DATA MINING 2
Anomaly & Outliers Detection

Riccardo Guidotti

a.a. 2020/2021

Slides edited from Tan, Steinbach, Kumar, Introduction to Data Mining and from Kriegel, Kröger, Zimek Tutorial on Outlier Detection Techniques

UNIVERSITÀ DI PISA

What is an Outlier?

Definition of Hawkins [Hawkins 1980]:

- "An outlier is an observation which deviates so much from the other observations as to arouse suspicions that it was generated by a different mechanism"

Statistics-based intuition

- Normal data objects follow a "generating mechanism", e.g. some given statistical process
- Abnormal objects deviate from this generating mechanism

Anomaly/Outlier Detection

- What are anomalies/outliers?
  - The set of data points that are considerably different than the remainder of the data

- Natural implication is that anomalies are relatively rare
  - One in a thousand occurs often if you have lots of data
  - Context is important, e.g., freezing temps in July

- Can be important or a nuisance
  - 10 foot tall 2 year old
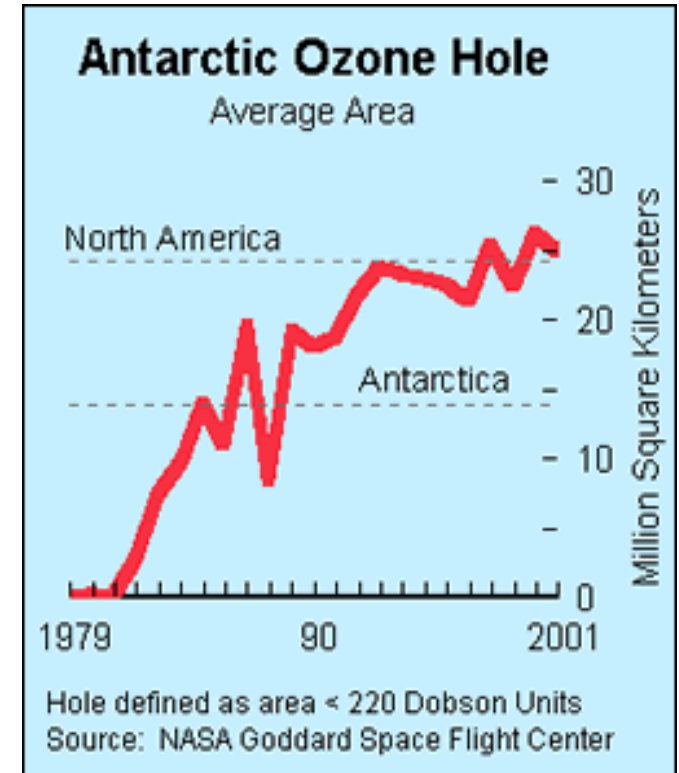 - Unusually high blood pressure
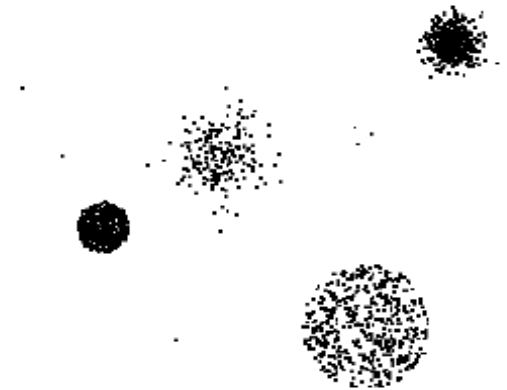
Applications of Outlier Detection

- Fraud detection
  - Purchasing behavior of a credit card owner usually changes when the card is stolen
  - Abnormal buying patterns can characterize credit card abuse
- Medicine
  - Unusual symptoms or test results may indicate potential health problems of a patient
  - Whether a particular test result is abnormal may depend on other characteristics of the patients (e.g. gender, age, …)
- Public health
  - The occurrence of a particular disease, e.g. tetanus, scattered across various hospitals of a city indicate problems with the corresponding vaccination program in that city
  - Whether an occurrence is abnormal depends

Importance of Anomaly Detection

Ozone Depletion History

- In 1985 three researchers (Farman, Gardinar and Shanklin) were puzzled by data gathered by the British Antarctic Survey showing that ozone levels for Antarctica had dropped 10% below normal levels

- Why did the Nimbus 7 satellite, which had instruments aboard for recording ozone levels, not record similarly low ozone concentrations?

- The ozone concentrations recorded by the satellite were so low they were being treated as outliers by a computer program and discarded!

Antarctic Ozone Hole
Average Area
North America
Antarctica
Million Square Kilometers
30
20
10
0
1979   90   2001
Hole defined as area < 220 Dobson Units
Source: NASA Goddard Space Flight Center

Causes of Anomalies

- Data from different classes
  - Measuring the weights of oranges, but a few grapefruit are mixed in

- Natural variation
  - Unusually tall people

- Data errors
  - 200 pound 2 year old

Distinction Between Noise and Anomalies

- Noise is erroneous, perhaps random, values or contaminating objects
  - Weight recorded incorrectly
  - Grapefruit mixed in with the oranges

- Noise doesn't necessarily produce unusual values or objects

- Noise is not interesting

- Anomalies may be interesting if they are not a result of noise

- Noise and anomalies are related but distinct concepts

General Issues: Number of Attributes

- Many anomalies are defined in terms of a single attribute
  - Height
  - Shape
  - Color

- Can be hard to find an anomaly using all attributes
  - Noisy or irrelevant attributes
  - Object is only anomalous with respect to some attributes

- However, an object may not be anomalous in any one attribute

General Issues: Anomaly Scoring

- Many anomaly detection techniques provide only a binary categorization
  - An object is an anomaly or it isn't
  - This is especially true of classification-based approaches

- Other approaches assign a score to all points
  - This score measures the degree to which an object is an anomaly
  - This allows objects to be ranked

- In the end, you often need a binary decision
  - Should this credit card transaction be flagged?
  - Still useful to have a score
- How many anomalies are there?

Other Issues for Anomaly Detection

- Find all anomalies at once or one at a time
  - Swamping
  - Masking

- Evaluation
  - How do you measure performance?
  - Supervised vs. unsupervised situations

- Efficiency

- Context

Variants of Anomaly Detection Problems

- Given a data set D, find all data points $\mathbf{x} \in$ D with anomaly scores greater than some threshold t

- Given a data set D, find all data points $\mathbf{x} \in$ D having the top-n largest anomaly scores

- Given a data set D, containing mostly normal (but unlabeled) data points, and a test point $\mathbf{x}$, compute the anomaly score of $\mathbf{x}$ with respect to D

Model-Based Anomaly Detection

Build a model for the data and see

- Unsupervised
  - Anomalies are those points that don't fit well
  - Anomalies are those points that distort the model
  - Examples:
    - Statistical distribution
    - Clusters
    - Regression
    - Geometric
    - Graph

- Supervised
  - Anomalies are regarded as a rare class
  - Need to have training data

Machine Learning for Outlier Detection

- If the ground truth of anomalies is available we can prepare a classification problem to unveil outliers.

- As classifiers we can use all the available machine learning approaches: Ensembles, SVM, DNN.

- The problem is that the dataset would be very unbalanced

- Thus, ad-hoc formulations/implementation should be adopted.

Additional Anomaly Detection Techniques

- **Proximity-based**
  - Anomalies are points far away from other points
  - Can detect this graphically in some cases

- **Density-based**
  - Low density points are outliers

- **Pattern matching**
  - Create profiles or templates of atypical but important events or objects
  - Algorithms to detect these patterns are usually simple and efficient

Outliers Detection Approaches Classification

- **Global vs local** outlier detection
  - Considers the set of reference objects relative to which each point's "outlierness" is judged

- **Labeling vs scoring** outliers
  - Considers the output of an algorithm

- **Modeling properties**
  - Considers the concepts based on which "outlierness" is modeled

Global versus Local Approaches

- Considers the resolution of the reference set w.r.t. which the "outlierness" of a particular data object is determined
- **Global approaches**
  - The reference set contains all other data objects
  - Basic assumption: there is only one normal mechanism
  - Basic problem: other outliers are also in the reference set and may falsify the results
- **Local approaches**
  - The reference contains a (small) subset of data objects
  - No assumption on the number of normal mechanisms
  - Basic problem: how to choose a proper reference set
- Notes
  - Some approaches are somewhat in between
  - The resolution of the reference set is varied e.g. from only a single object (local) to the entire database (global) automatically or by a user-defined input parameter

Labeling versus Scoring

- Considers the output of an outlier detection algorithm
- **Labeling approaches**
  - Binary output
  - Data objects are labeled either as normal or outlier
- **Scoring approaches**
  - Continuous output
  - For each object an outlier score is computed (e.g. the probability for being an outlier)
  - Data objects can be sorted according to their scores
- Notes
  - Many scoring approaches focus on determining the top-n outliers (parameter n is usually given by the user)
  - Scoring approaches can usually also produce binary output if necessary (e.g. by defining a suitable threshold on the scoring values)

Model-based Approaches

Approaches classified by the properties of the underlying modeling

- Rational
  - Apply a model to represent normal data points
  - Outliers are points that do not fit to that model

- Sample approaches
  - Probabilistic tests based on statistical models
  - Depth-based approaches
  - Deviation-based approaches
  - Some subspace outlier detection approaches

Model-based Approaches

Proximity-based Approaches

- Rational
    - Examine the spatial proximity of each object in the data space
    - If the proximity of an object considerably deviates from the proximity of other objects it is considered an outlier

- Sample approaches
    - Distance-based approaches
    - Density-based approaches
    - Some subspace outlier detection approaches

Model-based Approaches

Angle-based approaches

- Rational
  - Examine the spectrum of pairwise angles between a given point and all other points
  - Outliers are points that have a spectrum featuring high fluctuation

Visual Approaches

- Boxplots or Scatter plots

- Limitations
  - Not automatic
  - Subjective
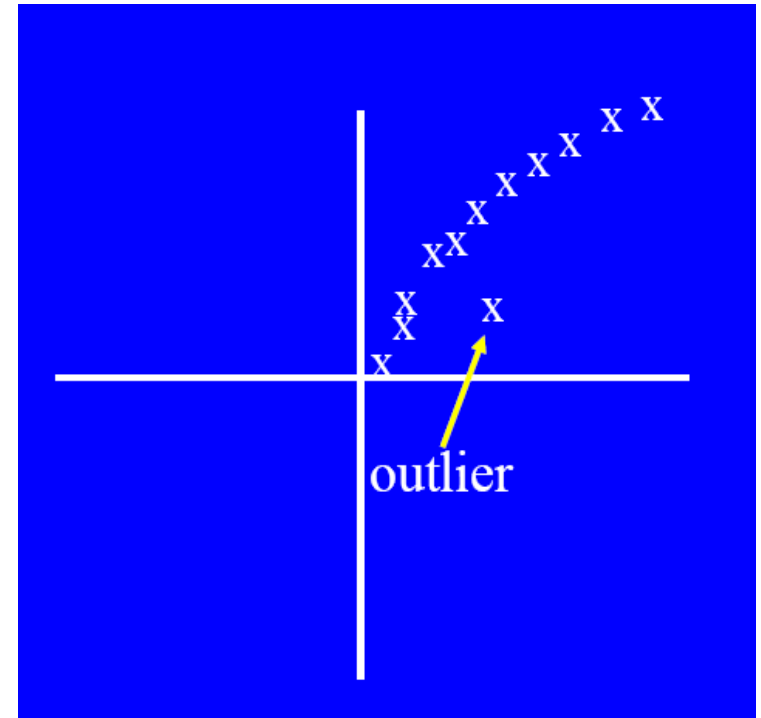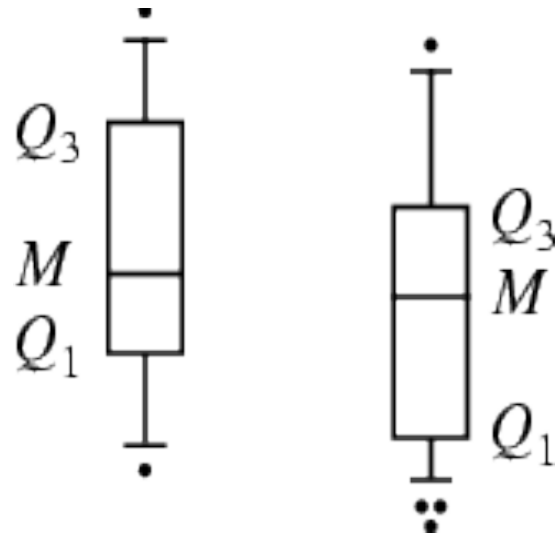
From Visual Box-plot to Automatic Approach

- The IQR of a set of values is calculated as the difference between the upper and lower quartiles, Q3 and Q1. *IQR = Q3 - Q1*

- x is an outlier if *x < Q1 − k IQR* or *x > Q3 + k IQR* (generally k=1.5)

- In a boxplot, the highest and lowest occurring value within this limit are indicated by *whiskers* of the box and any outliers as individual points.
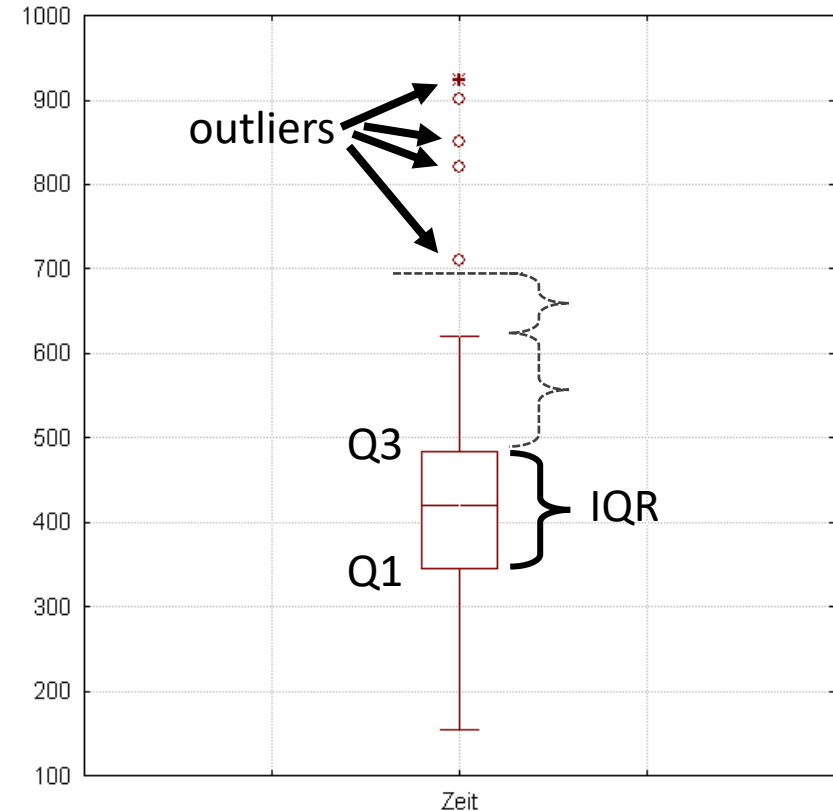
Statistical Approaches

Statistical Approaches

Probabilistic definition of an outlier: An outlier is an object that has a low probability with respect to a probability distribution model of the data.

- Usually assume a parametric model describing the distribution of the data (e.g., normal distribution)

- Apply a statistical test that depends on
  - Data distribution
  - Parameters of distribution (e.g., mean, variance)
  - Number of expected outliers (confidence limit)

- Issues
  - Identifying the distribution of a data set
    - Heavy tailed distribution
  - Number of attributes
  - Is the data a mixture of distributions?

Normal Distributions
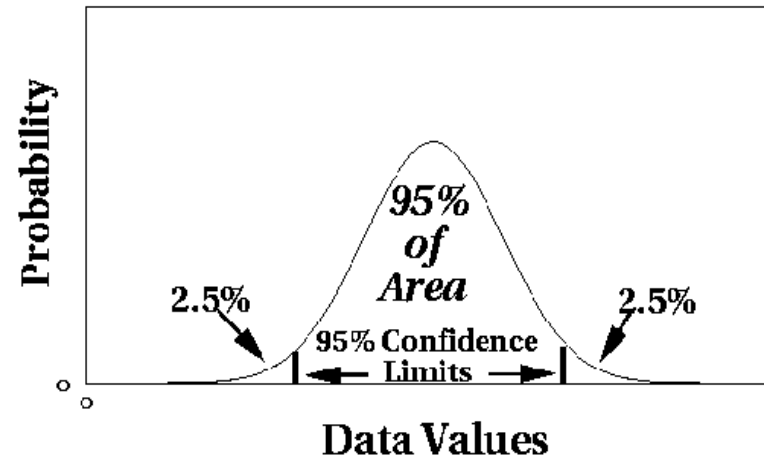
One-dimensional Gaussian
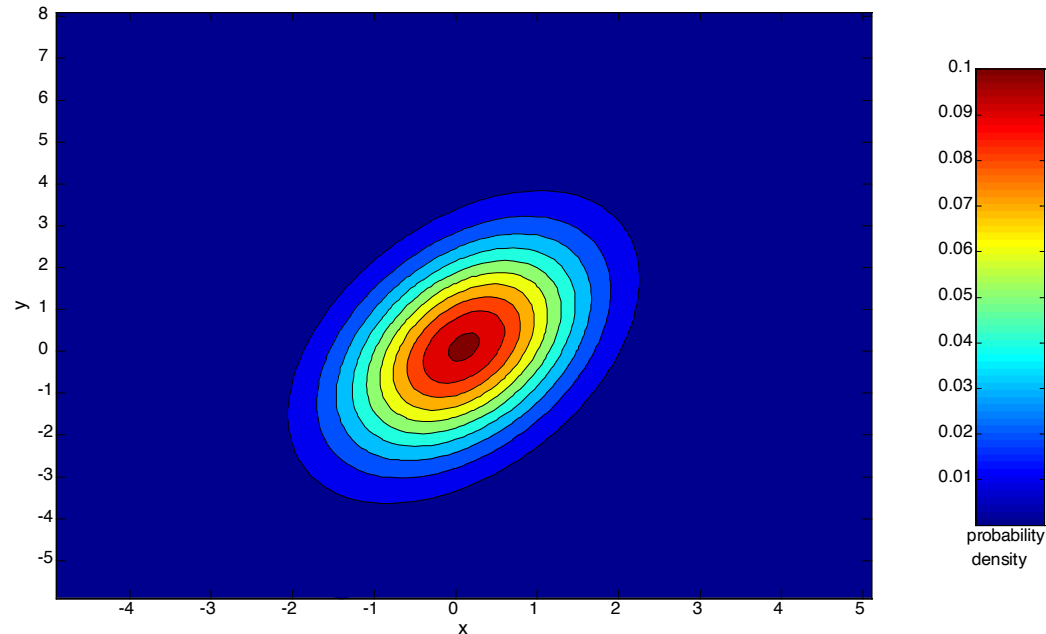
Two-dimensional Gaussian

Statistical-based – Grubbs' Test

- Detect outliers in univariate data

- Assume data comes from normal distribution

- Detects one outlier at a time, remove the outlier, and repeat
  - H_0: There is no outlier in data
  - H_A: There is at least one outlier

- Grubbs' test statistic:

  one-sided test with alpha/N
  two-sided test with alpha/2N

$$G = \frac{\max\left|X - \overline{X}\right|}{s}$$

mean

std dev

alpha significance
t – Student's distribution

- Reject null hypothesis H_0 of no outliers if:

$$G > \frac{(N-1)}{\sqrt{N}} \sqrt{\frac{t^2_{(\alpha/N, N-2)}}{N - 2 + t^2_{(\alpha/N, N-2)}}}$$

degrees of freedom

upper critical value of t-distribution

Statistical-based – Likelihood Approach

- Assume the data set D contains samples from a mixture of two probability distributions:
    - M (majority distribution)
    - A (anomalous distribution)
- General Approach:
    - Initially, assume all the data points belong to M
    - Let $L_t(D)$ be the log likelihood of D at time t
    - For each point x_t that belongs to M, move it to A
        - Let $L_{t+1}(D)$ be the new log likelihood.
        - Compute the difference, $\Delta = L_t(D) - L_{t+1}(D)$
        - If $\Delta > c$ (some threshold), then x_t is declared as an anomaly and moved permanently from M to A

Statistical-based – Likelihood Approach

- Data distribution, *D = (1 − λ) M + λ A*

- *M* is a probability distribution estimated from data
  - Can be based on any modeling method (naïve Bayes, maximum entropy, etc.)

- *A* is initially assumed to be uniform distribution

- Likelihood at time t:

$$L_t(D) = \prod_{i=1}^{N} P_D(x_i) = \left((1-\lambda)^{|M_t|} \prod_{x_i \in M_t} P_{M_t}(x_i) \right) \left(\lambda^{|A_t|} \prod_{x_i \in A_t} P_{A_t}(x_i) \right)$$

$$LL_t(D) = |M_t| \log(1-\lambda) + \sum_{x_i \in M_t} \log P_{M_t}(x_i) + |A_t| \log \lambda + \sum_{x_i \in A_t} \log P_{A_t}(x_i)$$

Strengths/Weaknesses of Statistical Approaches

Pros

- Firm mathematical foundation
- Can be very efficient
- Good results if distribution is known

Cons

- In many cases, data distribution may not be known
- For high dimensional data, it may be difficult to estimate the true distribution
- Anomalies can distort the parameters of the distribution
  - Mean and standard deviation are very sensitive to outliers

Depth-based Approaches

Depth-based Approaches

- General idea
  - Search for outliers at the border of the data space but independent of statistical distributions
  - Organize data objects in convex hull layers
  - Outliers are objects on outer layers

- Basic assumption
  - Outliers are located at the border of the data space
  - Normal objects are in the center of the data space
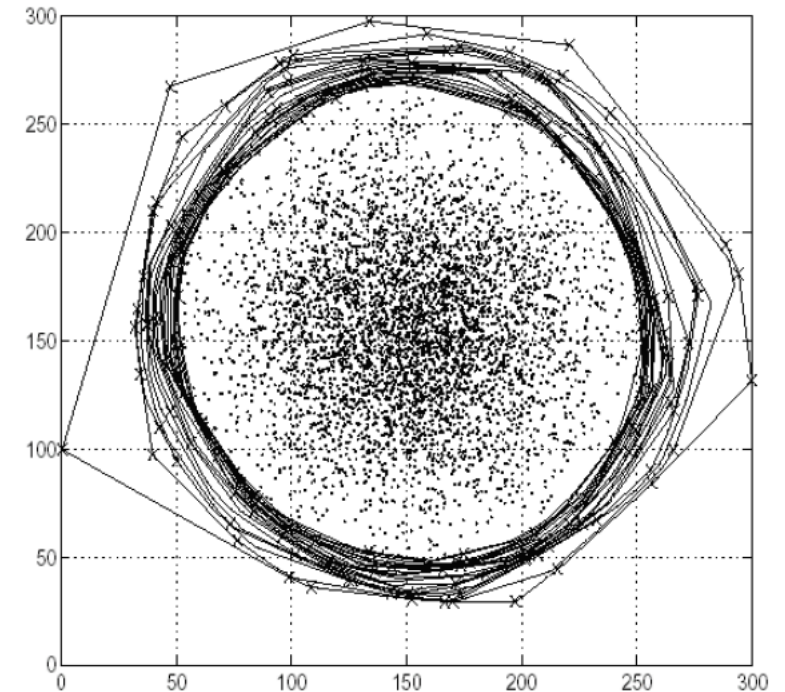
Depth-based Approaches

Model [Tukey 1977]

- Points on the convex hull of the full data space have depth = 1

- Points on the convex hull of the data set after removing all points with depth = 1 have depth = 2

- – …

- Points having a depth ≤ k are reported as outliers

(a) the data set   (b) depths and convex hulls
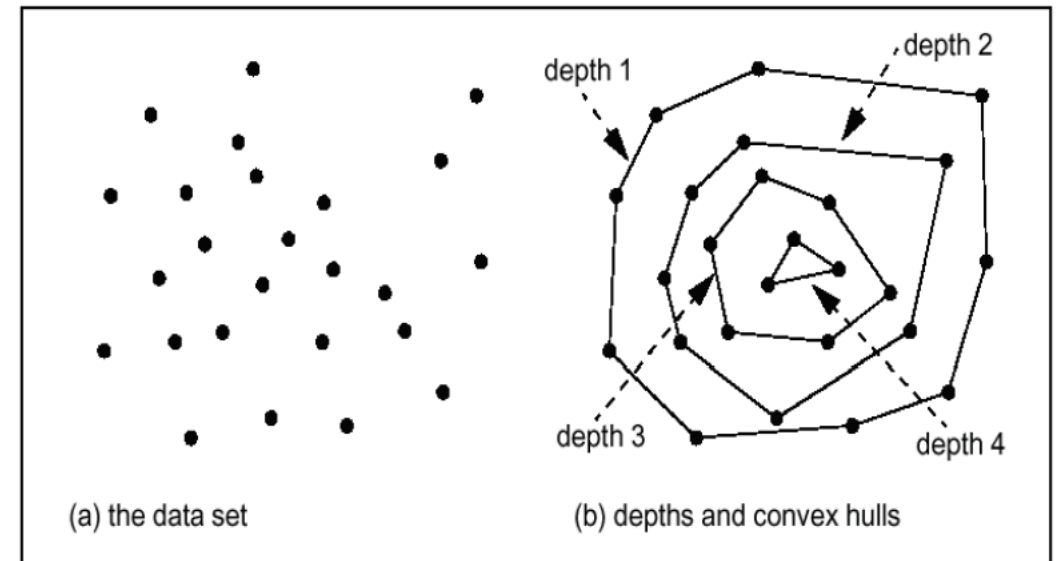
Depth-based Approaches

- Similar idea like classical statistical approaches ($k = 1$ distributions) but independent from the chosen kind of distribution

- Convex hull computation is usually only efficient in 2D / 3D spaces

- Originally outputs a label but can be extended for scoring easily (take depth as scoring value)

- Uses a global reference set for outlier detection

- Sample algorithms
  - ISODEPTH [Ruts and Rousseeuw 1996]
  - FDC [Johnson et al. 1998]

Deviation-based Approaches

Deviation-based Approaches

- General idea
  - Given a set of data points (local group or global set)
  - Outliers are points that do not fit to the general characteristics of that set, i.e., the variance of the set is minimized when removing the outliers

- Basic assumption
  - Outliers are the outermost points of the data set

Deviation-based Approaches

Model [Arning et al. 1996]

- Given a smoothing factor SF(I) that computes for each I ⊆ DB how much the variance of DB is decreased when I is removed from DB

- With equal decrease in variance, a smaller exception set E is better

- The outliers are the elements of E ⊆ DB for which the following holds: SF(E) ≥ SF(I) for all I ⊆ DB

Discussion:

- Similar idea like classical statistical approaches (k = 1 distributions) but independent from the chosen kind of distribution

- Naïve solution is in O(2n) for *n* data objects

- Heuristics like random sampling or best first search are applied

- Applicable to any data type (depends on the definition of SF)

- Originally designed as a global method

- Outputs a labeling

Distance-based Approaches

Distance-based Approaches

- General Idea
  - Judge a point based on the distance(s) to its neighbors
  - Several variants proposed

- Basic Assumption
  - Normal data objects have a dense neighborhood
  - Outliers are far apart from their neighbors, i.e., have a less dense neighborhood

Distance-based Approaches

- Several different techniques

- Approach 1: An object is an outlier if a specified fraction of the objects is more than a specified distance away (Knorr, Ng 1998)
  - Some statistical definitions are special cases of this

- Approach 2: The outlier score of an object is the distance to its k-th nearest neighbor

One Nearest Neighbor - One Outlier
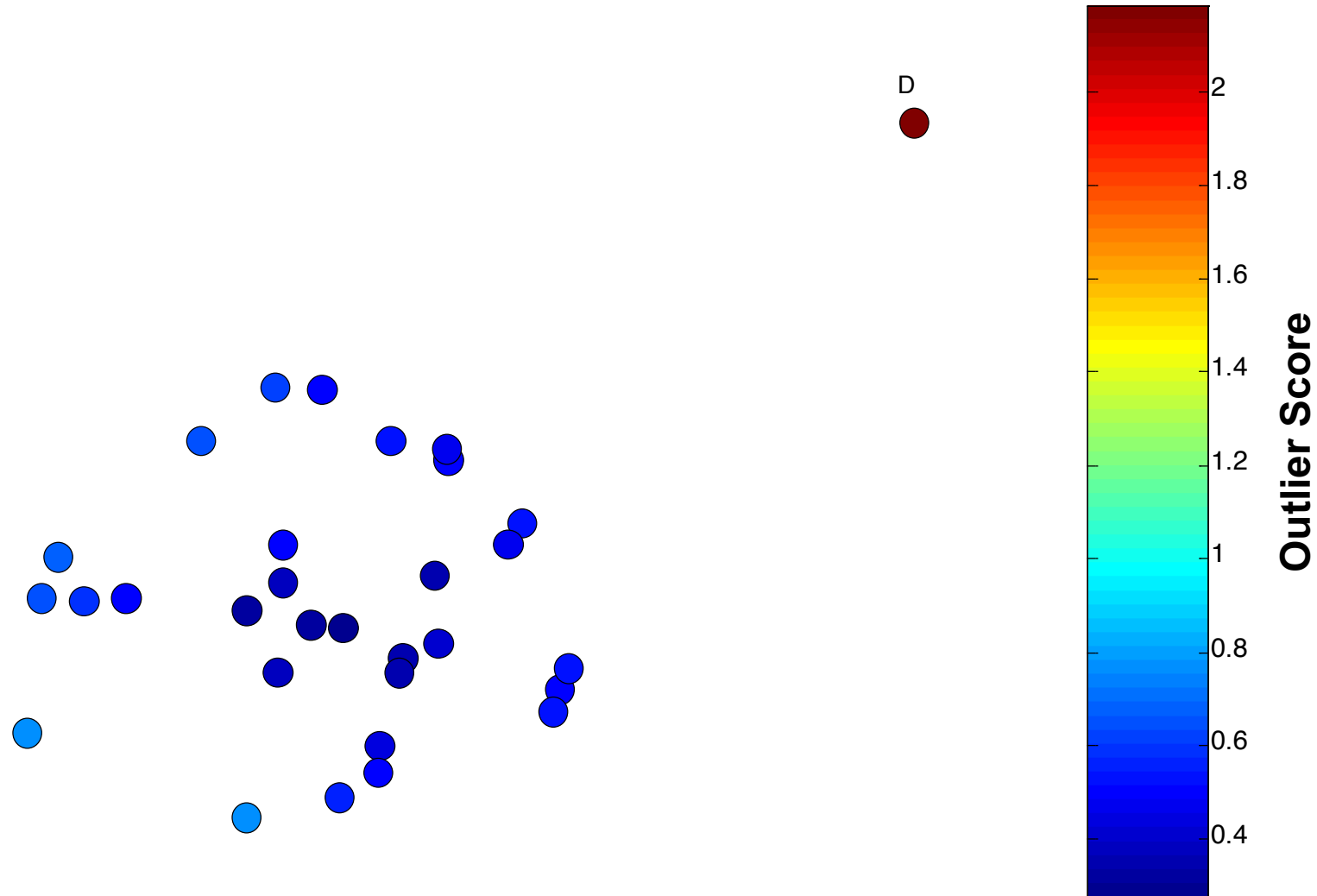
One Nearest Neighbor - Two Outliers
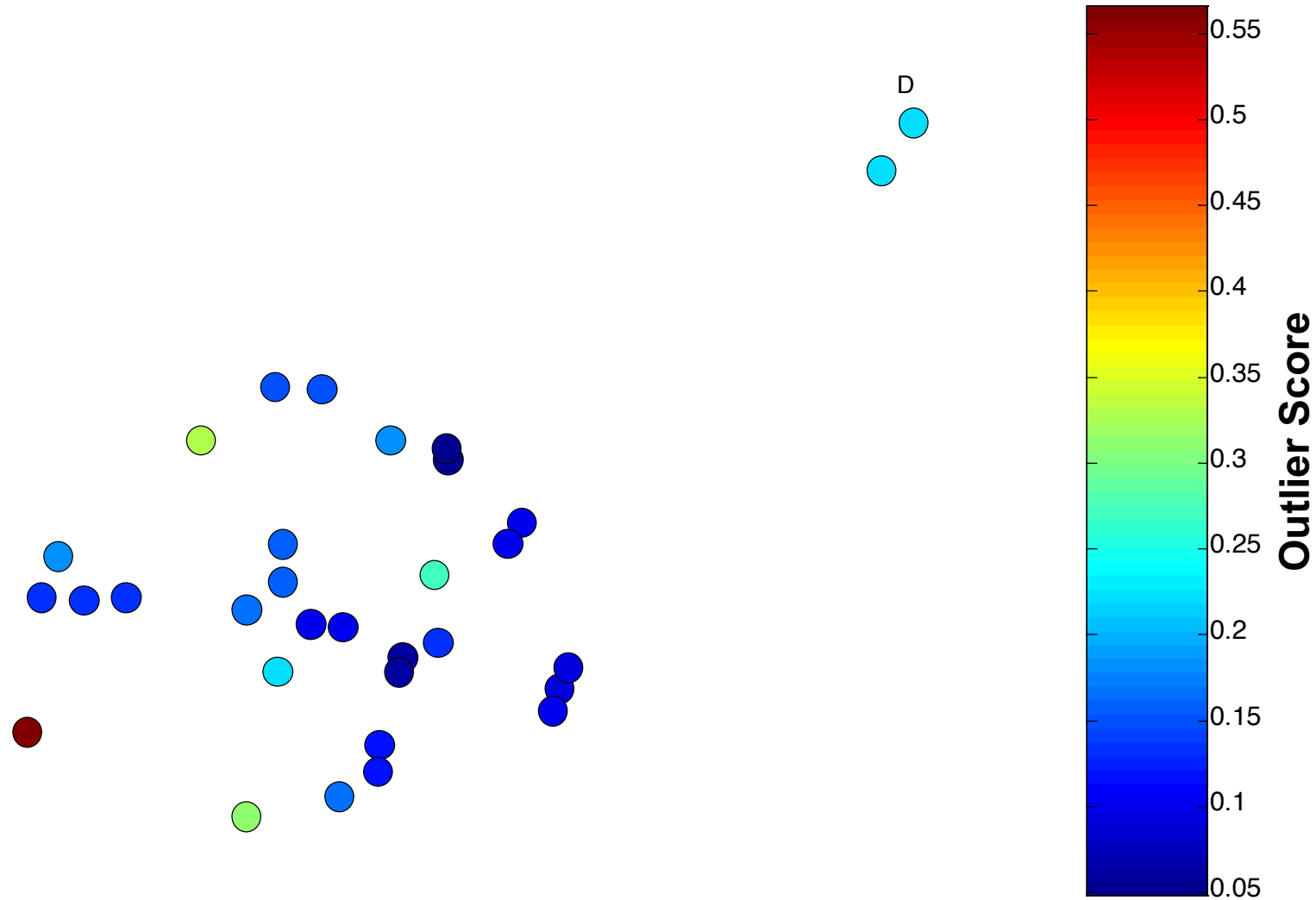
Six Nearest Neighbors - Small Cluster
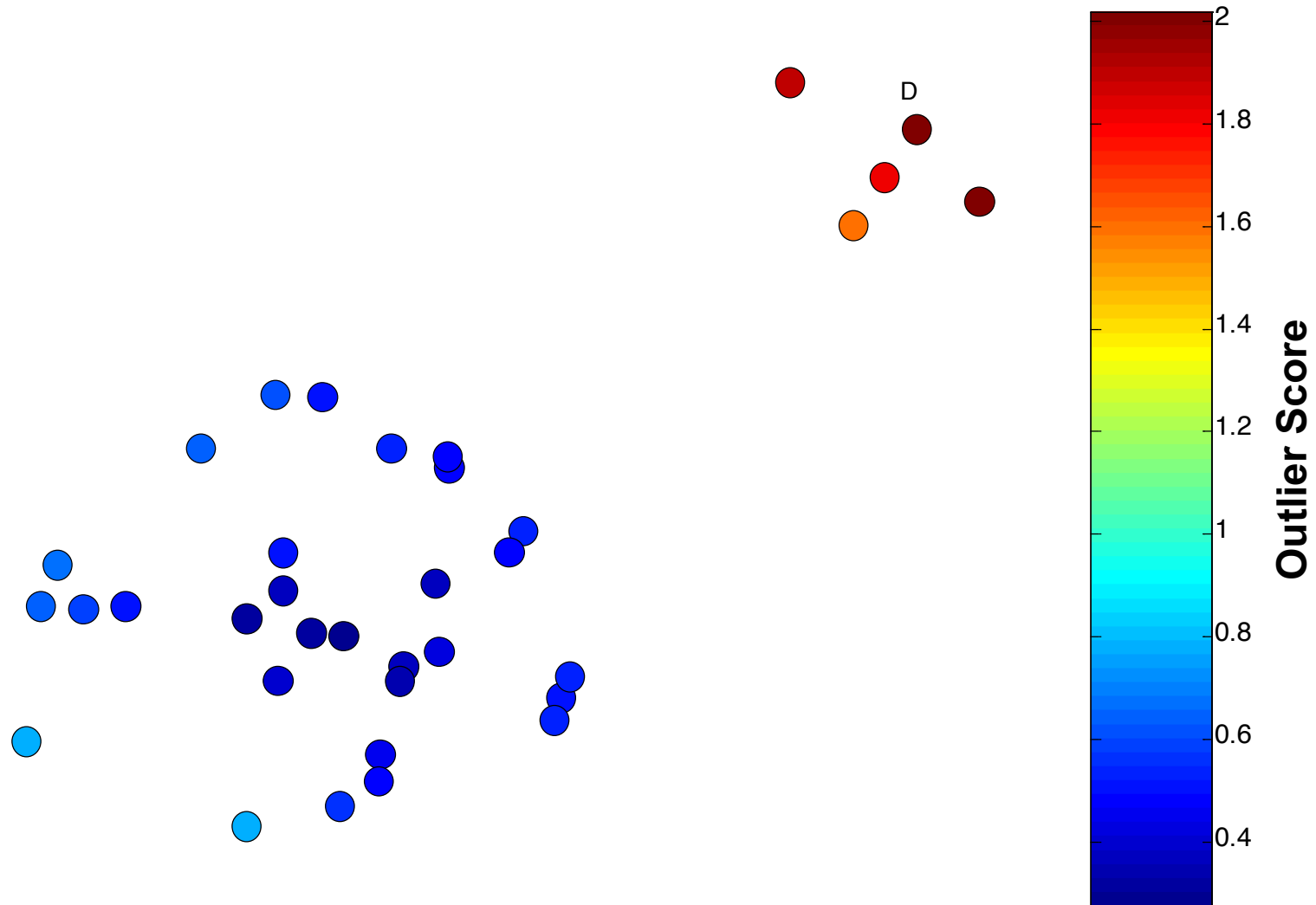
Five Nearest Neighbors - Differing Density
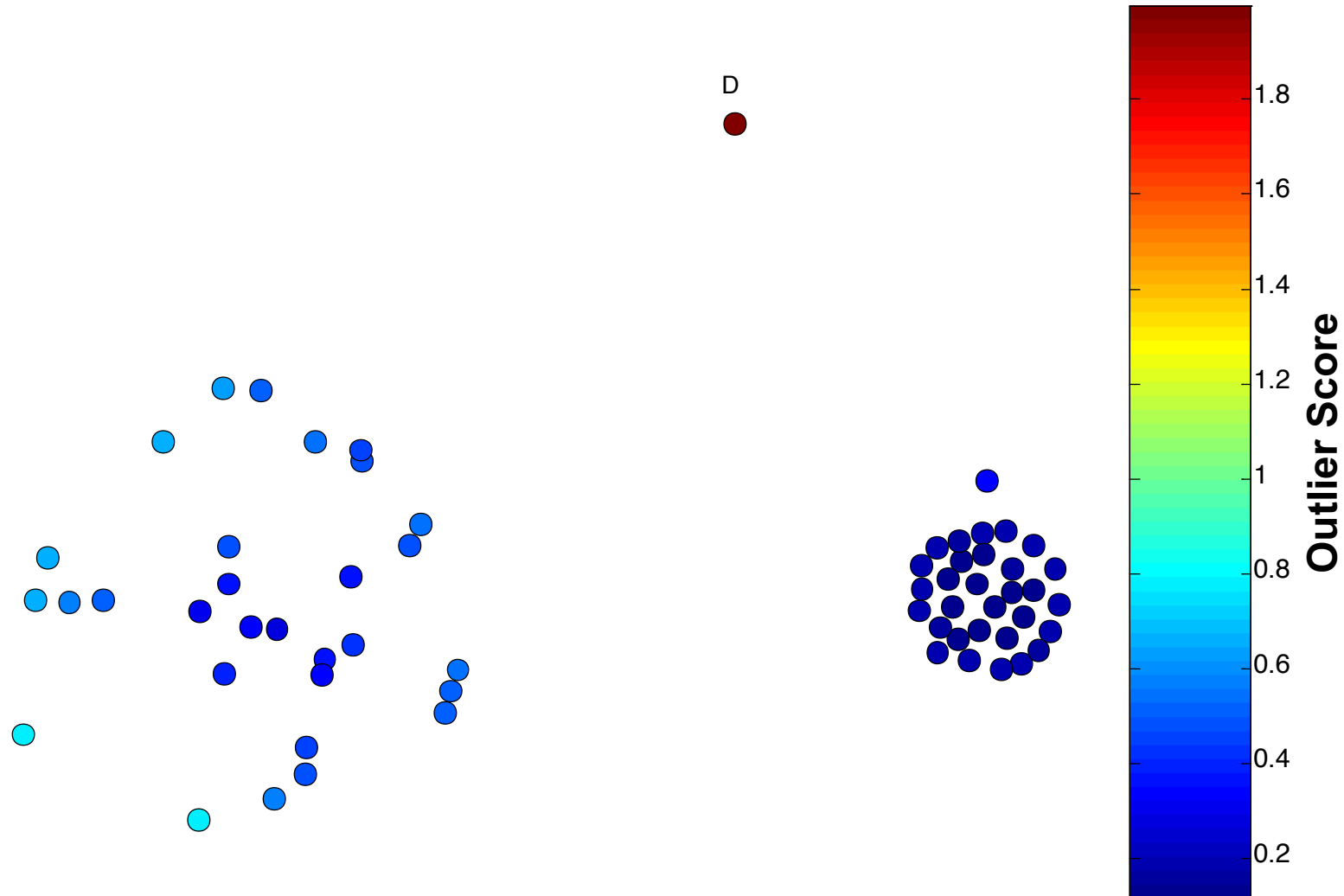
Distance-based Approaches

DB(ε,π)-Outliers

- Basic model [Knorr and Ng 1997]

- Given a radius ε and a percentage π

- A point p is considered an outlier if at most π percent of all other points have a distance to p less than ε, *i.e., it is close to few points*
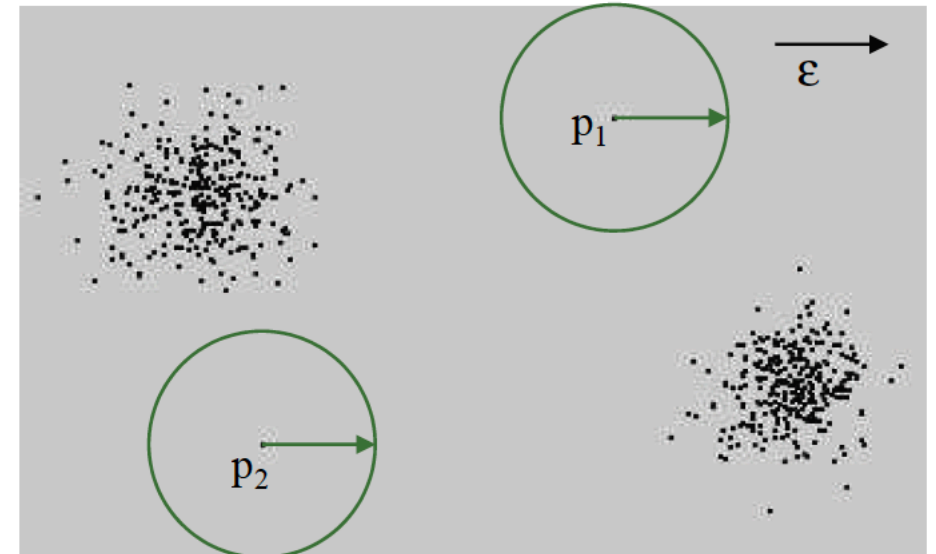
$$OutlierSet(\varepsilon, \pi) = \{p \mid \frac{Card(\{q \in DB \mid dist(p,q) < \varepsilon\})}{Card(DB)} \leq \pi\}$$

range-query with radius ε

Distance-based Approaches - Algorithms

- Index-based [Knorr and Ng 1998]
  - Compute distance range join using spatial index structure
  - Exclude point from further consideration if its ε-neighborhood contains more than Card(DB) π points

- Nested-loop based [Knorr and Ng 1998]
  - Divide buffer in two parts
  - Use second part to scan/compare all points with the points from the first part

- Grid-based [Knorr and Ng 1998]
  - Build grid such that any two points from the same grid cell have a distance of at most ε to each other
  - Points need only compared with points from neighboring cells

Outlier scoring based on kNN distances

General models

- Take the kNN distance of a point as its outlier score [Ramaswamy et al 2000]
- Aggregate the distances of a point to all its 1NN, 2NN, …, kNN as an outlier score [Angiulli and Pizzuti 2002]

Algorithms - General approaches

- Nested-Loop
  - Naïve approach: For each object: compute kNNs with a sequential scan
  - Enhancement: use index structures for kNN queries
- Partition-based
  - Partition data into micro clusters
  - Aggregate information for each partition (e.g. minimum bounding rectangles)
  - Allows to prune micro clusters that cannot qualify when searching for the kNNs of a particular point

Outlier Detection using In-degree Number

- Idea: Construct the kNN graph for a data set
  - Vertices: data points
  - Edge: if $q \in kNN(p)$ then there is a directed edge from p to q
  - A vertex that has an indegree less than equal to T (user threshold) is an outlier
- Discussion
  - The indegree of a vertex in the kNN graph equals to the number of reverse kNNs (RkNN) of the corresponding point
  - The RkNNs of a point p are those data objects having p among their kNNs
  - Intuition of the model: outliers are
    - points that are among the kNNs of less than T other points
    - have less than T RkNNs
  - Outputs an outlier label
  - Is a local approach (depending on user defined parameter k)

Strengths/Weaknesses of Distance-Based Approaches

Pros

• Simple

Cons

• Expensive – $O(n^2)$

• Sensitive to parameters

• Sensitive to variations in density

• Distance becomes less meaningful in high-dimensional space

Density-based Approaches

Density-based Approaches

- General idea
    - Compare the density around a point with the density around its local neighbors
    - The relative density of a point compared to its neighbors is computed as an outlier score
    - Approaches differ in how to estimate density
- Basic assumption
    - The density around a normal data object is similar to the density around its neighbors
    - The density around an outlier is considerably different to the density around its neighbors

Density-based Approaches

- **Density-based Outlier:** The outlier score of an object is the inverse of the density around the object.
  - Can be defined in terms of the k nearest neighbors
  - One definition: Inverse of distance to kth neighbor
  - Another definition: Inverse of the average distance to k neighbors
  - DBSCAN definition

- If there are regions of different density, this approach can have problems

Relative Density Outlier Scores
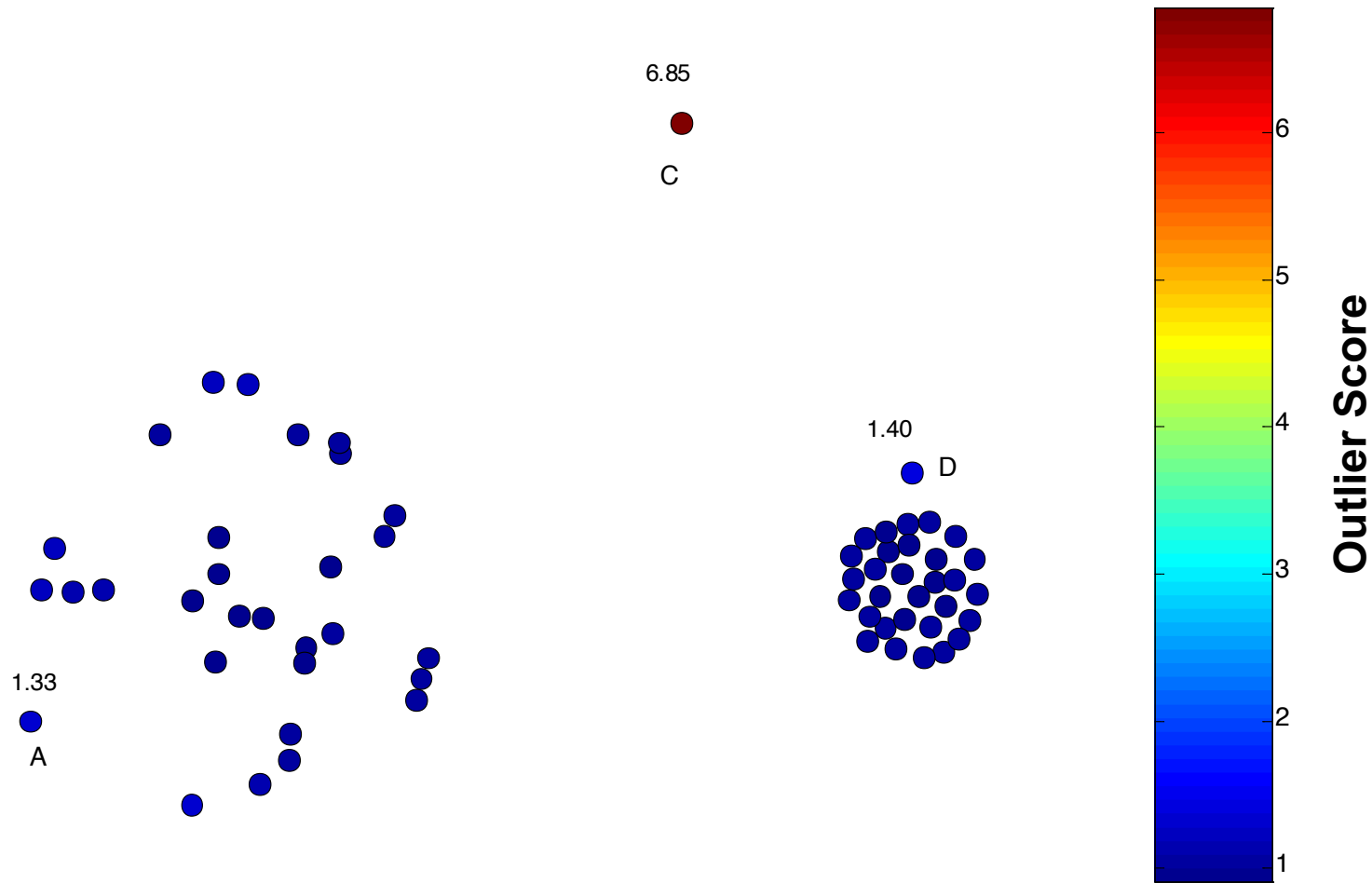
Relative Density

- Consider the density of a point relative to that of its k nearest neighbors

$$average\ relative\ density(\mathbf{x}, k) = \frac{density(\mathbf{x}, k)}{\sum_{\mathbf{y} \in N(\mathbf{x},k)} density(\mathbf{y}, k)/|N(\mathbf{x}, k)|}. \quad (10.7)$$

Algorithm 10.2 Relative density outlier score algorithm.

1: $\{k$ is the number of nearest neighbors$\}$
2: **for all** objects $\mathbf{x}$ **do**
3:     Determine $N(\mathbf{x}, k)$, the k-nearest neighbors of $\mathbf{x}$.
4:     Determine $density(\mathbf{x}, k)$, the density of $\mathbf{x}$, using its nearest neighbors, i.e., the objects in $N(\mathbf{x}, k)$.
5: **end for**
6: **for all** objects $\mathbf{x}$ **do**
7:     Set the $outlier\ score(\mathbf{x}, k) = average\ relative\ density(\mathbf{x}, k)$ from Equation 10.7.
8: **end for**

Local Outlier Factor (LOF) [Breunig et al. 1999], [Breunig et al. 2000]

Motivation:

- Distance-based outlier detection models have problems with different densities

- How to compare the neighborhood of points from areas of different densities?

Example

- DB(ε,π)-outlier model
  - Parameters ε and π cannot be chosen so that o_2 is an outlier but none of the points in cluster C_1 (e.g. q) is an outlier
- Outliers based on kNN-distance
  - kNN-distances of objects in C_1 (e.g. q) are larger than the kNN-distance of o_2

Solution: consider relative density
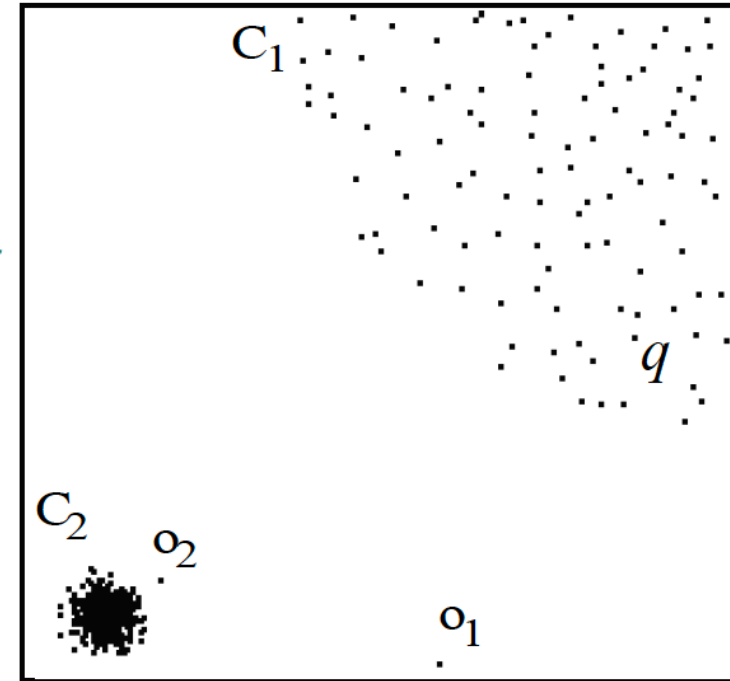
Local Outlier Factor (LOF)

- For each point, compute the density of its local neighborhood

- Compute local outlier factor (LOF) of a sample p as the average of the ratios of the density of sample p and the density of its nearest neighbors

- Outliers are points with largest LOF value
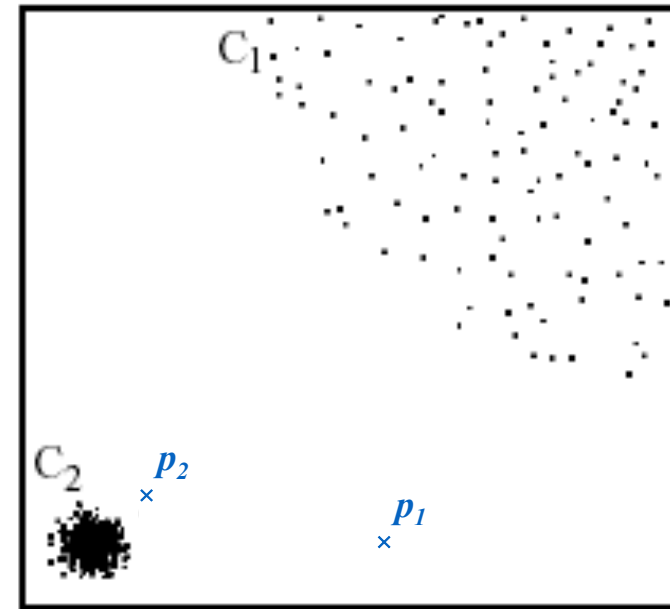
In the NN approach, p_2 is not considered as outlier, while LOF approach find both p_1 and p_2 as outliers

Local Outlier Factor (LOF)

- Reachability distance
  - Introduces a smoothing factor

$$reach - dist_k(p,o) = \max\{k - \text{distance}(o), dist(p,o)\}$$

$reach\text{-}dist_k(p_1, o) = k\text{-}distance(o)$
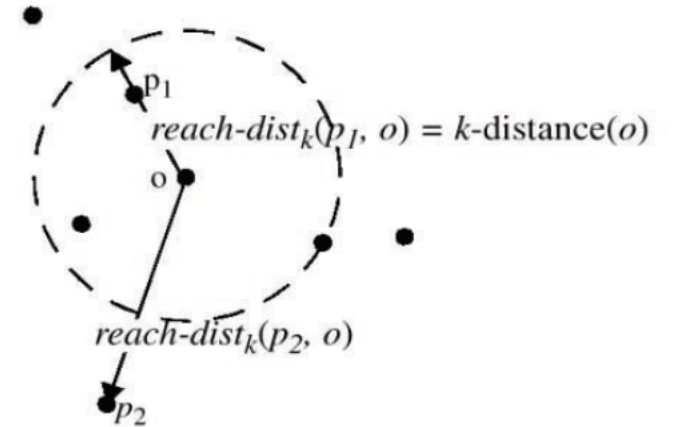
$reach\text{-}dist_k(p_2, o)$

- Local reachability distance (*lrd*) of point *p*
  - Inverse of the average reach-dists of the kNNs of *p*

$$lrd_k(p) = 1 / \left(\frac{\sum\limits_{o \in kNN(p)} reach - dist_k(p,o)}{Card(kNN(p))} \right)$$

- Local outlier factor (LOF) of point *p*
  - Average ratio of *lrds* of neighbors of *p* and *lrd* of *p*

$$LOF_k(p) = \frac{\sum\limits_{o \in kNN(p)} \dfrac{lrd_k(o)}{lrd_k(p)}}{Card(kNN(p))}$$

Local Outlier Factor (LOF)

Properties

- LOF ≈ 1: point is in a cluster (region with homogeneous density around the point and its neighbors)

- LOF >> 1: point is an outlier

Data set

Discussion

- Choice of k (MinPts in the original paper) specifies the reference set

- Originally implements a *local* approach (resolution depends on the user's choice for k)

- Outputs a scoring (assigns an LOF value to each point)

LOFs (*MinPts* = 40)
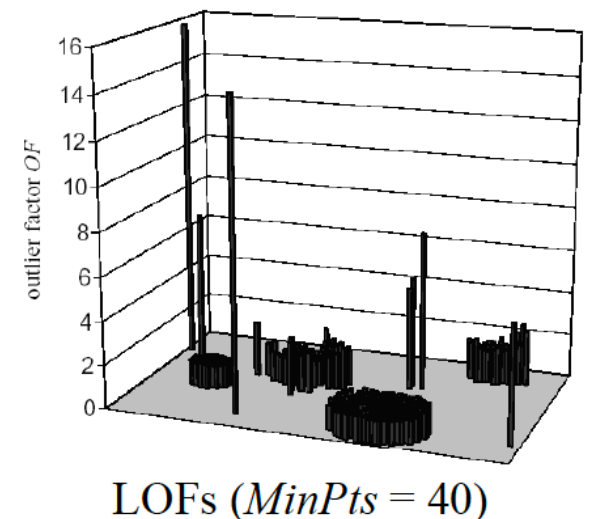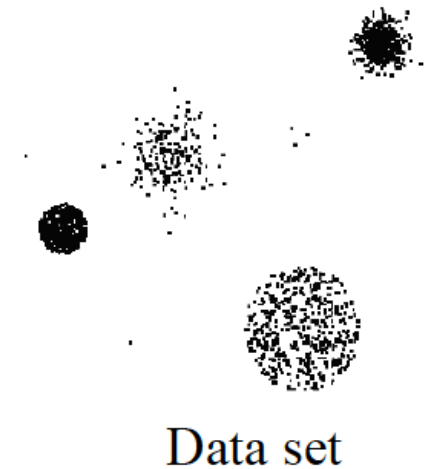
Mining Top-n Local Outliers [Jin et al. 2001]

Idea:

- Usually, a user is only interested in the **top-n** outliers
- Do not compute the LOF for all data objects => save runtime

Method

- Compress data points into micro clusters using the CFs of BIRCH [Zhang et al. 1996]
- Derive upper and lower bounds of the reachability distances, lrd-values, and LOF-values for points within a micro clusters
- Compute upper and lower bounds of LOF values for micro clusters and sort results w.r.t. ascending lower bound
- Prune micro clusters that cannot accommodate points among the top-n outliers (n highest LOF values)
- Iteratively refine remaining micro clusters and prune points accordingly

Connectivity-based outlier factor (COF) [Tang et al. 2002]

- Motivation
  - In regions of low density, it may be hard to detect outliers
  - Choose a low value for k is often not appropriate

- Solution
  - Treat "low density" and "isolation" differently

- Example
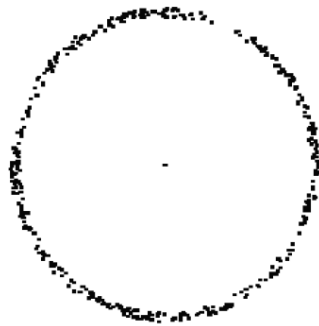
Data set
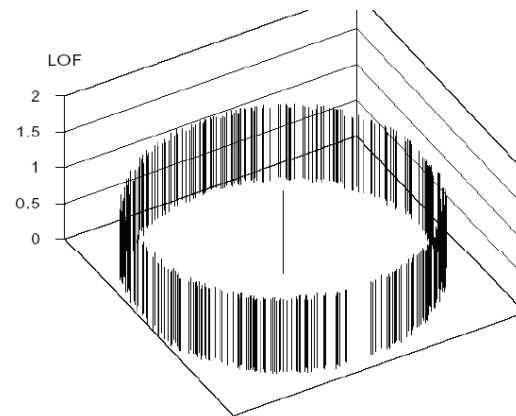
LOF
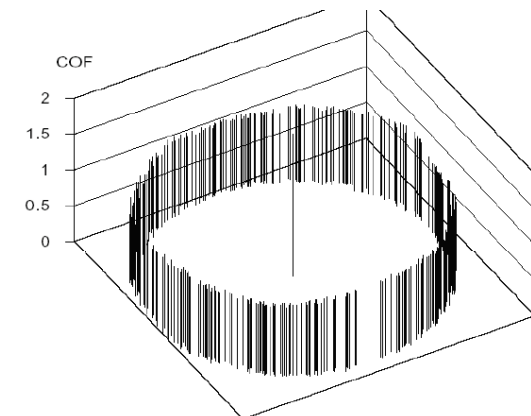
COF

Influenced Outlierness (INFLO) [Jin et al. 2006]

Motivation

- If clusters of different densities are not clearly separated, LOF will have problems
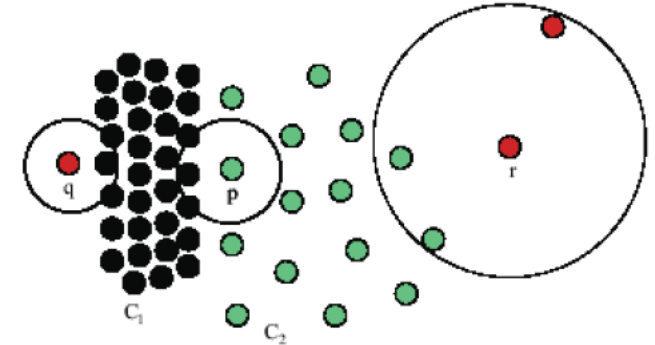
Point p will have a higher LOF than points q or r which is counter intuitive

Idea

- Take symmetric neighborhood relationship into account

- Influence space $kIS(p)$ of a point p includes its kNNs $(kNN(p))$ and its reverse kNNs $(RkNN(p))$
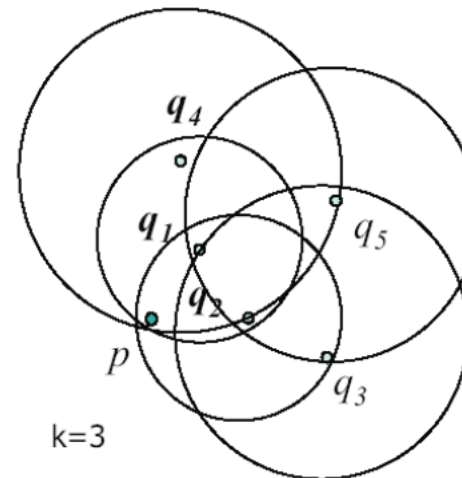
$kIS(p) = kNN(p) \cup RkNN(p))$

$= \{q_1, q_2, q_4\}$

Influenced Outlierness (INFLO) [Jin et al. 2006]

Model

- Density is simply measured by the inverse of the kNN distance, i.e.,
  - *den(p) = 1/k-distance(p)*

- Influenced outlierness of a point *p*

$$INFLO_k(p) = \frac{\sum_{o \in kIS(p)} den(o) \Big/ Card(kIS(p))}{den(p)}$$

- INFLO takes the ratio of the average density of objects in the neighborhood of a point *p* (i.e., in *kNN(p) ∪ RkNN(p)*) to *p*'s density

Proposed algorithms for mining top-n outliers

- Index-based

- Two-way approach

- Micro cluster based approach

Influenced Outlierness (INFLO) [Jin et al. 2006]

Properties

- Similar to LOF
- INFLO ≈ 1: point is in a cluster
- INFLO >> 1: point is an outlier

Discussion

- Outputs an outlier score
- Originally proposed as a *local* approach (resolution of the reference set kIS can be adjusted by the user setting parameter k)

Strengths/Weaknesses of Density-Based Approaches

Pros

- Simple

Cons

- Expensive – $O(n^2)$
- Sensitive to parameters
- Density becomes less meaningful in high-dimensional space

Clustering-based Approaches

Clustering and Anomaly Detection

- Are outliers just a side product of some clustering algorithms?
  - Many clustering algorithms do not assign all points to clusters but account for noise objects (e.g. DBSCAN, OPTICS)
  - Look for outliers by applying one algorithm and retrieve the noise set
- Problem:
  - Clustering algorithms are optimized to find clusters rather than outliers
  - Accuracy of outlier detection depends on how good the clustering algorithm captures the structure of clusters
  - A set of many abnormal data objects that are similar to each other would be recognized as a cluster rather than as noise/outliers

Clustering-Based Approaches

- **Clustering-based Outlier:** An object is a cluster-based outlier if it does not strongly belong to any cluster
  - For prototype-based clusters, an object is an outlier if it is not close enough to a cluster center
  - For density-based clusters, an object is an outlier if its density is too low
  - For graph-based clusters, an object is an outlier if it is not well connected

- Other issues include the impact of outliers on the clusters and the number of clusters
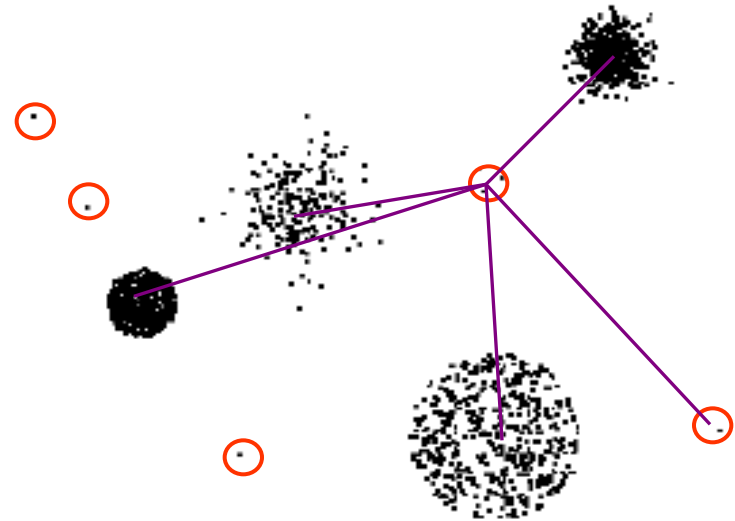
Distance of Points from Closest Centroids
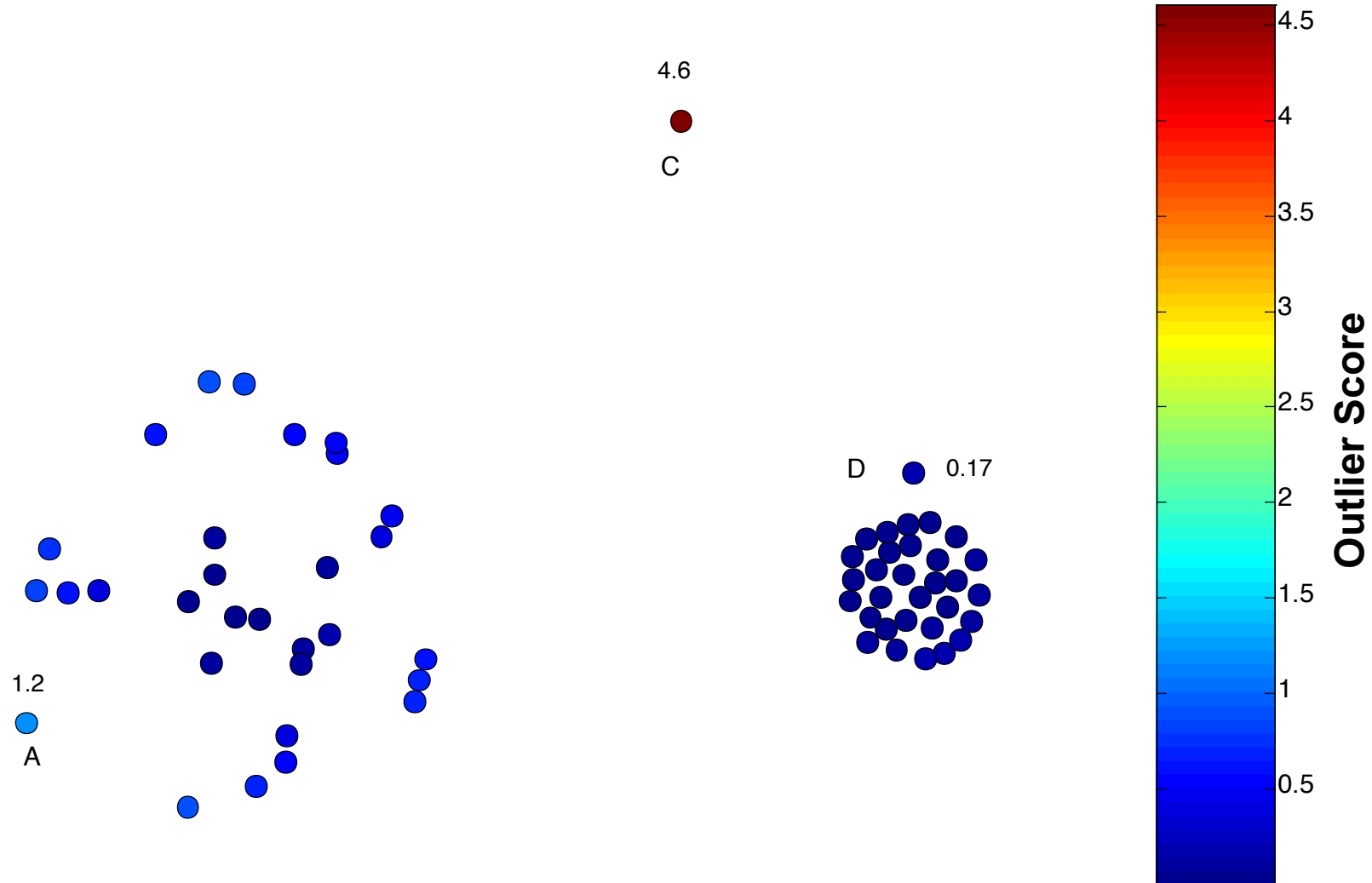
Relative Distance of Points from Closest Centroid
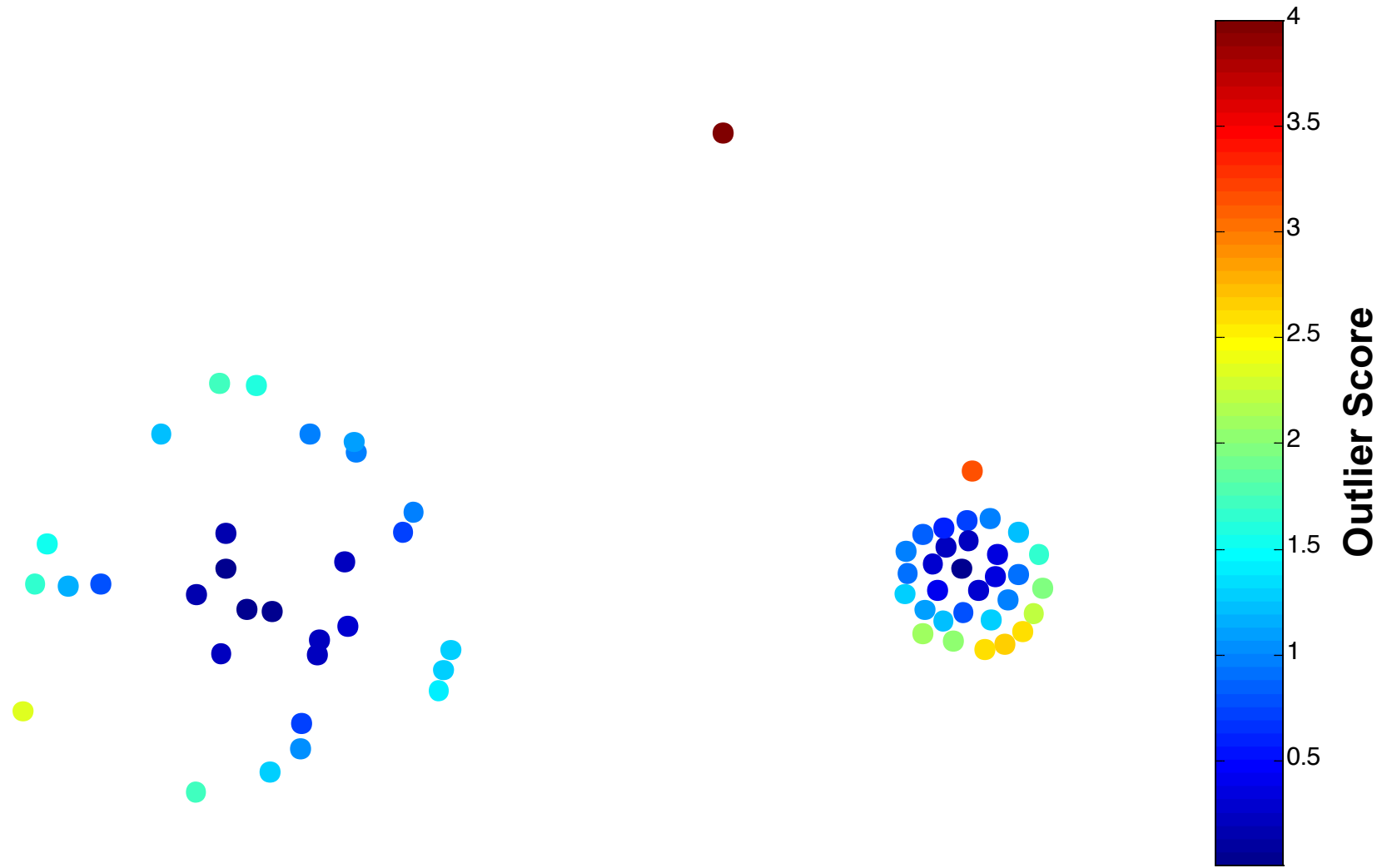
Strengths/Weaknesses of Clustering-Based Approaches

Pros

- Simple
- Many clustering techniques can be used

Cons

- Can be difficult to decide on a clustering technique
- Can be difficult to decide on number of clusters
- Outliers can distort the clusters

High-dimensional Approaches

Challenges

Curse of dimensionality

- Relative contrast between distances decreases with increasing dimensionality

- Data is very sparse, almost all points are outliers

- Concept of neighborhood becomes meaningless

Solutions

- Use more robust distance functions and find full-dimensional outliers

- Find outliers in projections (subspaces) of the original feature space

ABOD – Angle-based Outlier Degree [Kriegel et al. 2008]

- Angles are more stable than distances in high dimensional spaces (e.g. the popularity of cosine-based similarity measures for text data)
- Object o is an outlier if most other objects are located in similar directions
- Object o is no outlier if many other objects are located in varying directions
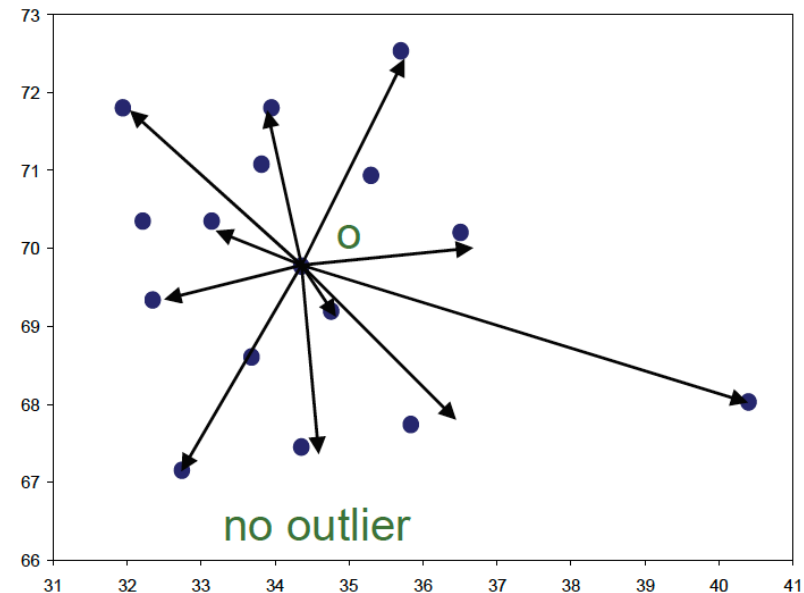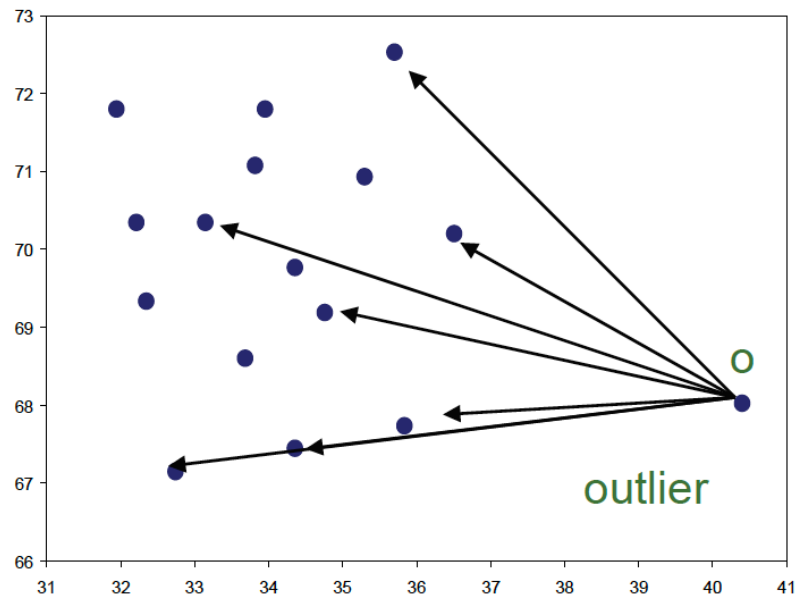
ABOD – Angle-based Outlier Degree [Kriegel et al. 2008]

- Basic assumption
  - Outliers are at the border of the data distribution
  - Normal points are in the center of the data distribution

- Model
  - Consider for a given point p the angle between any two instances x and y
  - Consider the spectrum of all these angles
  - The broadness of this spectrum is a score for the outlierness of a point
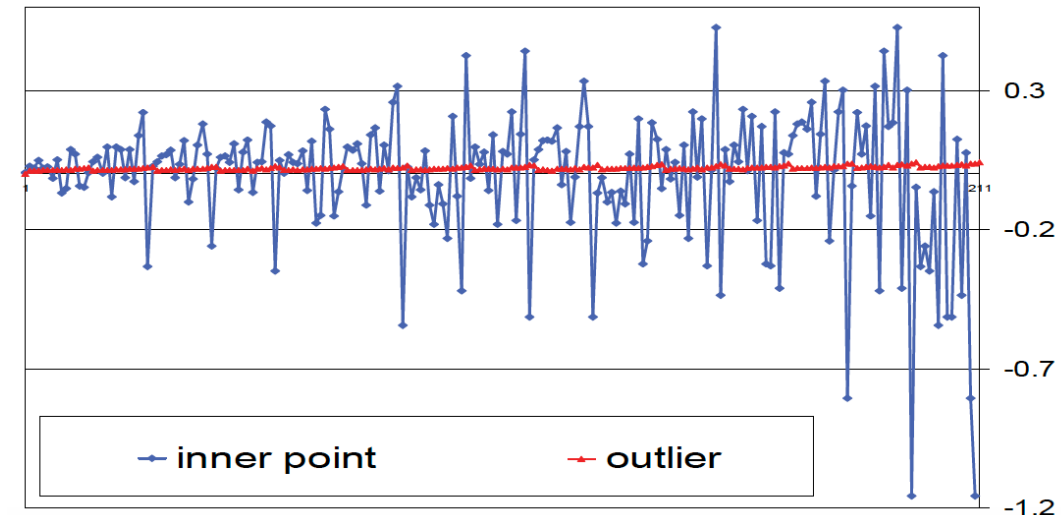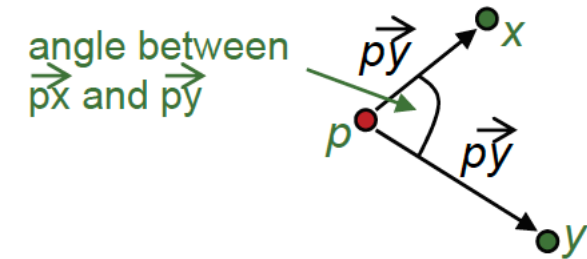
ABOD – Angle-based Outlier Degree [Kriegel et al. 2008]

- Model
  - Measure the variance of the angle spectrum
  - Weighted by the corresponding distances (for lower dimensional data sets where angles are less reliable)

$$ABOD(p) = \underset{x,y \in DB}{VAR} \left(\frac{\left\langle \overrightarrow{xp}, \overrightarrow{yp} \right\rangle}{\left\| \overrightarrow{xp} \right\|^2 \cdot \left\| \overrightarrow{yp} \right\|^2} \right)$$

$\overrightarrow{xp}$ denotes the difference vector x-p
$\langle \overrightarrow{xp}, \overrightarrow{yp} \rangle$ denotes the scalar product
scalar product $\langle a,b \rangle = \sum a_i b_i$

- Properties
  - Small ABOD => outlier
  - High ABOD => no outlier

ABOD – Angle-based Outlier Degree [Kriegel et al. 2008]

Algorithms

- Naïve algorithm is in $O(n^3)$

- Approximate algorithm based on random sampling for mining top-n outliers
  - Do not consider all pairs of other points *x, y* in the database to compute the angles
  - Compute ABOD based on samples => lower bound of the real ABOD
  - Filter out points that have a high lower bound
  - Refine (compute the exact ABOD value) only for a small number of points

Discussion

- Global approach to outlier detection
- Outputs an outlier score

Grid-based Subspace Outlier Detection [Aggarwal and Yu 2000]

Model

- Partition data space by an equi-depth grid (Φ = number of cells in each dimension)

- Sparsity coefficient $S(C)$ for a k-dimensional grid cell C

$$S(C) = \frac{count(C) - n \cdot \left(\frac{1}{\Phi}\right)^k}{\sqrt{n \cdot \left(\frac{1}{\Phi}\right)^k \cdot \left(1 - \left(\frac{1}{\Phi}\right)^k\right)}}$$

- where count(C) is the number of data objects in C

- $S(C) < 0 \Rightarrow count(C)$ is lower than expected

- Outliers are those objects that are located in lower-dimensional cells with negative sparsity coefficient
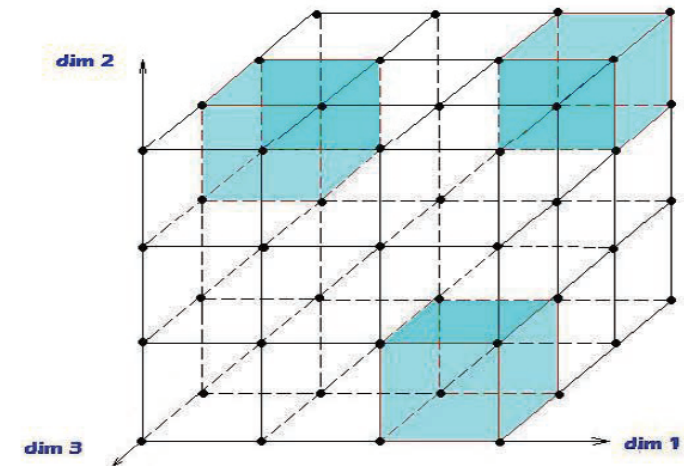
k = nbr dimensions (e.g. 3)
φ = nbr of equi-depth ranges (e.g 3)

Grid-based Subspace Outlier Detection [Aggarwal and Yu 2000]

- Algorithm
    - Find the *m* grid cells (projections) with the lowest sparsity coefficients
    - Brute-force algorithm is *in O(Φd)*
    - Evolutionary algorithm (input: m and the dimensionality of the cells)

- Discussion
    - Results need not be the points from the optimal cells
    - Very coarse model (all objects that are in cell with less points than to be expected)
    - Quality depends on grid resolution and grid position
    - Outputs a labeling
    - Implements a global approach (key criterion: globally expected number of points within a cell)

Model-based Approaches

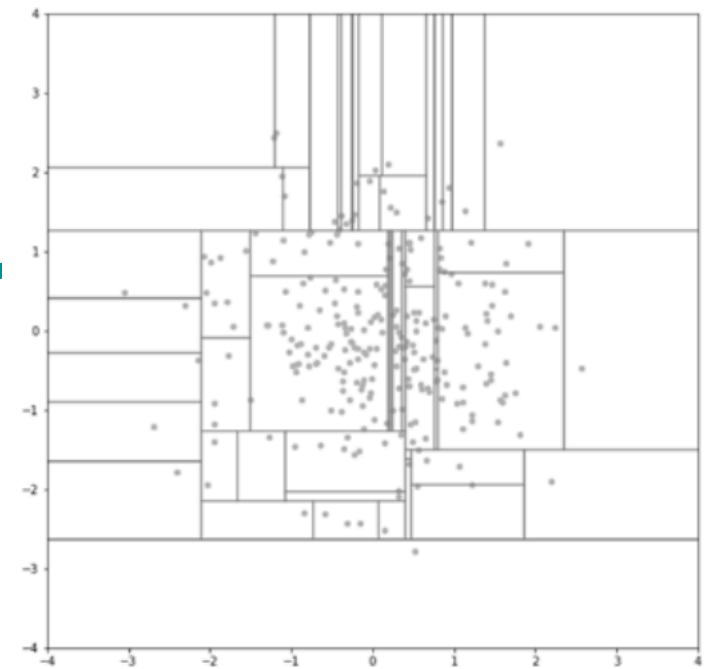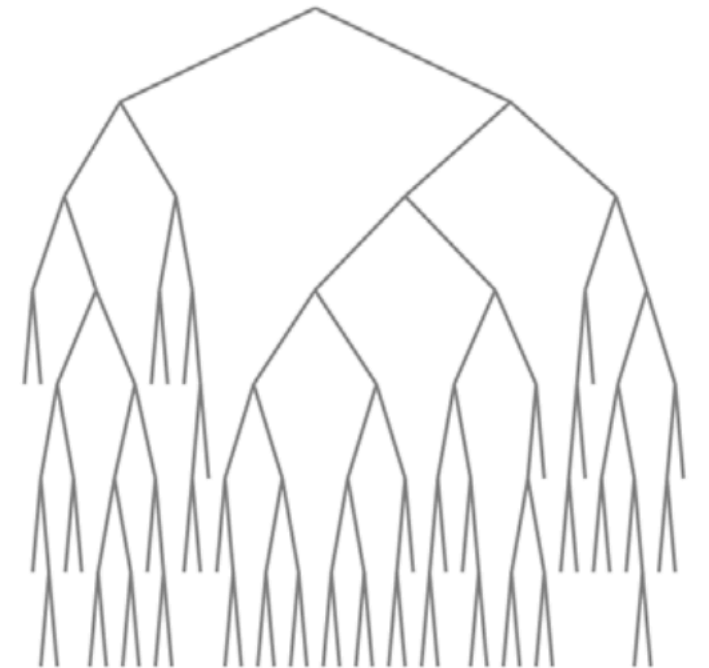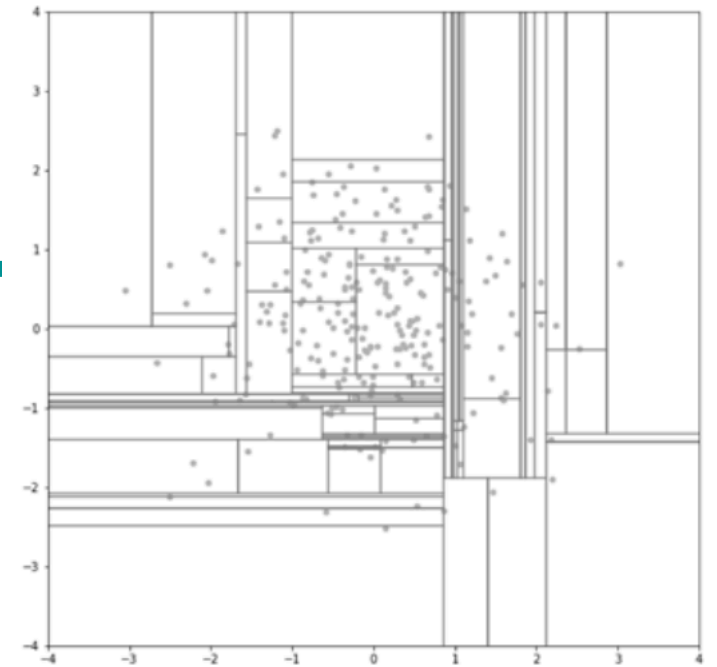Slides revisited from Isolation Forest for Anomaly Detection, Sahand Hariri

Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.
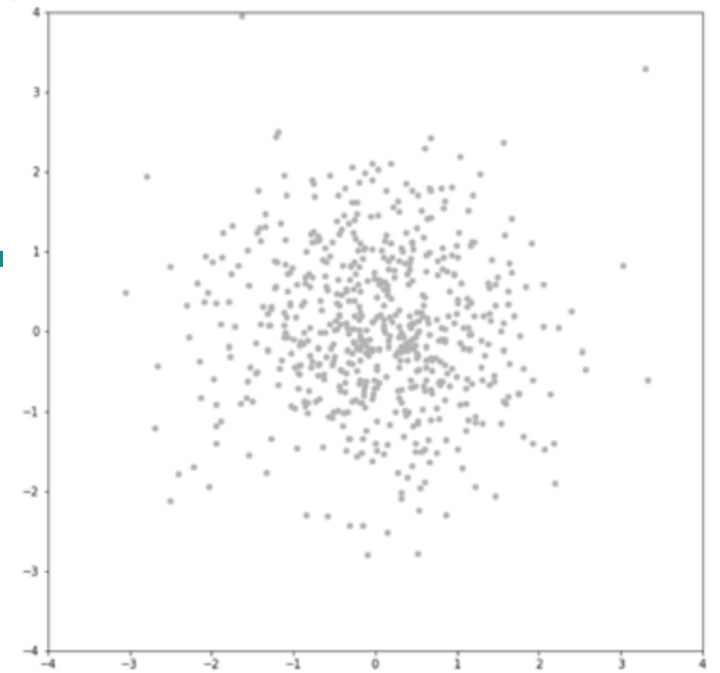
https://scikit-learn.org/stable/auto_examples/miscellaneous/plot_anomaly_comparison.html#sphx-glr-auto-examples-miscellaneous-plot-anomaly-comparison-py
https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html#sklearn.ensemble.IsolationForest
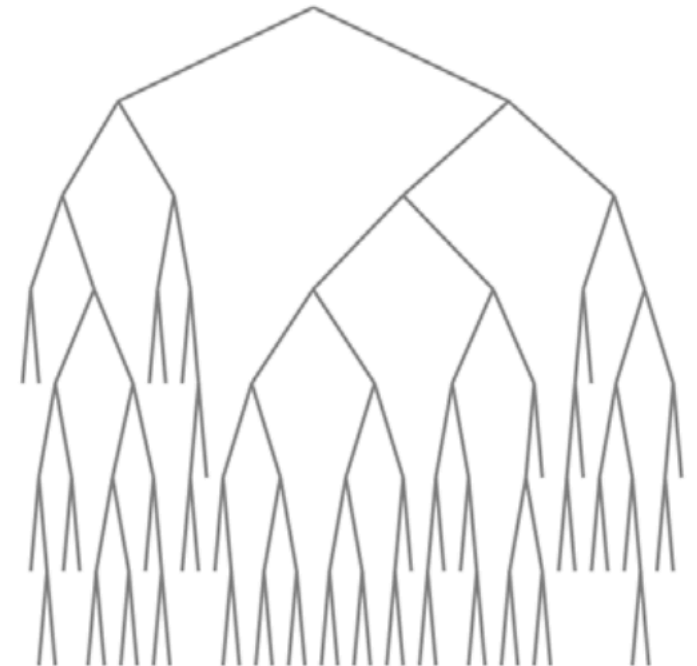https://scikit-learn.org/stable/auto_examples/ensemble/plot_isolation_forest.html
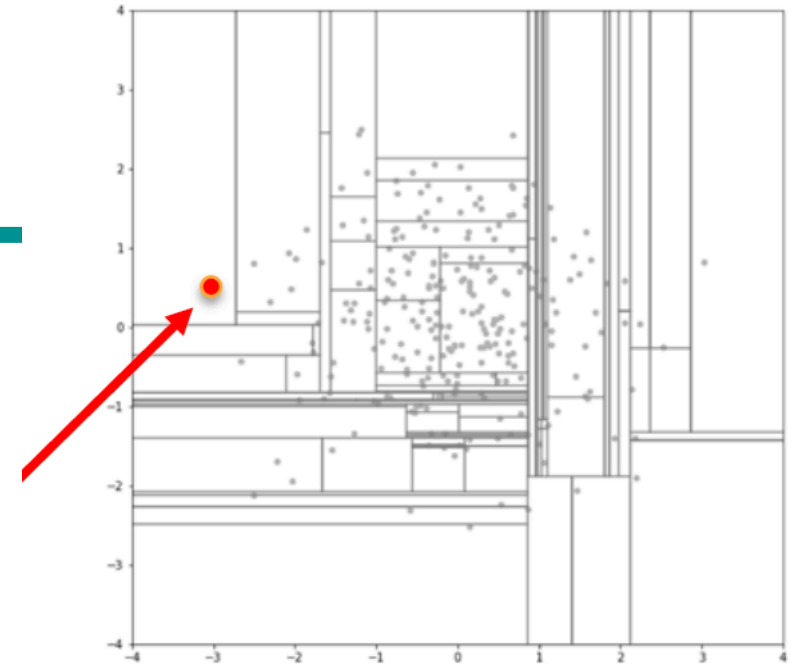
Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.

- For each tree:
  - Get a sample of the data

Isolation Forest

y

- Idea: Few and different instances can be isolated quicker
- Given the dataset build a forest of trees.
- For each tree:
  - Get a sample of the data
  - Randomly select a dimension
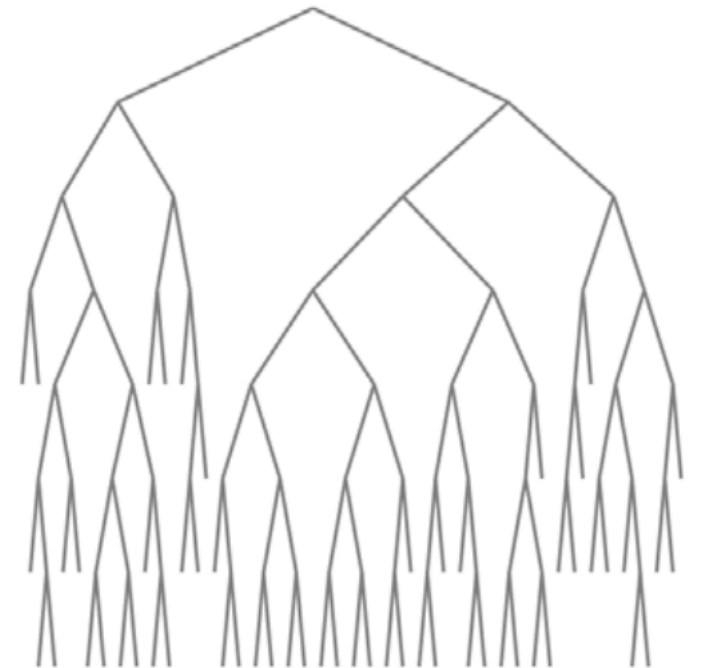 - Randomly pick a value in that dimension
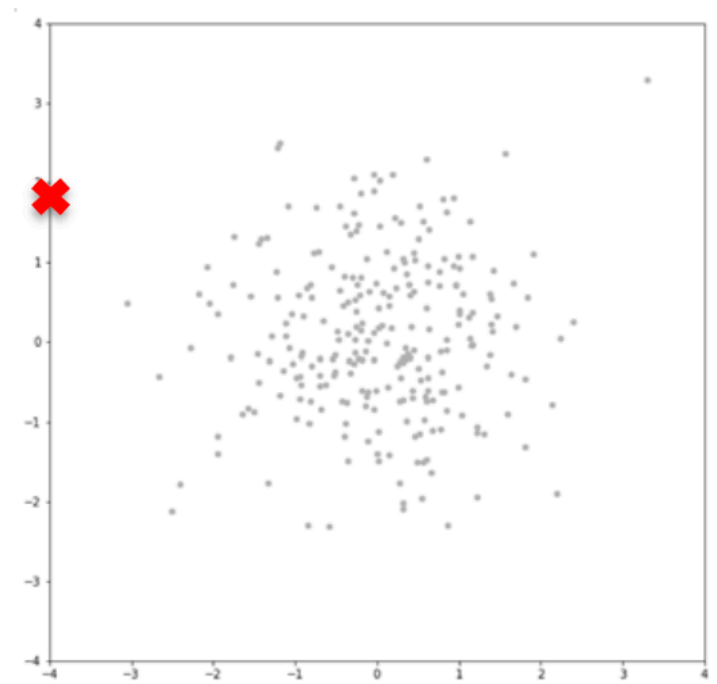
Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.

- For each tree:
  - Get a sample of the data
  - Randomly select a dimension
  - Randomly pick a value in that dimension
  - Draw a straight line through the data at that value and split data
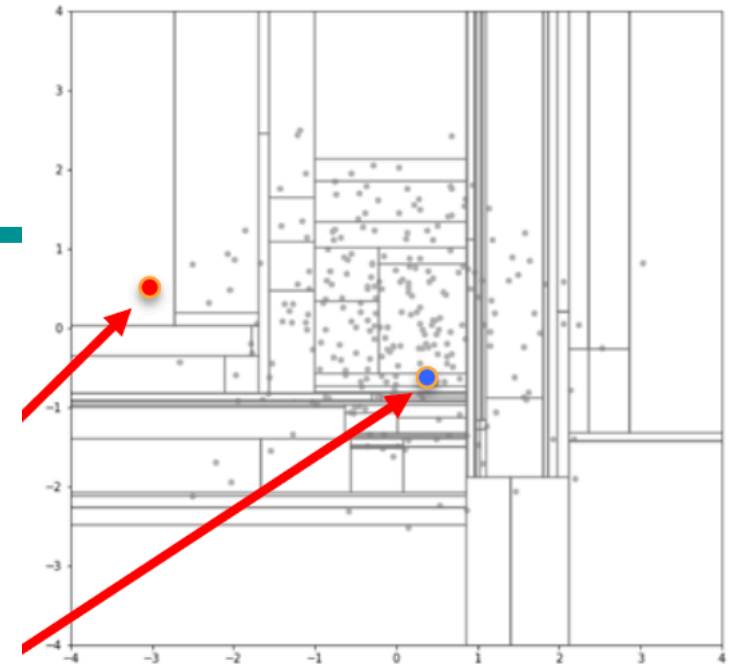
Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.

- For each tree:
  - Get a sample of the data
  - Randomly select a dimension
  - Randomly pick a value in that dimension
  - Draw a straight line through the data at that value and split data
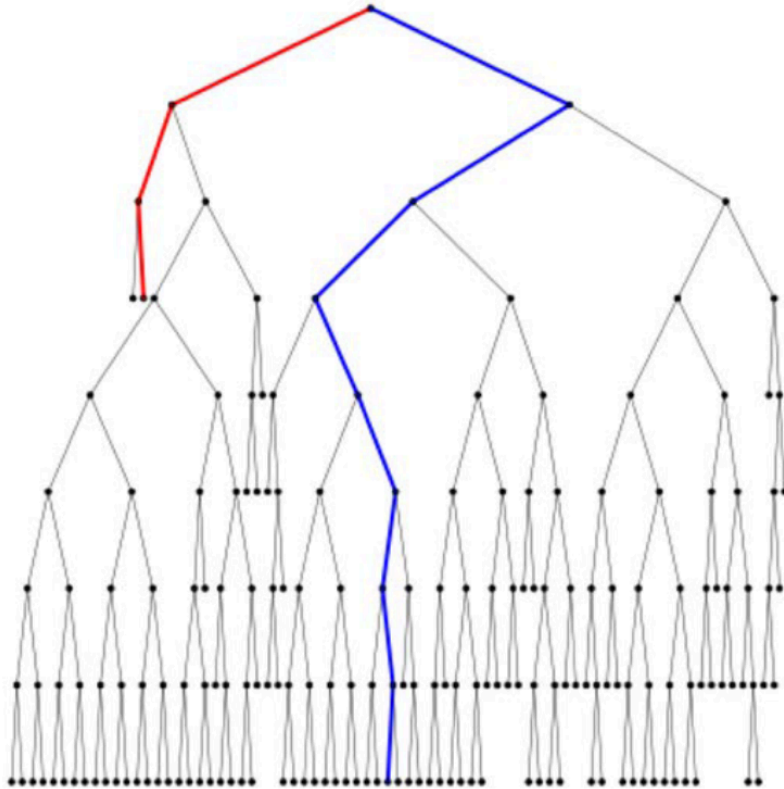 - Repeat until tree is complete

Isolation Forest

- Idea: Few and different instances can be isolated quicker
- Given the dataset build a forest of trees.
- For each tree:
  - Get a sample of the data
  - Randomly select a dimension
  - Randomly pick a value in that dimension
  - Draw a straight line through the data at that value and split data
  - Repeat until tree is complete

Isolation Forest

- Idea: Few and different instances can be isolated quicker
- Given the dataset build a forest of trees.
- For each tree:
  - Get a sample of the data
  - Randomly select a dimension
  - Randomly pick a value in that dimension
  - Draw a straight line through the data at that value and split data
  - Repeat until tree is complete

Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.

- For each tree:
  - Get a sample of the data
  - Randomly select a dimension
  - Randomly pick a value in that dimension
  - Draw a straight line through the data at that value and split data
  - Repeat until tree is complete

- Generate multiple trees -> forest

Isolation Forest

- Idea: Few and different instances can be isolated quicker
- Given the dataset build a forest of trees.
- For each tree:
  - Get a sample of the data
  - Randomly select a dimension
  - Randomly pick a value in that dimension
  - Draw a straight line through the data at that value and split data
  - Repeat until tree is complete
- Generate multiple trees -> forest

Isolation Forest

- Idea: Few and different instances can be isolated quicker
- Given the dataset build a forest of trees.
- For each tree:
  - Get a sample of the data
  - Randomly select a dimension
  - Randomly pick a value in that dimension
  - Draw a straight line through the data at that value and split data
  - Repeat until tree is complete
- Generate multiple trees -> forest
- Anomalies will be isolated in only few steps
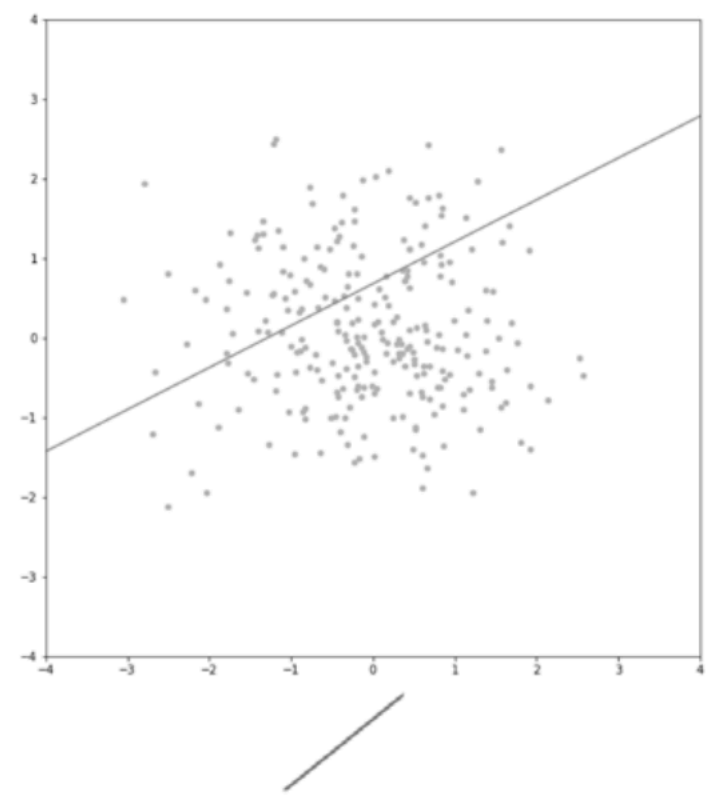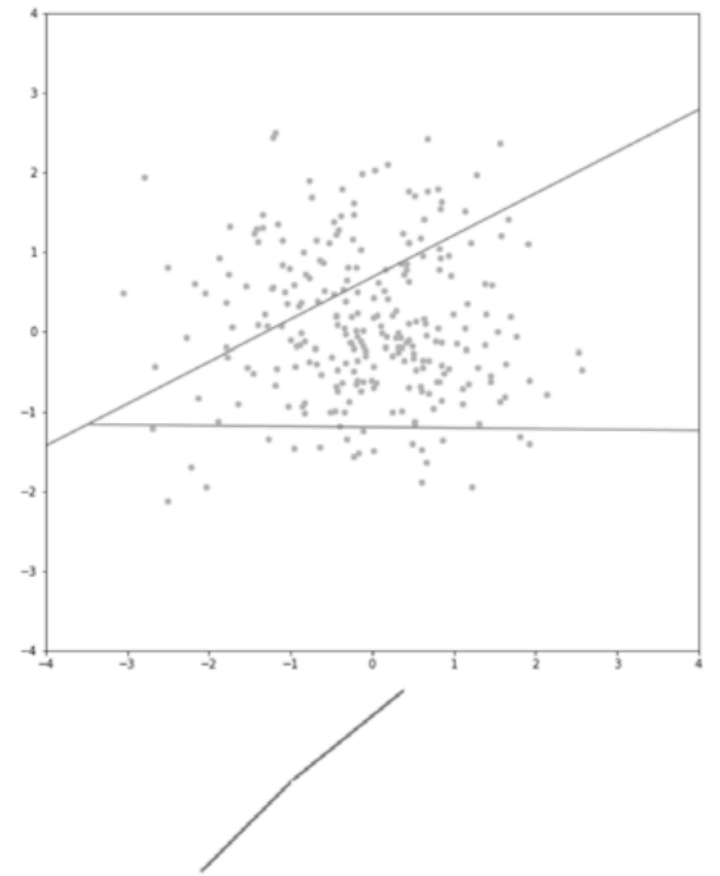
Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.

- For each tree:
    - Get a sample of the data
    - Randomly select a dimension
    - Randomly pick a value in that dimension
    - Draw a straight line through the data at that value and split data
    - Repeat until tree is complete

- Generate multiple trees -> forest

- Anomalies will be isolated in only few steps

- Nominal points in more

Isolation Forest

Single Tree scores for
anomaly and nominal points

Forest plotted radially.
Scores for anomaly and
nominal shown as lines
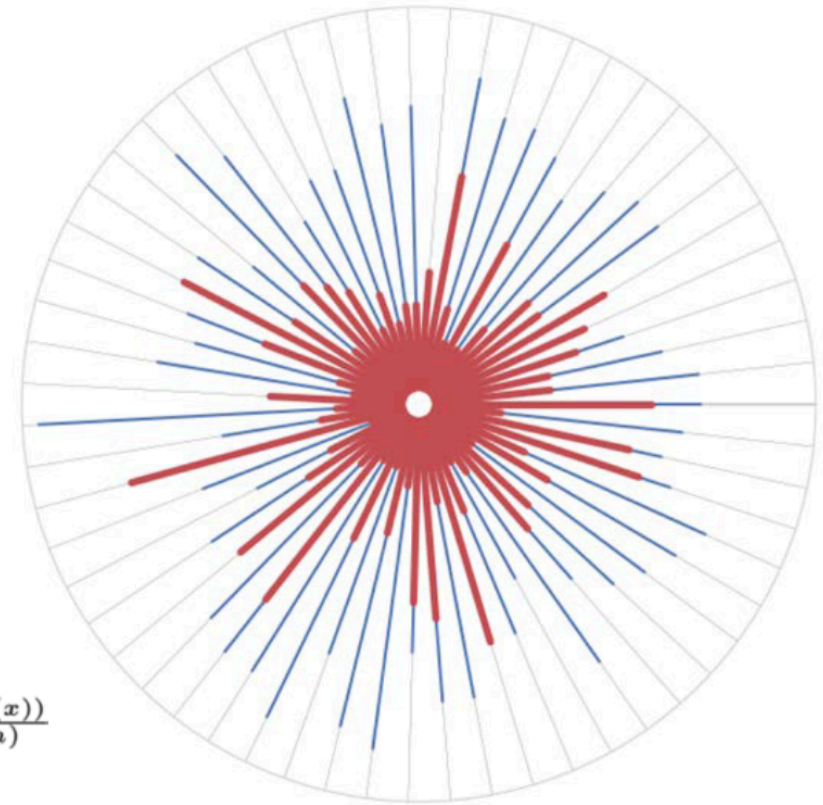
$$s(x, n) = 2^{-\frac{E(h(x))}{c(n)}}$$

Anomaly Detection with Isolation Forest

- Isolation Forest
  - Computationally Efficient
  - Parallelizable
  - Handle high dimensional data
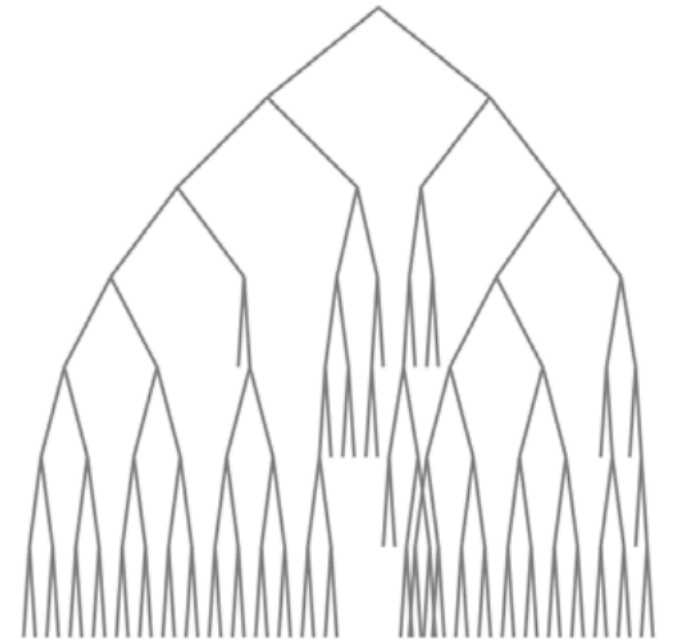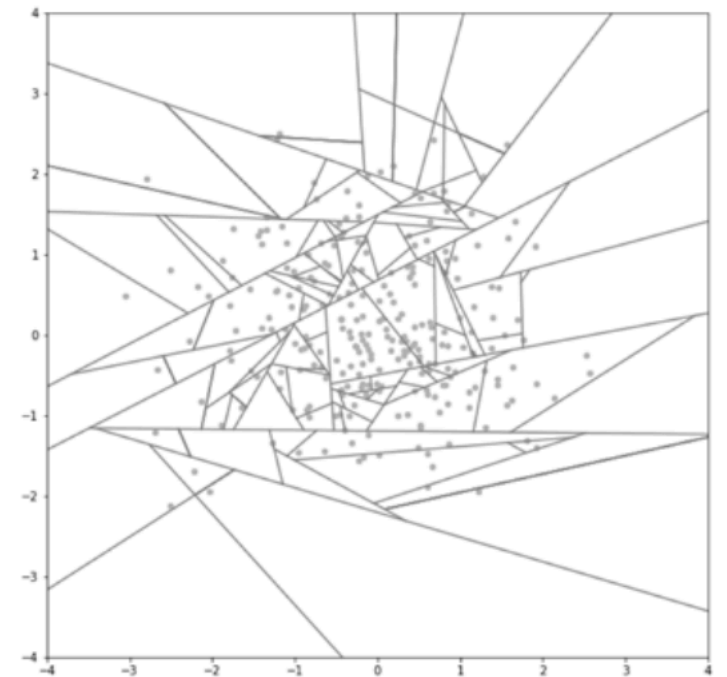 - Inconsistent scoring can be observed
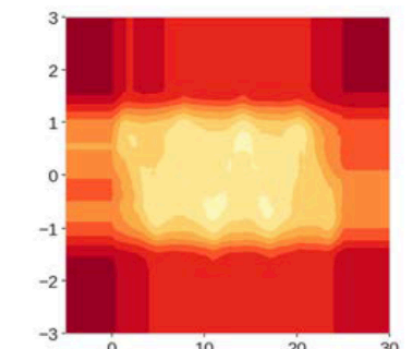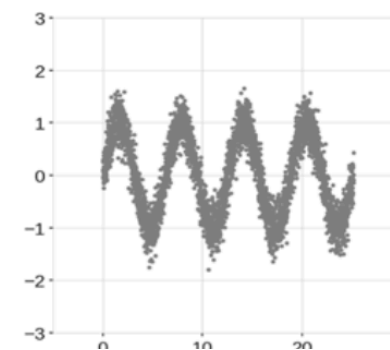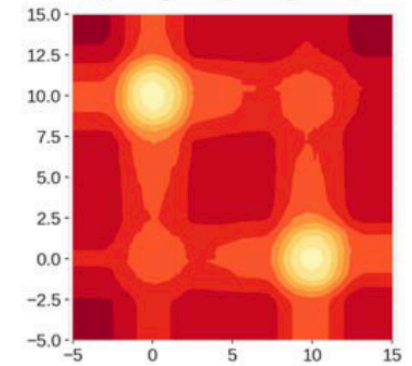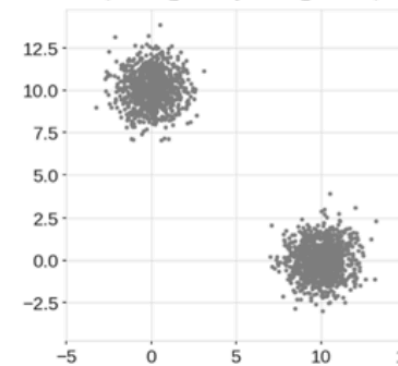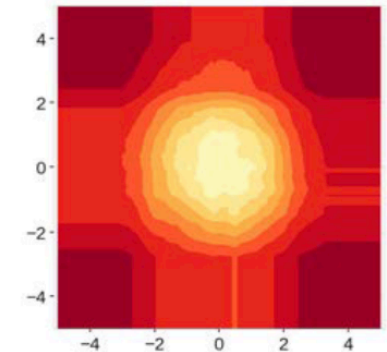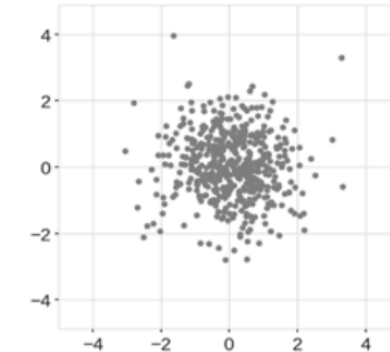
Extended Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.

- For each tree:
  - Get a sample of the data
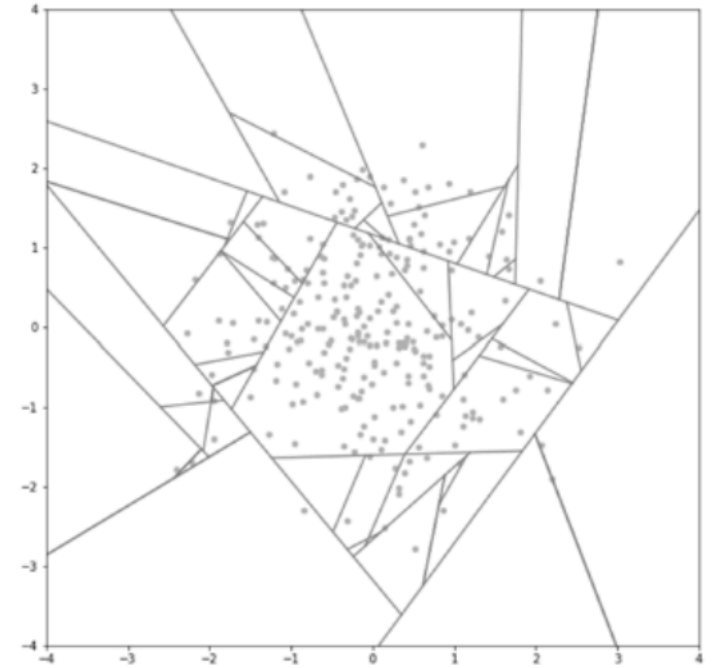 - Randomly select a normal vector
  - Randomly select an intercept

Extended Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.

- For each tree:
  - Get a sample of the data
  - Randomly select a normal vector
  - Randomly select an intercept
 - Draw a straight line through the data at that value and split data

Extended Isolation Forest

- Idea: Few and different instances can be isolated quicker
- Given the dataset build a forest of trees.
- For each tree:
  - Get a sample of the data
  - Randomly select a normal vector
  - Randomly select an intercept
  - Draw a straight line through the data at that value and split data
 - Repeat until the tree is complete

Extended Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.

- For each tree:
  - Get a sample of the data
  - Randomly select a normal vector
  - Randomly select an intercept
  - Draw a straight line through the data at that value and split data
  - Repeat until the tree is complete

Extended Isolation Forest

- Idea: Few and different instances can be isolated quicker

- Given the dataset build a forest of trees.

- For each tree:
  - Get a sample of the data
  - Randomly select a normal vector
  - Randomly select an intercept
  - Draw a straight line through the data at that value and split data
  - Repeat until the tree is complete

- Generate multiple trees –> forest

Anomaly Detection with Isolation Forest

- Isolation Forest
  - Computationally Efficient
  - Parallelizable
  - Handle high dimensional data
  - Inconsistent scoring can be observed
- Extended Isolation Forest
  - Computationally Efficient
  - Parallelizable
  - Handle high dimensional data
 - Consistent scoring
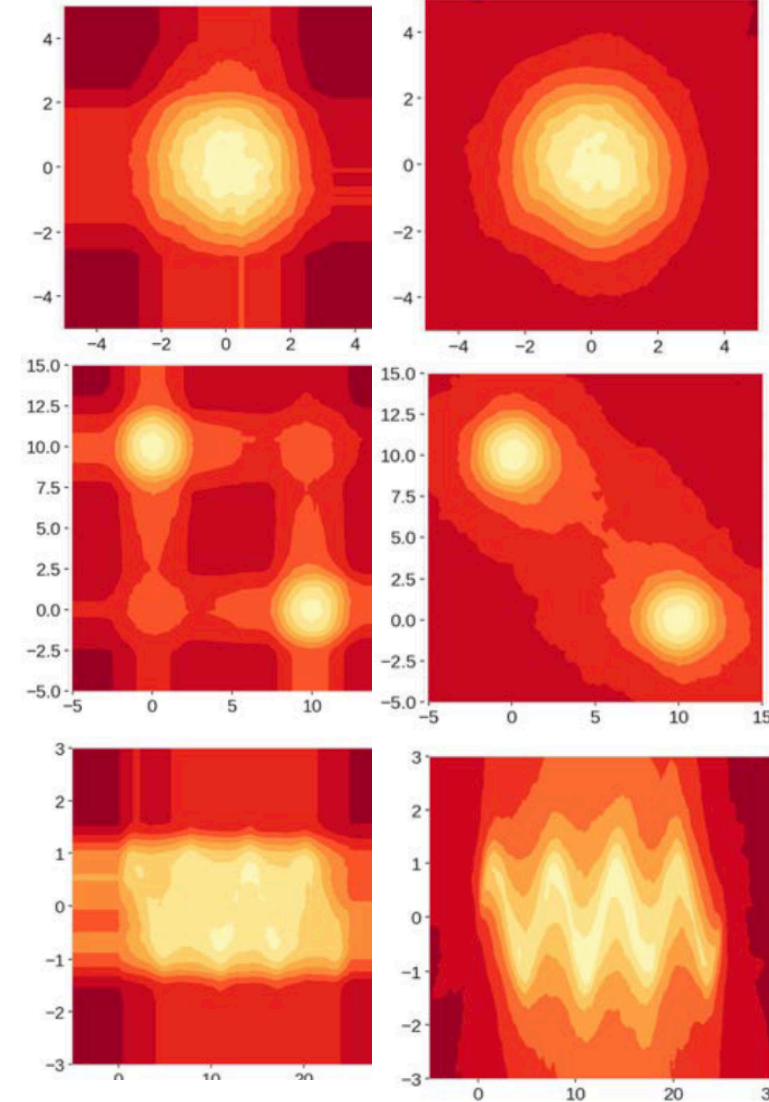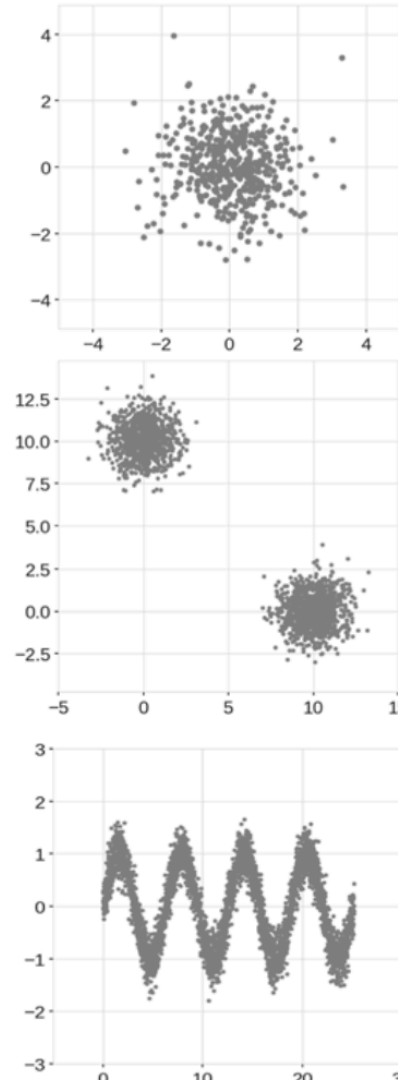
Summary

- Different models are based on different assumptions
- Different models provide different types of output (labeling/scoring)
- Different models consider outlier at different resolutions (global/local)
- Thus, different models will produce different results
- A thorough and comprehensive comparison between different models and approaches is still missing

References

- Anomaly Detection. Chapter 10. Introduction to Data Mining.

- Liu, Fei Tony; Ting, Kai Ming; Zhou, Zhi-Hua (December 2008). "Isolation Forest". 2008 Eighth IEEE International Conference on Data Mining: 413–422

- Chandola, V., Banerjee, A., & Kumar, V. (2009). Anomaly detection: A survey. ACM computing surveys (CSUR), 41(3), 1-58.
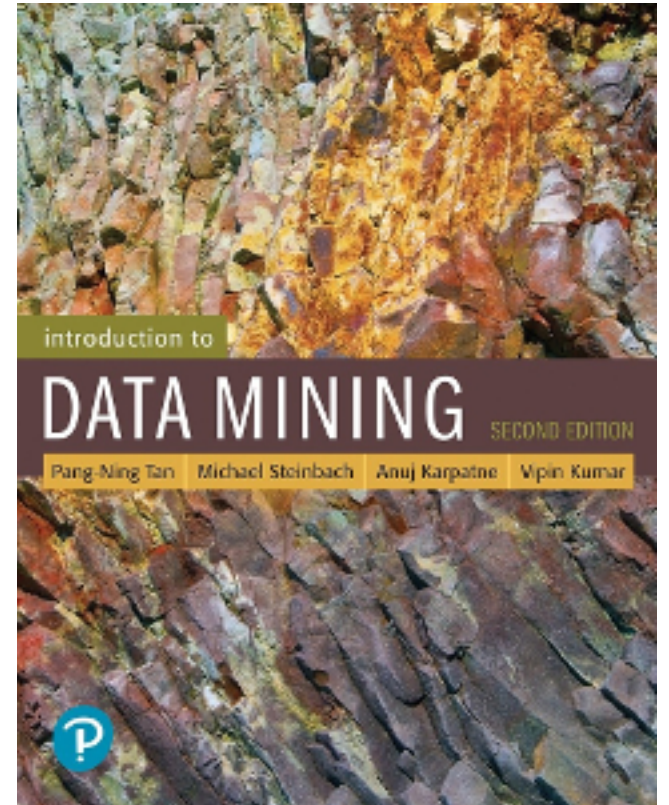
Exercises – Outlier Detection

Outlier Detection – Exercise 1

Given the dataset of 10 points below, consider the outlier detection problem for points A and B, adopting the following three methods:

a) Distance-based: DB(ε,п)   (**2 points**)
Are A and/or B outliers, if thresholds are forced to ε = 2.5 and п = 0.15 ? The point itself should not be counted.

b) Density-based: LOF   (**2 points**)
Compute the LOF score for points A and B by taking k=2, i.e. comparing each point with its 2 NNs (not counting the point itself). In order to simplify the calculations, the reachability-distance used by LOF can be replaced by the simple Euclidean distance.

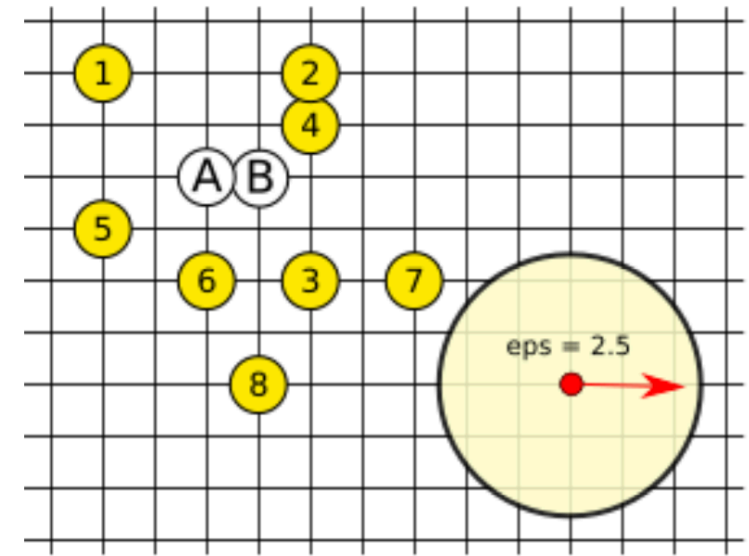c) Depth-based   (**2 points**)
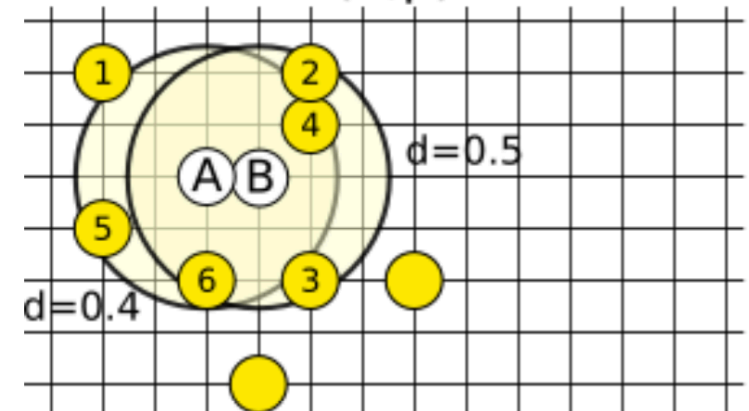Compute the depth score of all points.
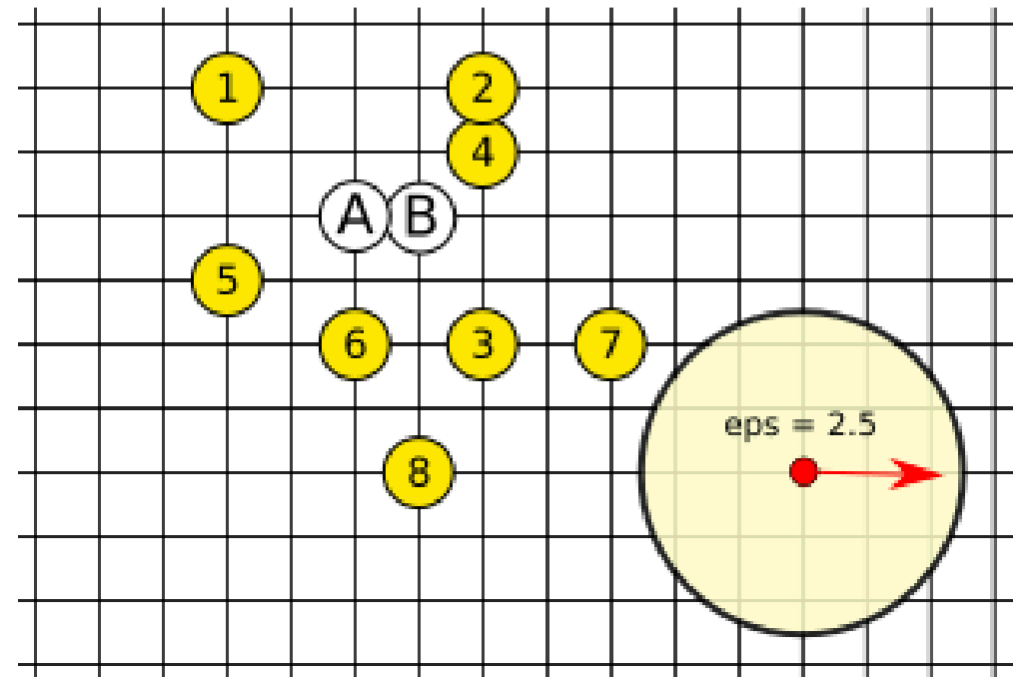
Outlier Detection – Exercise 1 – Solution

Distance-based

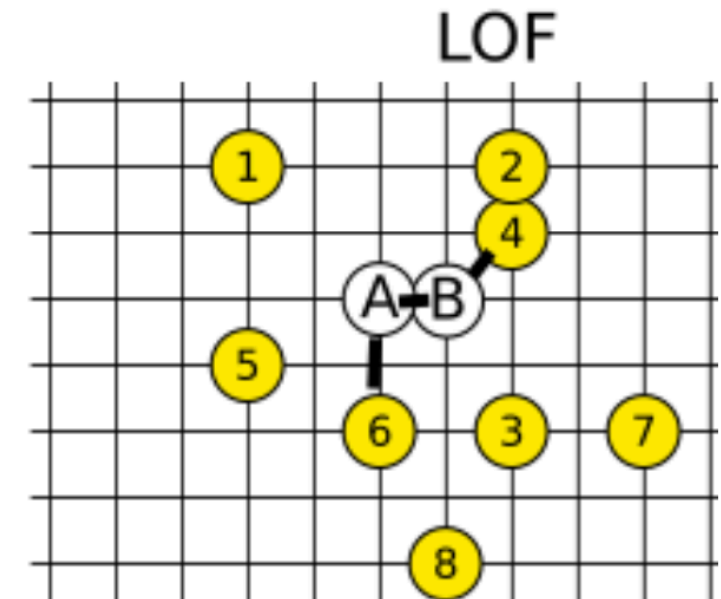- No outliers because within their radius there are 0.4 and 0.5 points for A and B, respectively

DB(e,p)

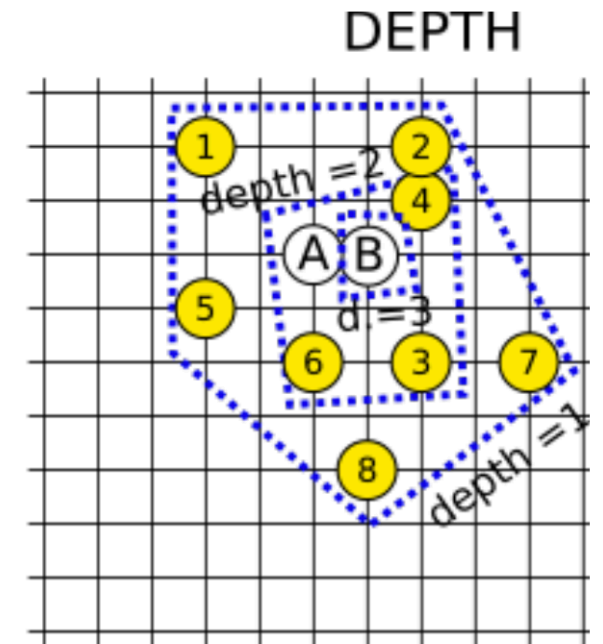# Outlier Detection – Exercise 1 – Solution

Density-based

- LRD(A) = 1/ [(1 + 2)/2] = 0.666

- LRD(B) = 1/ [(1 + √2)/2] = 0.828

- LRD(6) = 1/ [(2 + 2)/2] = 0.500

- LOF(A) = ([LRD(B) + LRD(6)]/2) / LRD(A) = [(0.828 + 0.500) / 2] / 0.666 = 1.003

- LRD(4) = 1/ [(1 + √2)/2] = 0.828

- LOF(B) = ([LRD(A) + LRD(4)]/2) / LRD(B) = [(0.666 + 0.828) / 2] / 0.828 = 0.902

- Both are smaller or very close to 1, so they are most likely no outliers.

LOF

Outlier Detection – Exercise 1 – Solution

Depth-based

- A is an outlier for depth = 2

- For depth <= 1 neither A or B are outliers

Outlier Detection – Exercise 2

Given the dataset of 10 points below, consider the outlier detection problem for points A and B, adopting the following three methods:

a) Distance-based: DB(ε,π)   **(2 points)**
Are A and/or B outliers, if thresholds are forced to ε = 2.1 and π = 0.15 ? The point itself should not be counted.

b) Density-based: LOF   **(2 points)**
Compute the LOF score for points A and B by taking k=2, i.e. comparing each point with its 2 NNs (not counting the point itself). In order to simplify the calculations, the reachability-distance used by LOF can be replaced by the simple Euclidean distance.
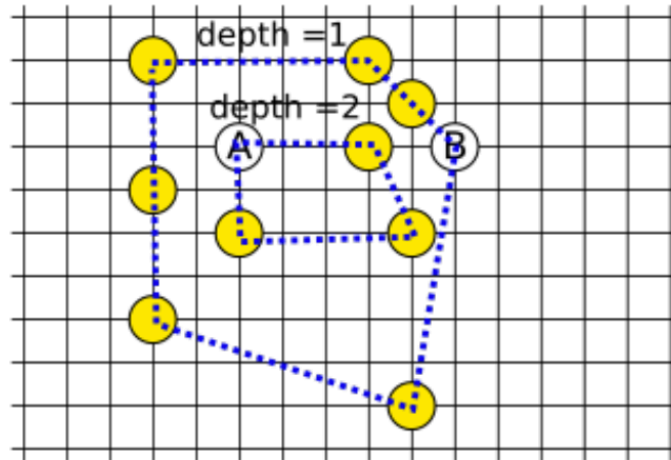
c) Depth-based   **(2 points)**
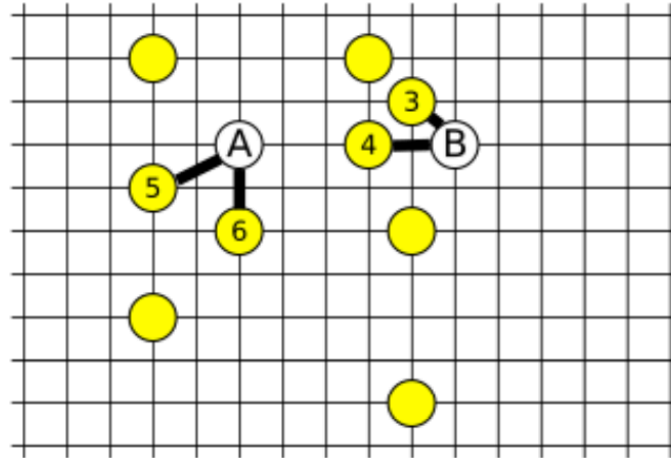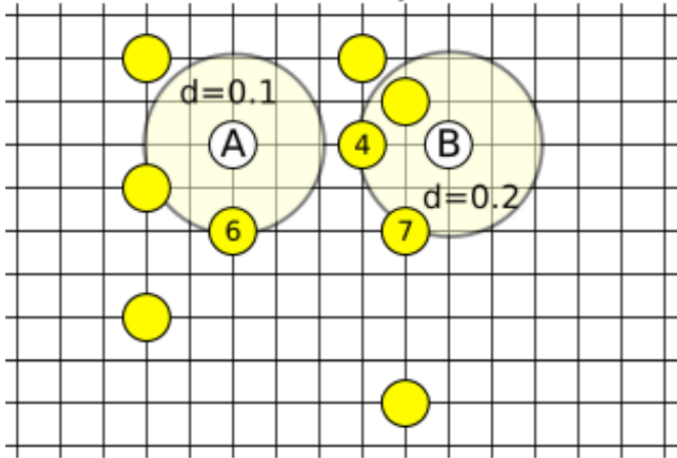Compute the depth score of all points. Are A and/or B outliers of depth 1?
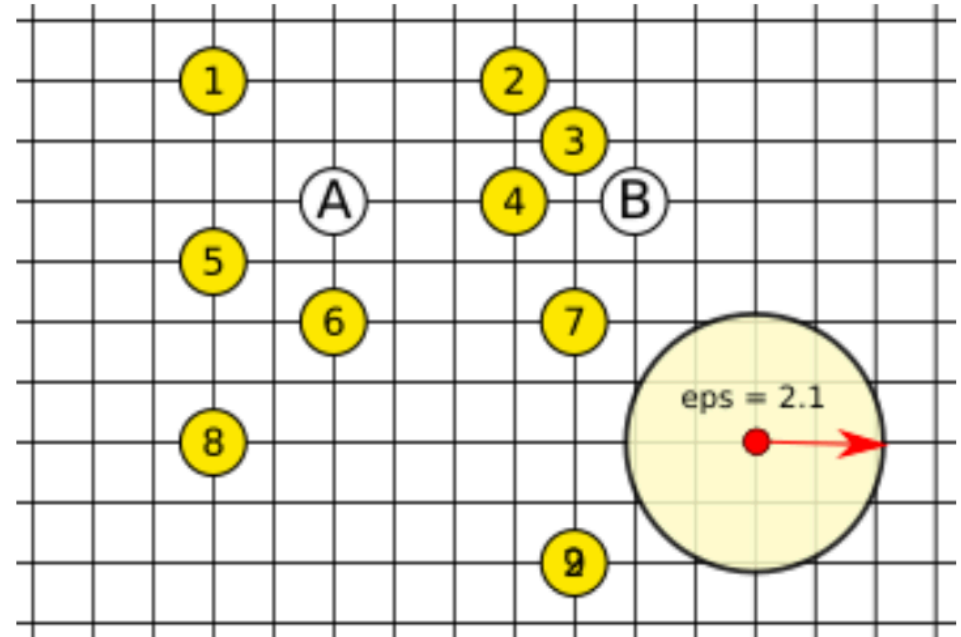
Outlier Detection – Exercise 2 – Solution
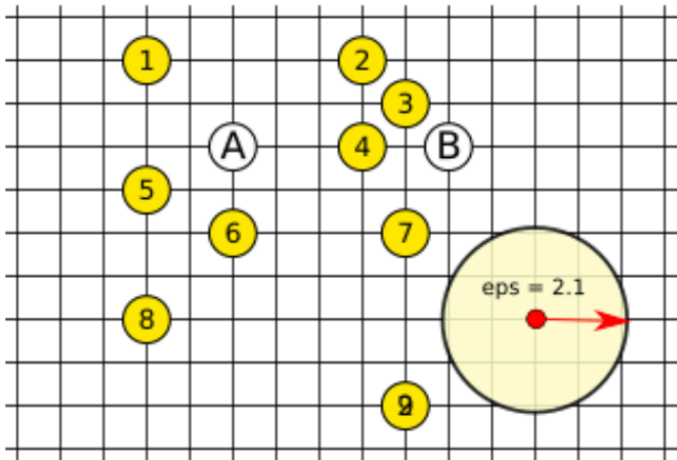
LRD(A) = 1/ [(2 + √5)/2] = 0.472

LRD(5) = 1/ [(√5 + √5)/2] = 0.447

LRD(6) = 1/ [(2 + √5)/2] = 0.472

LOF(A) = ([LRD(5) + LRD(6)]/2) / LRD(A)
= [(0.472 + 0.447) / 2] / 0.472 = 0.973

DB(e,p)

LOF

LRD(B) = 1/ [(2 + √2)/2] = 0.586

LRD(3) = 1/ [(√2 + √2 + √2)/3] = 0.707

LRD(4) = 1/ [(2 + 2 + √2)/3] = 0.554

LOF(B) = ([LRD(3) + LRD(4)]/2) / LRD(B)
= [(0.707 + 0.554) / 2] / 0.586 = 0.929

Outlier Detection – Exercise 3

Given the dataset of 10 points below (A, B, 1, 2, …, 8), consider the outlier detection problem for points A and B, adopting the following three methods:

a) Distance-based: DB(ε,π) **(2 points)**
Are A and/or B outliers, if thresholds are forced to ε = 2.5 and π = 0.3? Show the density of the two points. (Notice: in computing the density of a point P, P itself should not be counted as neighbour).

b) Density-based: LOF **(3 points)**
Compute the LOF score for points A and B by taking k=2, i.e. comparing each point with its 2-NNs (not counting the point itself). In order to simplify the calculations, the reachability-distance used by LOF can be replaced by the simple Euclidean distance.

c) Depth-based **(1 points)**
Compute the depth score of all points.