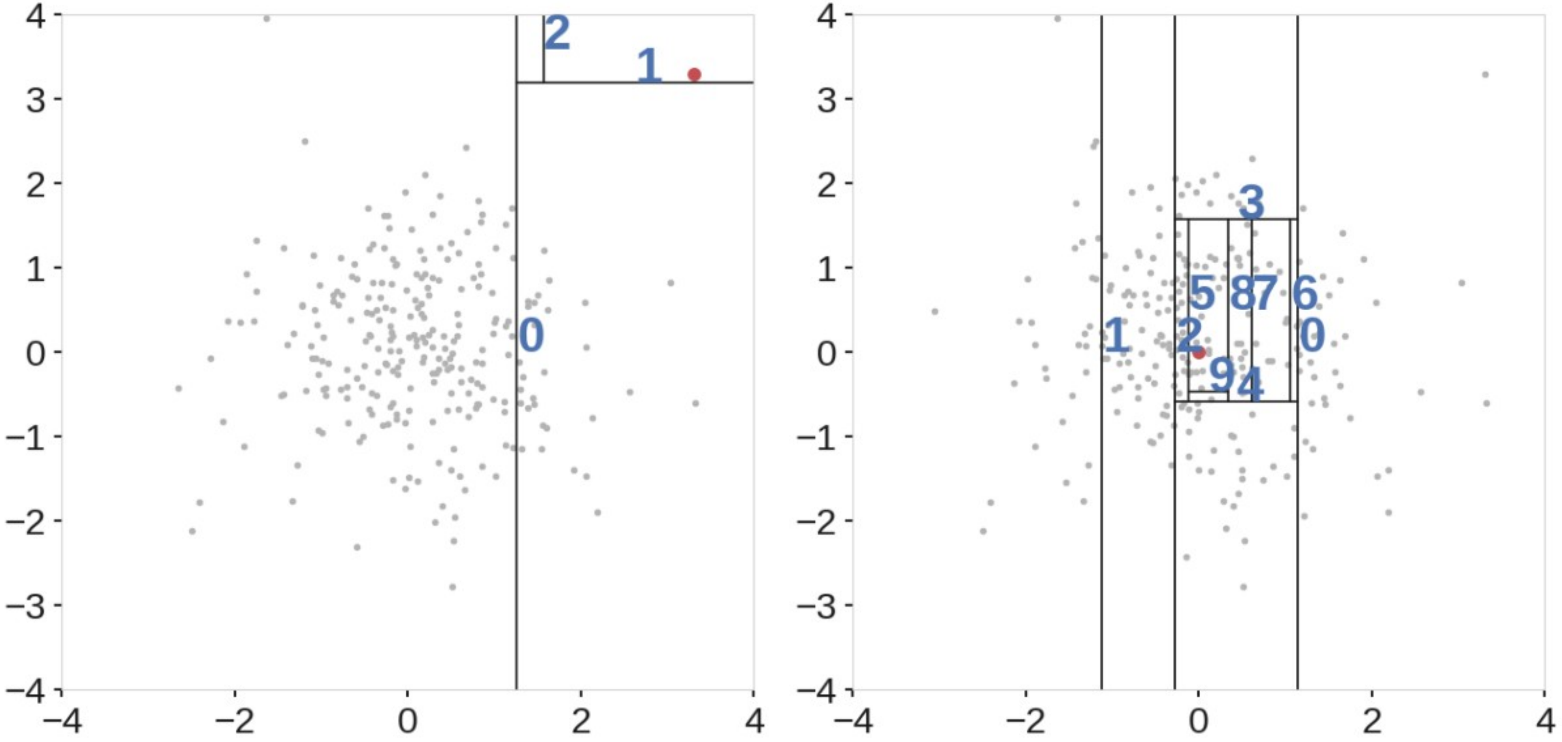
Stopping criteria for recursion

- 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

https://towardsdatascience.com/outlier-detection-with-extended-isolation-forest-1e248a3fe97b

Outlier score

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

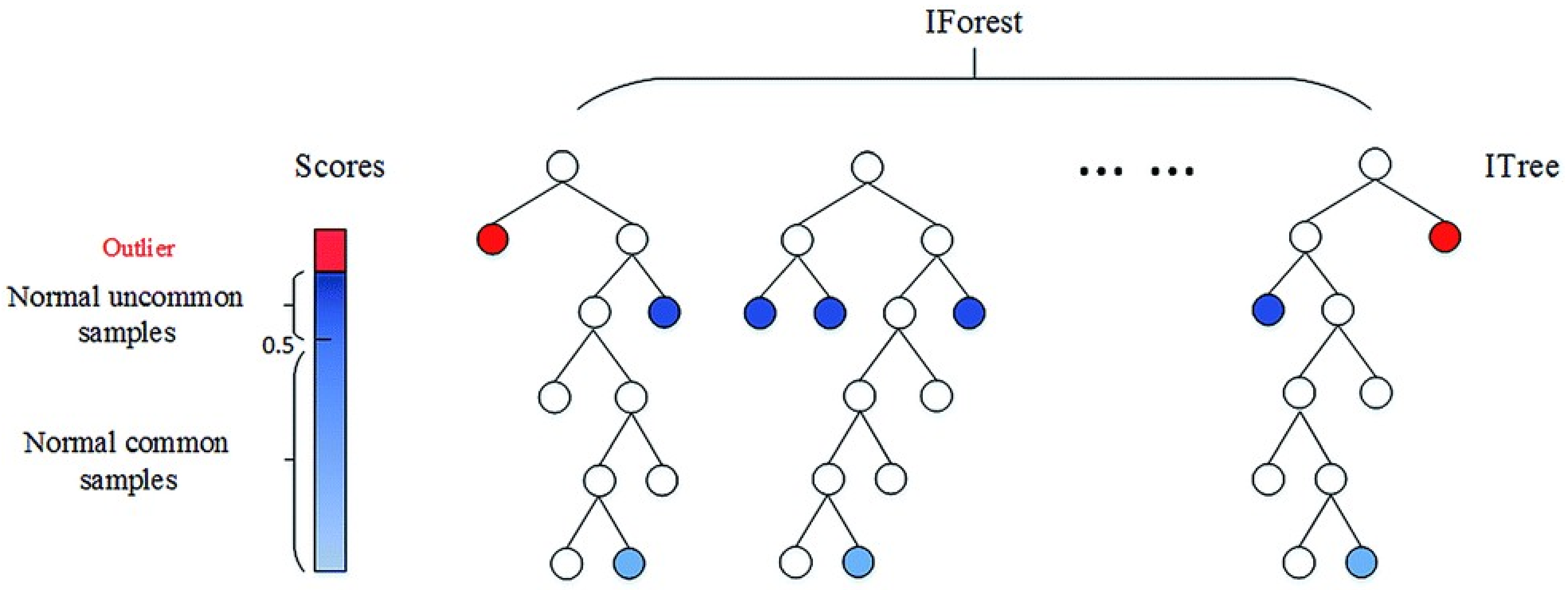
$$c(n) = 2H(n-1) - (2(n-1)/n) \qquad H(n) = \sum_{k=1}^{n} \frac{1}{k}$$

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

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

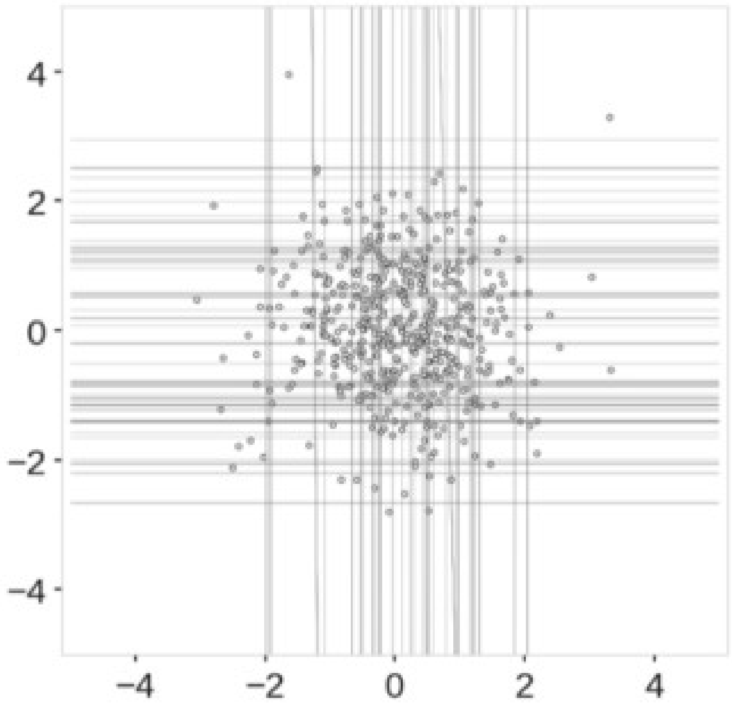
Outlier scores in isolation forests

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

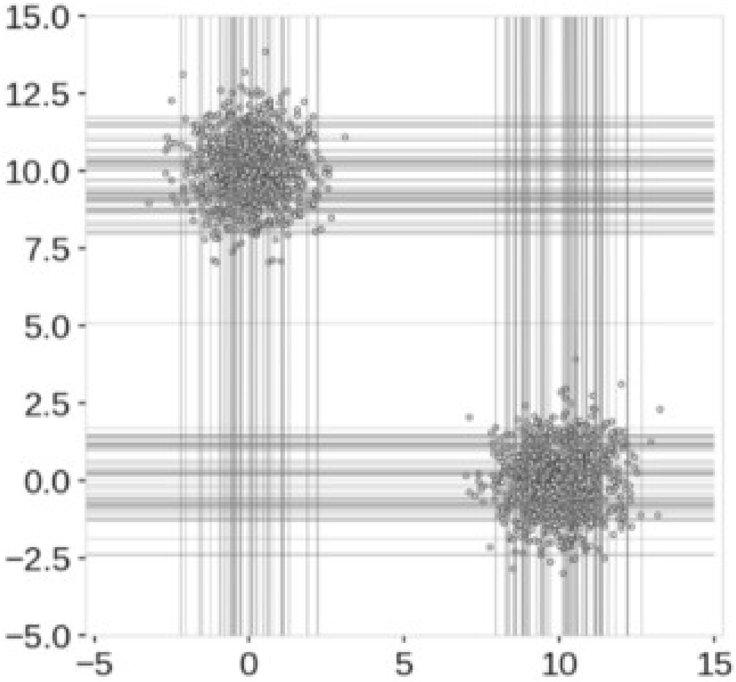


https://donghwa-kim.github.io/iforest.html

Example



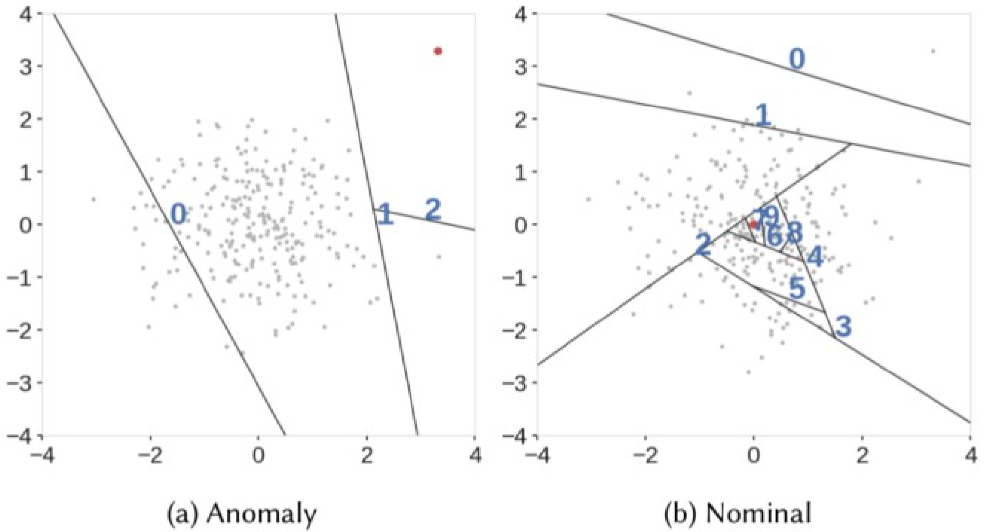
(a) Single blob



(b) Multiple Blobs

Extended Isolation Forest

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

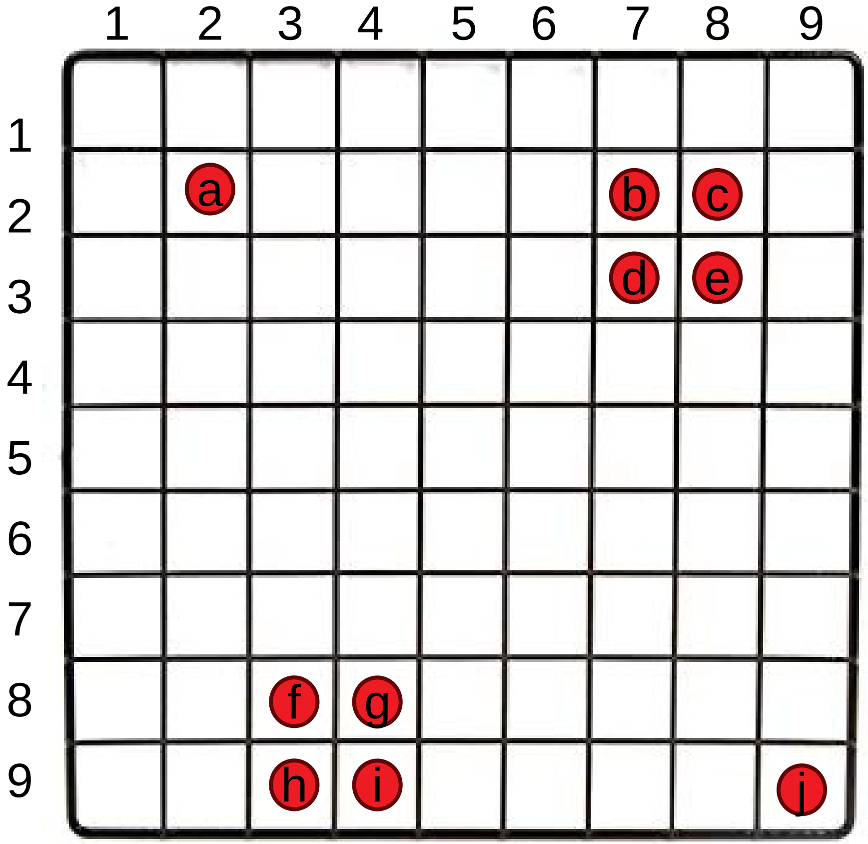


https://towardsdatascience.com/outlier-detection-with-extended-isolation-forest-1e248a3fe97b

Exercise

Answer in
Nearpod Draw-it

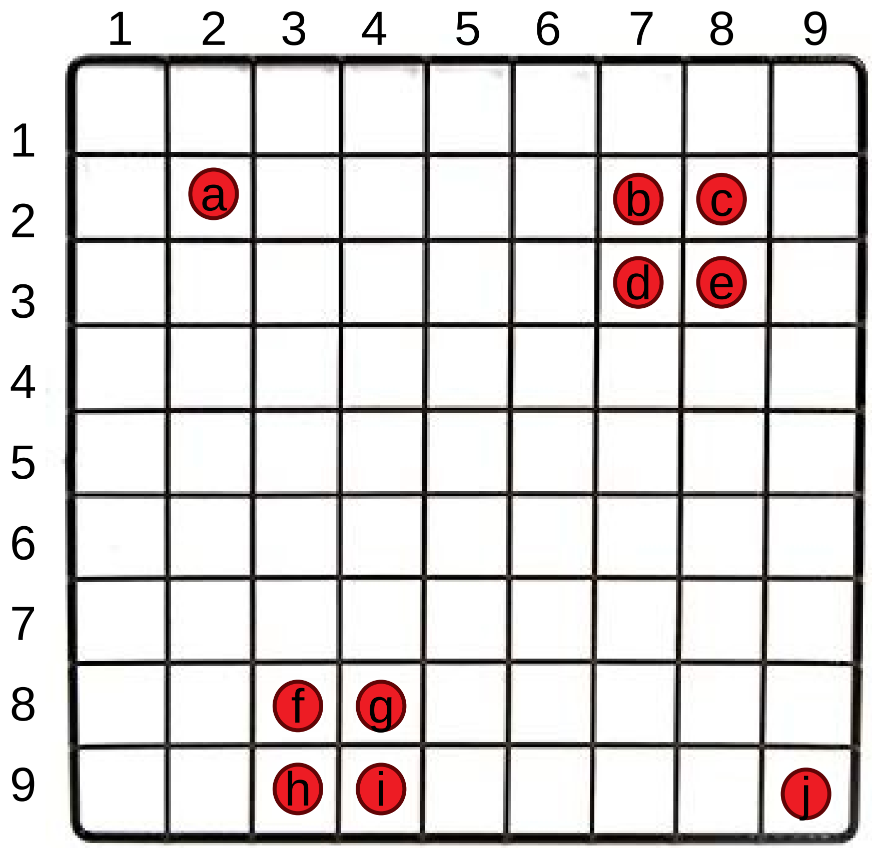
- Create one tree of the isolation forest by repeating 4 times:
  - Picking a sector containing >1 element
  - Picking a random dimension
  - Picking a random cut-off between min and max value along that dimension
- Draw the lines of your cuts
- Label each point with its depth h(x)



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) = 2xH(9) – (2x9/10) ≃ 3.857 ≃ **4**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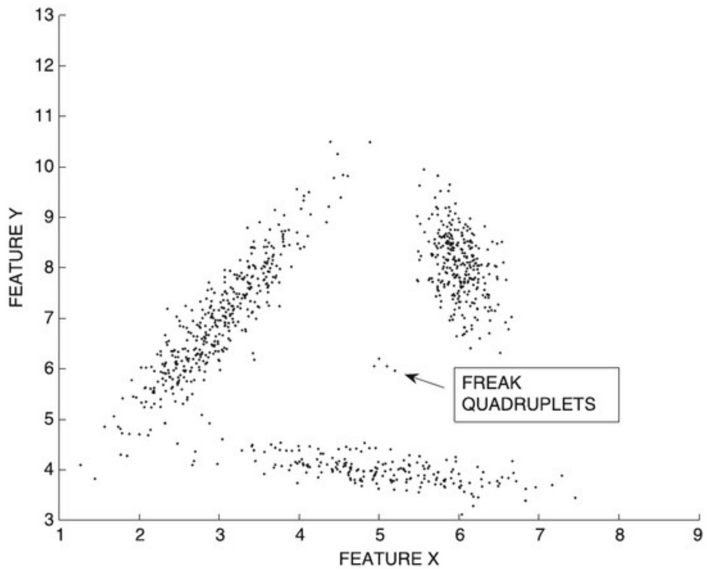
Additional materials

[NOT FOR THE EXAM]

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 $k > 3$

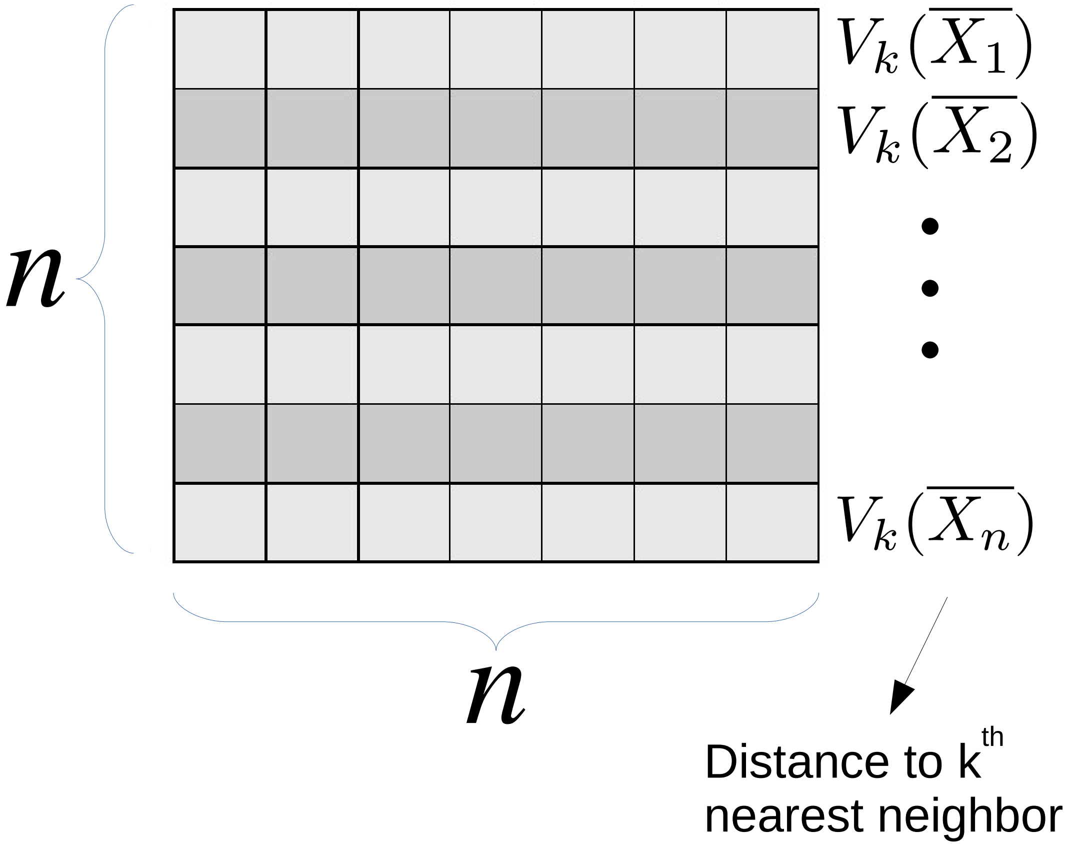


Problem: computational cost

- 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

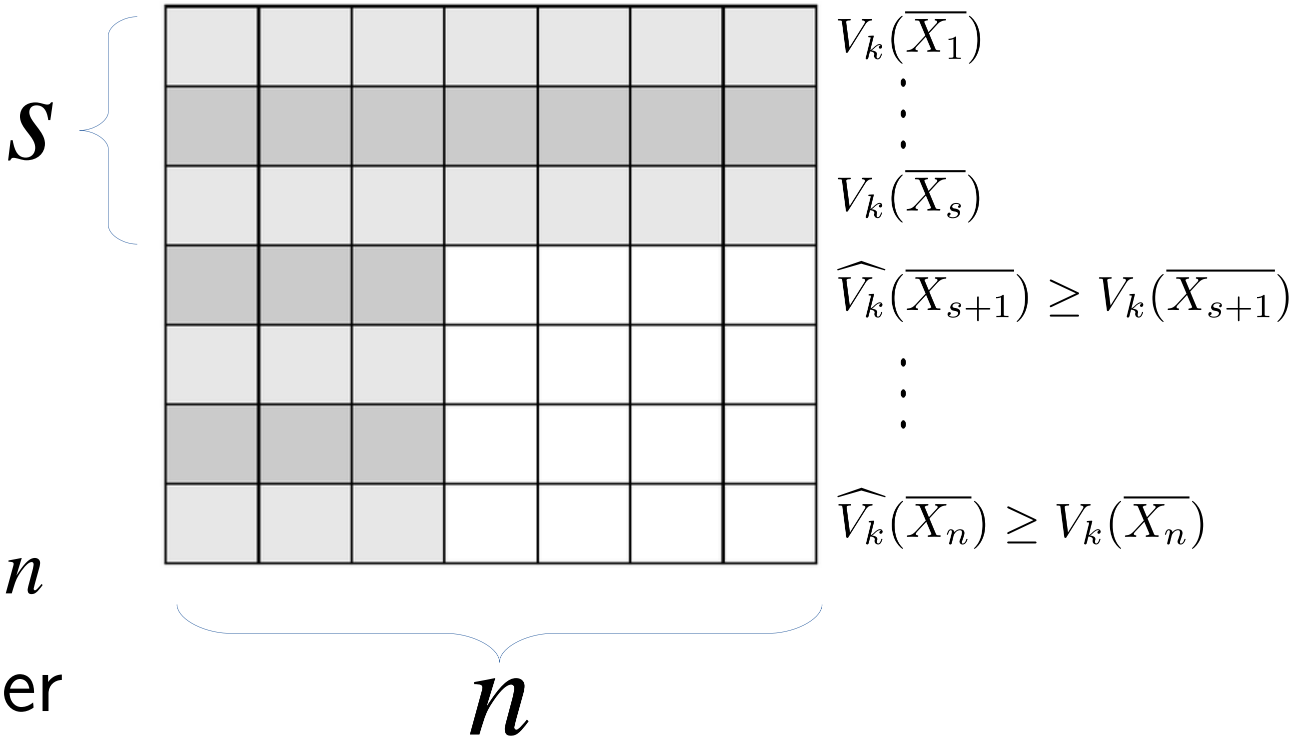
Problem: computational cost

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



Pruning method: sampling

- Evaluate s x n distances
- For points *1…s* we are OK
- For points *(s+1)…n* we know only upper bounds



Pruning method: sampling (cont.)

From points

$1 \ldots s$ we already know the

"winners"

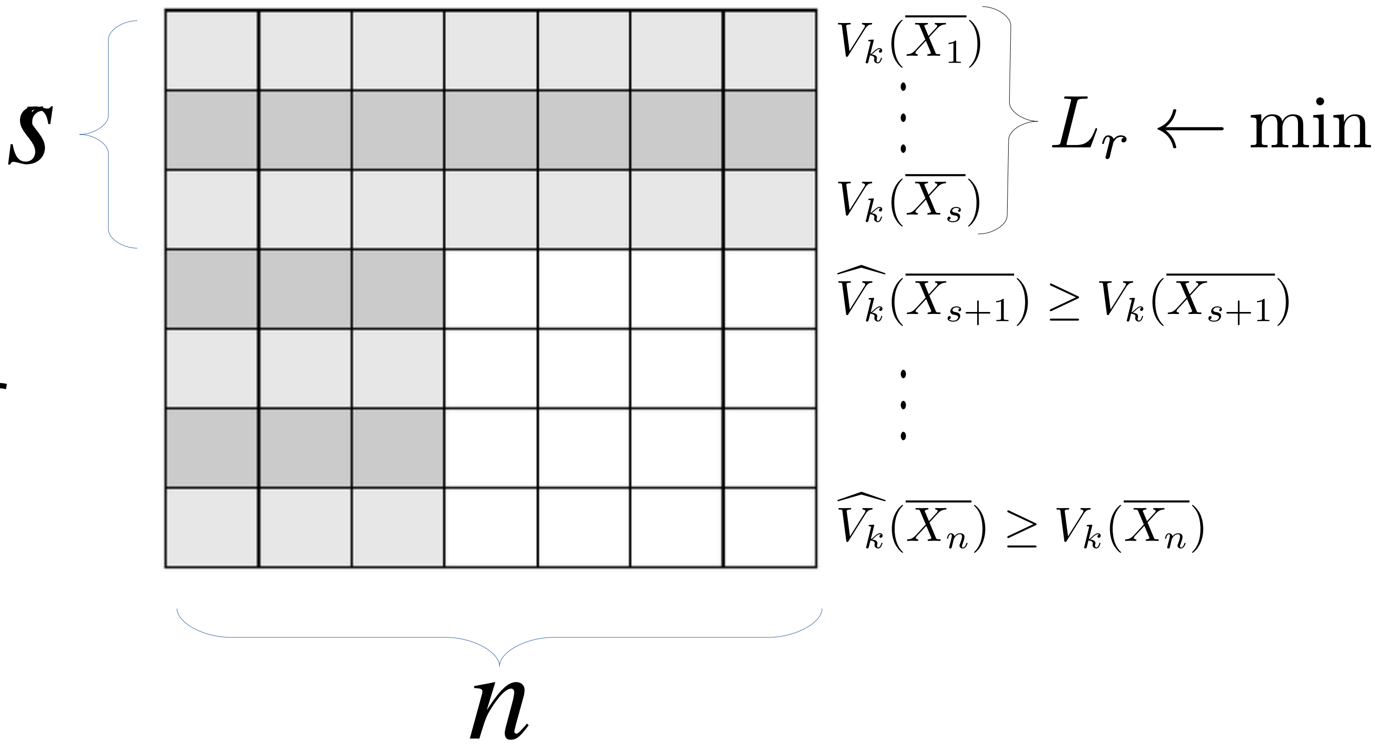
($r \leq s$ nodes with the larger distance to their

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 s

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($r \leq s$ nodes with the larger distance to their

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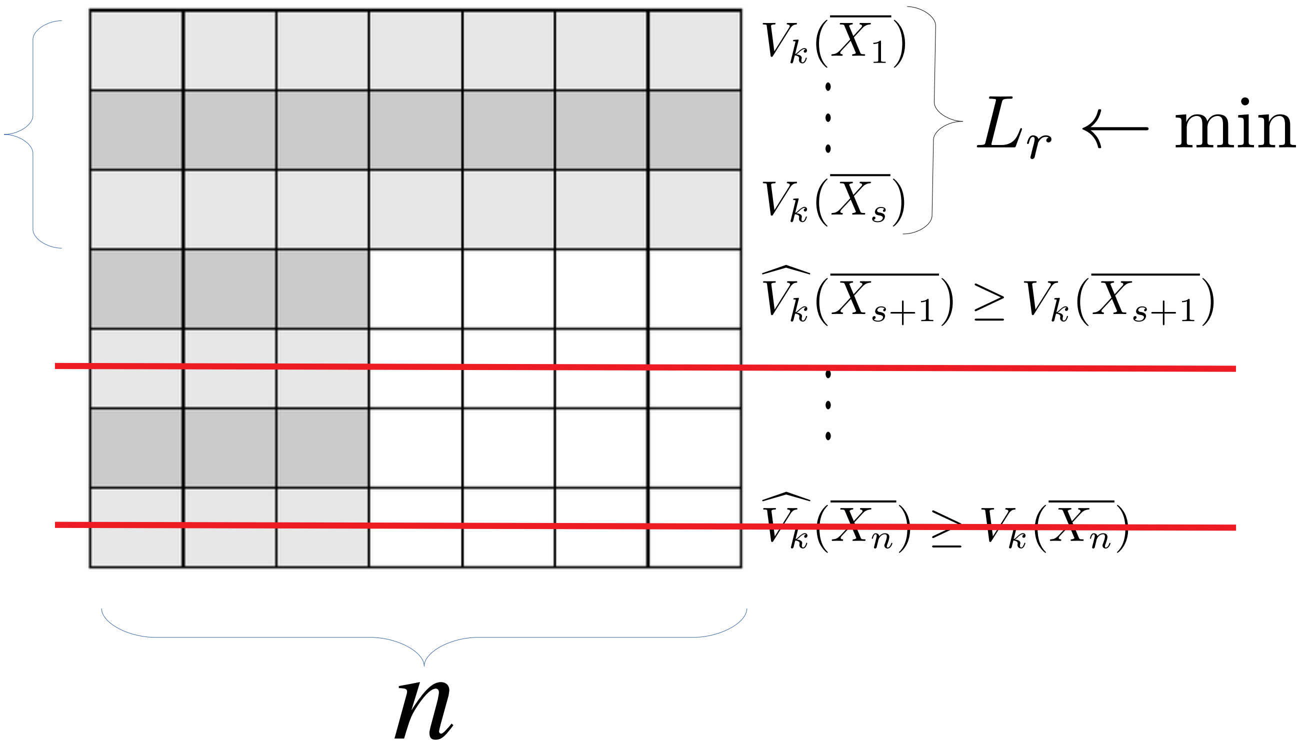


Any point having

$V_k < L_s$ cannot be among

the top r outliers

Pruning method: sampling (cont.)

Remove points

having $\widehat{V_k} \leq L_r$

Update L_r keeping

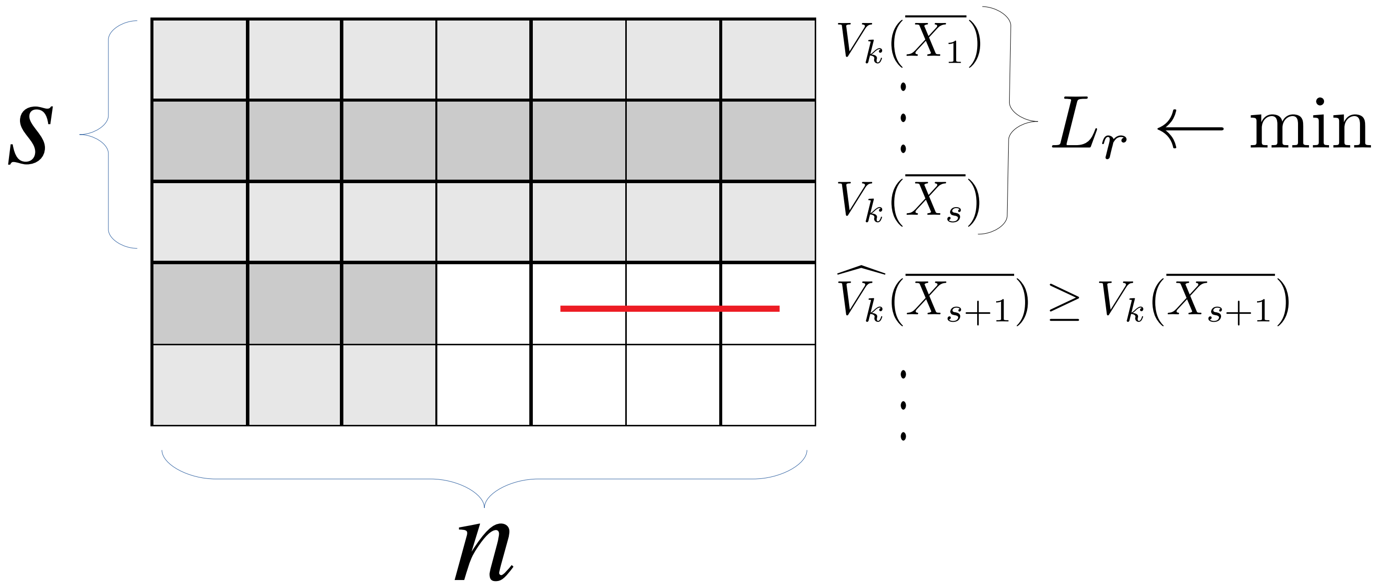
r largest values, and

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

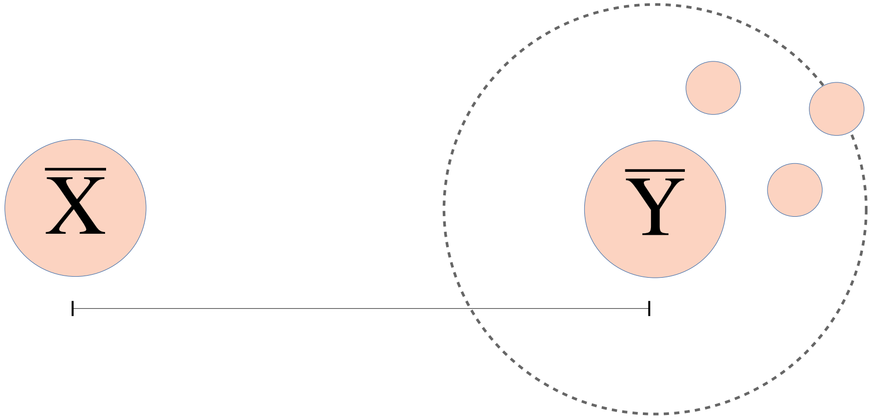
$$R_k(\overline{X}, \overline{Y}) = \max\{\mathrm{Dist}(\overline{X}, \overline{Y}), V_k(\overline{Y})\}$$

Local Outlier Factor (LOF) (cont.)

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

$$R_k(\overline{X}, \overline{Y}) = \max\{\mathrm{Dist}(\overline{X}, \overline{Y}), V_k(\overline{Y})\}$$

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



Local Outlier Factor (LOF) (cont.)

- Reachability distance

$$R_k(\overline{X}, \overline{Y}) = \max\{\mathrm{Dist}(\overline{X}, \overline{Y}), V_k(\overline{Y})\}$$

- Average reachability distance

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

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

Local Outlier Factor (LOF) (cont.)

$$R_k(\overline{X}, \overline{Y}) = \max\{\mathrm{Dist}(\overline{X}, \overline{Y}), V_k(\overline{Y})\}$$

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

- Local outlier factor

$$\mathrm{LOF}_k(\overline{X}) = \underset{\overline{Y} \in L_k(\overline{X})}{E} \frac{AR_k(\overline{X})}{AR_k(\overline{Y})}$$

Outlier score

$$\max_k \mathrm{LOF}_k(\overline{X})$$

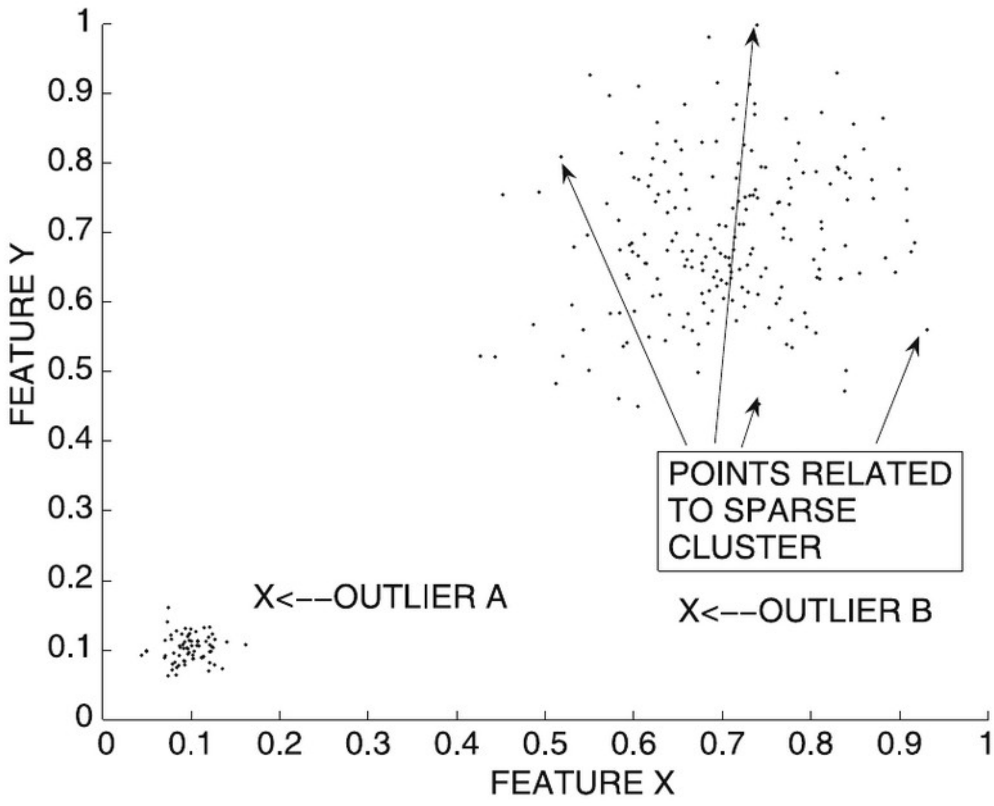
- Large for outliers, close to 1 for others

Local Outlier Factor (LOF) (cont.)

- Local outlier factor

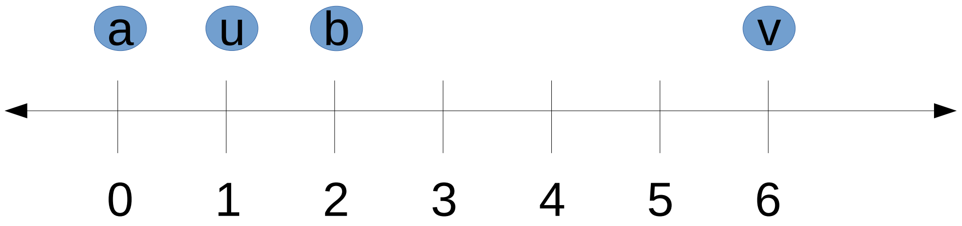
$$\mathrm{LOF}_k(\overline{X}) = \underset{\overline{Y} \in L_k(\overline{X})}{E} \frac{AR_k(\overline{X})}{AR_k(\overline{Y})}$$

- 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 **LOF(u), LOF(v)**



- Let k=2
- $LOF_2(u) = E[\ \{AR_2(u)\ /AR_2(a),\ AR_2(u)/AR_2(b)\}] =$ ________
- $LOF_2(v) = E[\ \{AR_2(v)\ /AR_2(b),\ AR_2(v)/AR_2(u)\}] =$ ________
- $AR_2(u) = E[\ \{R_k(u,a),\ R_k(u,b)\ \}] =$ _______
- $AR_2(v) = E[\ \{R_k(v,b),\ R_k(v,u)\ \}] =$ _______
- $AR_2(a) = E[\ \{R_k(a,u),\ R_k(a,b)\ \}] =$ ______
- $AR_2(b) = E[\ \{R_k(b,u),\ R_k(b,a)\ \}] =$ ______
- **$R_k(a,u)$ = ____;** $R_k(a,b) =$ _____; $R_k(b,u) =$ ______; $R_k(b,a) =$ _______
- $R_k(u,a) =$ _____; $R_k(u,b) =$ ______; $R_k(v,b) =$ _______; $R_k(v,u) =$ ______
- V_2 = distance to 2nd nearest neighbor: $V_2(u) =$ _____ ; $V_2(v) =$ _____; $V_2(a) =$ _____ ; $V_2(b) =$ _____

$$\mathrm{LOF}_k(\overline{X}) = \underset{\overline{Y} \in L_k(\overline{X})}{E} \frac{AR_k(\overline{X})}{AR_k(\overline{Y})}$$

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

$$R_k(\overline{X}, \overline{Y}) = \max\{\mathrm{Dist}(\overline{X}, \overline{Y}), V_k(\overline{Y})\}$$

Summary

Things to remember

- Density-based methods
- Isolation forest
- Distance-based methods

Exercises for TT19-TT21

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