

Lecture: Machine Learning for Data Science

Winter semester 2021/22

Lecture 15: Outlier detection

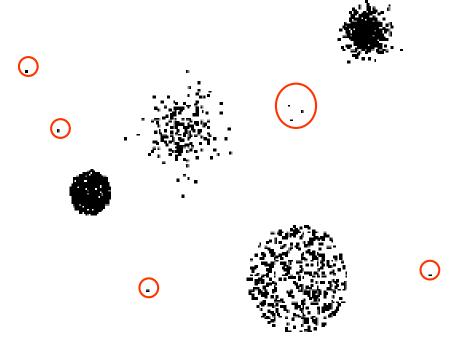
Prof. Dr. Eirini Ntoutsi

Outline

- Introduction
- Approaches for outlier detection
- Model-based or Statistical approaches
- Distance-based approaches
- Density-based approaches
- Clustering-based approaches
- Things you should know from this lecture & reading material

Outlier detection/ anomaly detection

- Goal: find objects that are considerably different from most other objects or unusual or in some way
 inconsistent with other objects
 - Outliers / anomalous objects / exceptions
 - Anomaly detection/ Outlier detection / Exception mining
- It is used either as a
 - Standalone task (anomalies are the focus)
 - Pre-processing task (to improve data quality)
 - Post-processing task (to improve pattern quality)



Applications 1/2

- Fraud detection, e.g., credit cards
 - 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 on different aspects like frequency, spatial correlation, etc.

Applications 2/2

Sports statistics

- □ In many sports, various parameters are recorded for players in order to evaluate the players' performances
- Outstanding (in a positive as well as a negative sense) players may be identified as having abnormal parameter values
- Sometimes, players show abnormal values only on a subset or a special combination of the recorded parameters
- Intrusion detection, e.g., in networks
 - Attack connections different than normal connections
- Detecting measurement errors
 - Data derived from sensors (e.g. in a given scientific experiment) may contain measurement errors
 - Abnormal values could provide an indication of a measurement error
 - Removing such errors can be important in other data analysis tasks

An example from sports

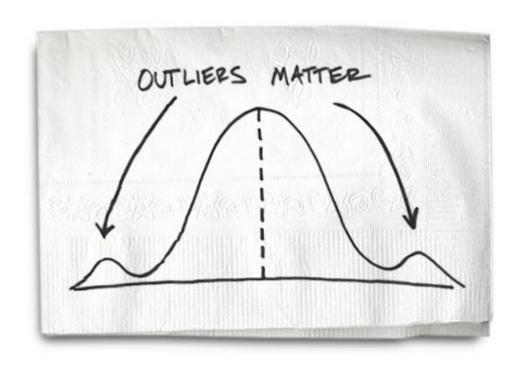
- Analysis of the SAT.1-Ran-Soccer-Database (Season 1998/99)
 - 375 players
 - □ Primary attributes: Name, #games, #goals, playing position (goalkeeper, defense, midfield, offense),
 - Derived attribute: Goals per game
 - Outlier analysis (playing position, #games, #goals)
- Result: Top 5 outliers

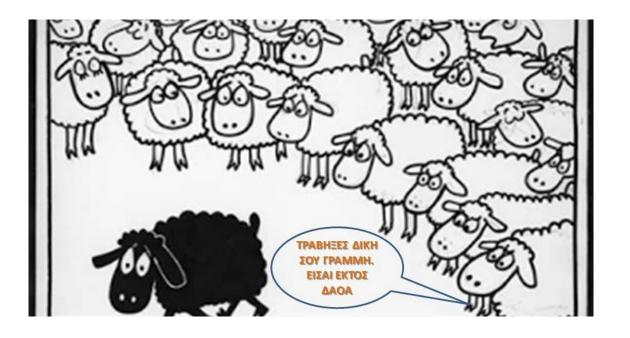
Rank	Name	# games	#goals	position	Explanation
1	Michael Preetz	34	23	Offense	Top scorer overall
2	Michael Schjönberg	15	6	Defense	Top scoring defense player
3	Hans-Jörg Butt	34	7	Goalkeeper	Goalkeeper with the most goals
4	Ulf Kirsten	31	19	Offense	2 nd scorer overall
5	Giovanne Elber	21	13	Offense	High #goals/per game

Being an "outlier" is not necessarily a negative term.

Outliers matter

• One person's noise could be another person's signal.

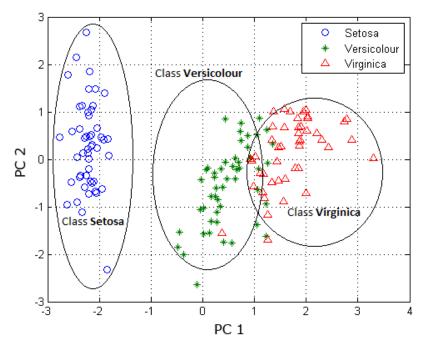




Causes of anomaly 1/3

Data from different "classes"

- An object might be different from other objects because it is from another class (it comes from another distribution).
 - E.g. an attack connection in a network has different characteristics from a normal connection.
 - Or, a person who commits credit card fraud belongs to a different class than persons using credit cards legally.

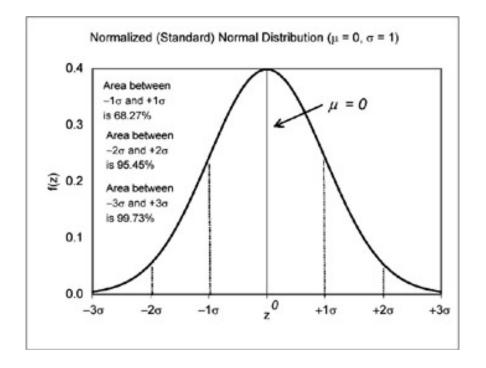


Machine Learning for Data Science: Lecture 15 - Outlier detection

Causes of anomaly 2/3

Natural variation

- Many datasets can be modeled by statistical distributions
 - e.g., Gaussian distribution (most objects are near the center, the likelihood that an object differs significantly from the avg object is small).
 - □ In that case an exceptional tall person is not anomalous (not from another distribution), but it has an extreme value



Causes of anomaly 3/3

- Data measurement errors and collection errors
 - erroneous measurements due to human/ measuring device errors, noise presence.
 - such errors should be eliminated since they just reduce the quality of data
- Other causes ...
- In practice, the techniques can be used for all those causes

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

Variants of outlier detection problems/tasks

- Compute anomaly score for a query instance
 - Given a dataset D, containing mostly normal (but unlabeled) data points, and a query point $x \in D$, compute the anomaly score of x w.r.t. D
- Detect all anomalies in the dataset w.r.t. an anomaly threshold t
 - Given a dataset D, find all the data points $x \in D$ with anomaly scores f(x) greater than a threshold t
- Detect top-n anomalies in the dataset
 - \Box Given a dataset D, find all the data points $x \in D$ having the top-n largest anomaly scores f(x)

Outline

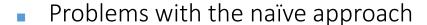
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Basic ML approaches for outlier detection

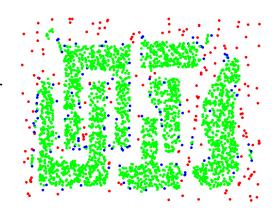
- Distinction based on the availability of class labels (for anomalies or normal instances)
- Supervised anomaly detection
 - In some applications, training data with both normal and abnormal data objects are provided
 - There may be multiple normal and/or abnormal classes
 - □ In such cases, the goal is to classify a new instance as anomaly or not
 - Often, the classification problem is highly imbalanced
- Unsupervised anomaly detection
 - In most applications there are no training data available
 - In such cases, the goal is to assign a score to each instance that reflects the degree to which the instance is anomalous.
 - This is the most common case.
- Semi-supervised anomaly detection
 - In some applications, only training data for the normal class(es) (or only the abnormal class(es)) are provided

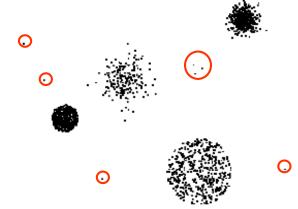
Outlier detection and clustering

- Many clustering algorithms do not assign all points to clusters but account for noise objects
 - E.g., DBSCAN.
- Naïve approach: Look for outliers by applying one of those algorithms and retrieve the noise set
 - □ In this case, outliers are just a side product of the clustering algorithms



- Clustering algorithms are optimized to find clusters rather than outliers
- Accuracy of outlier detection depends on how well 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
- So, outlier detection is a problem on its own.





A variety of different outlier detection methods

- A variety of approaches that can be categorized according to the following aspects:
 - 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
- NOTE: we focus on models and methods for Euclidean data but many of those can be also used for other data types (because they only require a distance measure)

Global vs local outlier detection approaches

 Considers the resolution of the reference set w.r.t. which the "outlierness" of a particular data object is determined

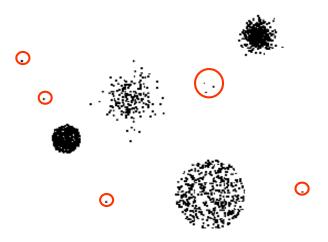
Global approaches

- □ 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

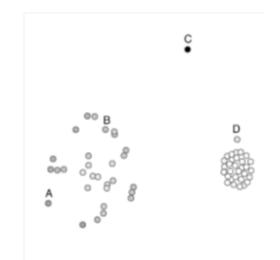
- □ The reference contains a (small) subset of data objects
- No assumption on the number of normal mechanisms
- Basic problem: how to choose a proper reference set
- Some approaches are somewhat in between (hybrid)
 - The resolution of the reference set varies e.g. from only a single object (local) to the entire database (global) automatically or by a user-defined input parameter





Labeling vs scoring outlier detection approaches

- Considers the output of an outlier detection algorithm
- Labeling approaches
 - Binary output
 - Data objects are labeled either as normal or outlier
 - E.g., points C and D are outliers
- Scoring approaches
 - Continuous output
 - For each object an outlier score is computed (e.g. the probability of 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 be turned into labeling approaches if necessary (e.g., by defining a suitable threshold on the scoring values)



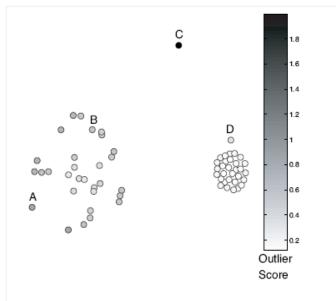
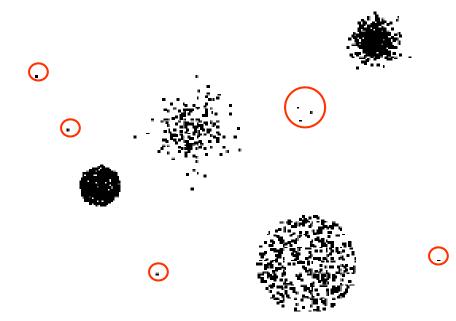


Figure 10.7. Outlier score based on the distance to the fifth nearest neighbor. Clusters of differing density.

Outlier detection approaches w.r.t. modeling properties

- General steps
 - Build a profile of the "normal" behavior
 - i.e., patterns or summary statistics for the overall population
 - Use the "normal" profile to detect anomalies
 - Anomalies are observations whose characteristics differ significantly from the normal profile
- Types of anomaly detection schemes
 - Model-based (or, statistical approaches)
 - Distance-based
 - Density-based
 - Clustering-based



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Model-based or Statistical approaches

- A model of the data is built and instances are evaluated w.r.t. how well they fit the model
- An outlier is an object that has a low probability w.r.t. a probability distribution model of the data.
- Most approaches here follow the following 2-step approach:
 - building a probability distribution model (by learning the distribution parameters from the data) and
 - considering how likely instances are under that model

Model-based or Statistical approaches at a glance

General idea

- Assuming a certain kind of statistical distribution (e.g., Gaussian)
- Compute the parameters assuming all data points have been generated by such a statistical distribution (e.g., mean and standard deviation in univariate Gaussian case)
- Outliers are points that have a low probability to be generated by the overall distribution (e.g., deviate more than 3 times the standard deviation from the mean)

Basic assumption

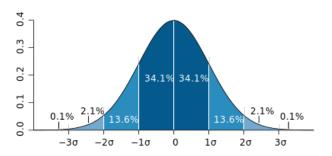
- Normal data objects follow a (known) distribution and occur in a high probability region of this model
- Outliers deviate strongly from this distribution
- A huge number of tests are available differing in
 - Type of data distribution (e.g. Gaussian)
 - Number of variables, i.e., dimensions of the data objects (univariate/multivariate)
 - Number of data distributions (mixture models)

Example: univariate Gaussian

- Assuming a univariate Gaussian distribution
- Compute the parameters of the model, μ and σ^2 , assuming all data points have been generated by such a statistical distribution
- Probability density function of a univariate normal distribution

$$f(x\mid \mu,\sigma^2) = rac{1}{\sqrt{2\sigma^2\pi}} \ e^{-rac{(x-\mu)^2}{2\sigma^2}}$$

- Most of the objects are within +-3 σ (99.7%)
- There is a little chance that an object will occur at the tails of the distribution
- Score outliers based on the distance of the points to the mean μ



- μ is the mean value of all points
- σ^2 is the variance

Example: multivariate Gaussian

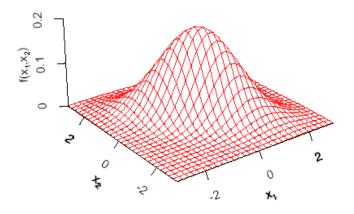
- Assuming a multivariate Gaussian distribution (1 model)
- Compute the parameters of the model, μ and Σ , assuming all data points have been generated by such a statistical distribution
- Probability density function of a multivariate normal distribution

$$N(x) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} e^{-\frac{(x-\mu)^T \Sigma^{-1} (x-\mu)}{2}}$$

 Score outliers based on Mahalanobis distance, a measure of the distance between a point x and a distribution

$$MDist(x, \mu) = (x - \mu)^{\mathrm{T}} \Sigma^{-1} (x - \mu)$$

- $(x-\mu)$ is the distance of x from the mean μ
- \Box Division by covariance Σ effect
 - If attributes are strongly correlated → high covariance → distance will be reduced
 - If attributes are not correlated → low covariance → distance will not be affected much



- μ is the mean of the population
- Σ is the covariance matrix

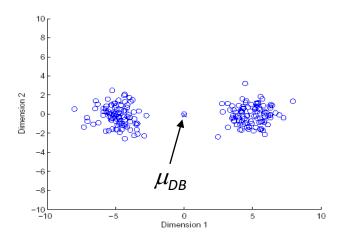
Model-based approaches overview

Robustness

- Mean and standard deviation are very sensitive to outliers
- These values are computed for the complete data set (including potential outliers)

Discussion

- Data distribution is fixed
- Low flexibility (no mixture model)
- Global method
- Outputs a label but it can also output a score



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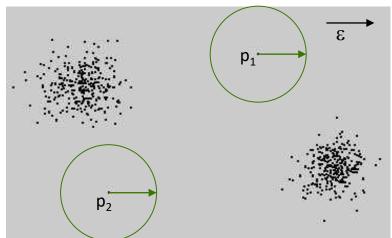
Distance-based approaches

- General idea: Judge a point based on the distance(s) to its neighbor(s)
- Basic assumption:
 - An object is an anomaly if it is distant from most points
 - Normal data objects have a dense neighborhood
 - Outliers are far apart from their neighbors, i.e., they have a less dense neighborhood
- More general and more easily applied than statistical approaches since its easier to find a suitable proximity measure than to determine the statistical distribution
- Several variations of what is an outlier
 - \Box Data points for which there are fewer than p neighboring points within a distance d
 - \Box The top-*n* data points whose distance to the *k*-th nearest neighbor is greatest
 - \Box The top-*n* data points whose average distance to the *k*-th nearest neighbors is greatest

Distance-based approaches: Basic model [Knorr and Ng 1997]

- Data points for which there are fewer than p neighboring points within a distance d
- DB(ε , π)-Outliers
 - Basic model [Knorr and Ng 1997]
 - Given a radius ε and a percentage π , the set of outlier points is defined as follows

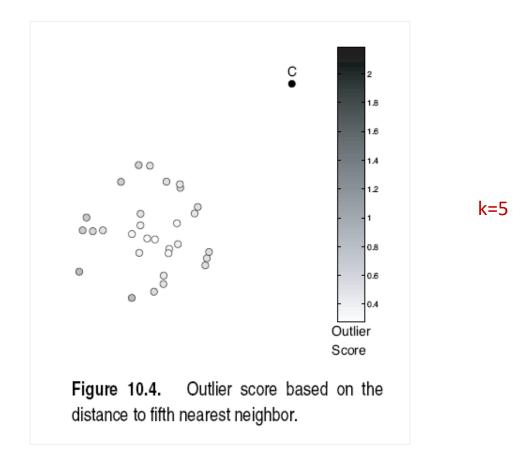
$$OutlierSet(\varepsilon,\pi) = \{p \mid \frac{Card(\{q \in DB \mid dist(p,q) < \varepsilon\})}{Card(DB)} \leq \pi \}$$



range-query with radius arepsilon

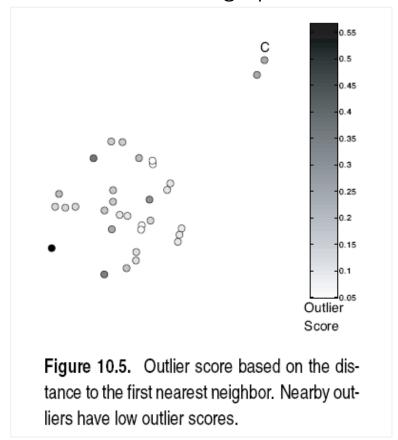
Distance-based approaches: kth nearest neighbor-based 1/3

- The outlier score of an object is given by its distance to its k-nearest neighbor (kNN distance).
 - Lowest outlier score 0.

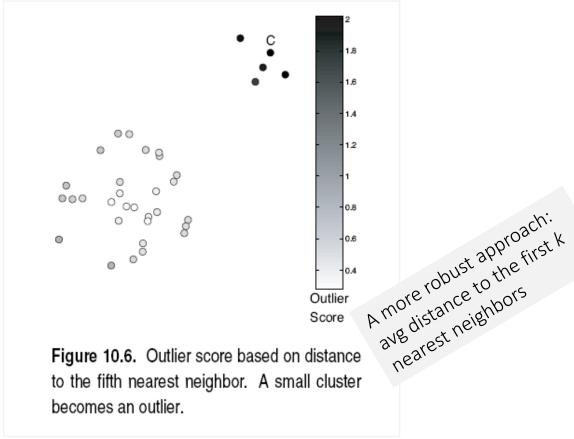


Distance-based approaches: kth nearest neighbor-based 2/3

The outlier score is highly sensitive to the value of k.



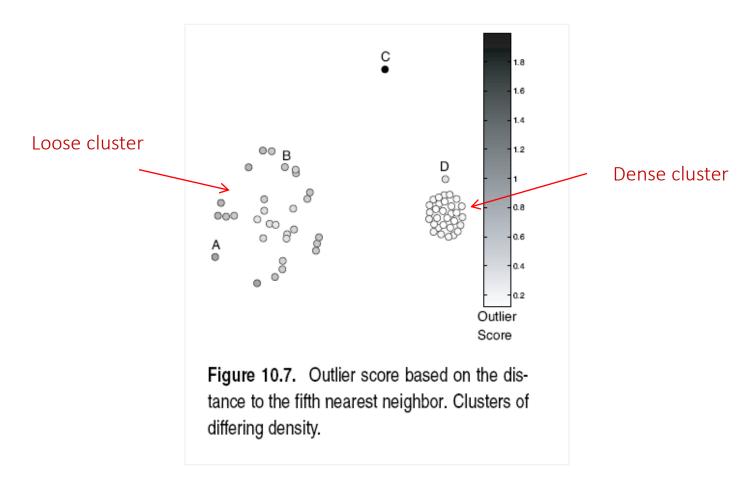
• If *k* is too small, then a small number of nearby outliers can cause low outlier scores.



• If *k* is too large, then all objects in a cluster with less than k objects might become outliers.

Distance-based approaches: kth nearest neighbor-based 3/3

It cannot handle datasets with regions of widely different densities due to the global threshold k



Distance-based approaches overview

- Simple schemes
- Expensive
 - Index structures or specialized algorithms have been proposed for performance improvement
- Sensitive to the choice of parameters
- In high-dimensional spaces, data is sparse and the notion of proximity becomes meaningless
 - Every point is an almost equally good outlier from the perspective of proximity-based definitions
 - Lower-dimensional projection methods have been proposed to tackle this issue.

Outline

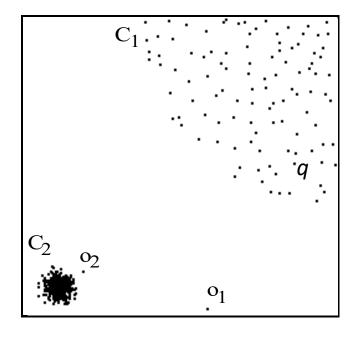
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Density-based approaches

- Outliers are instances in regions of low density
- 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' density is computed as an outlier score
 - Approaches essentially differ on how they 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 from the density around its neighbors
- Closely related to distance-based methods, since density is usually defined in terms of proximity.

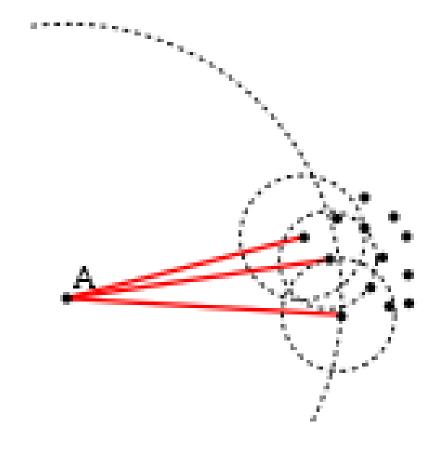
LOF(Local Outlier Factor): Motivation

- 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?
- Existing solutions
 - \square DB($arepsilon,\pi$)-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., point 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



LOF(Local Outlier Factor): Basic idea

- Basic idea of LOF: compare the local density of a point with the densities of its neighbors.
- Outlier points will have a much lower density
 - E.g., A has a much lower density than its neighbors.



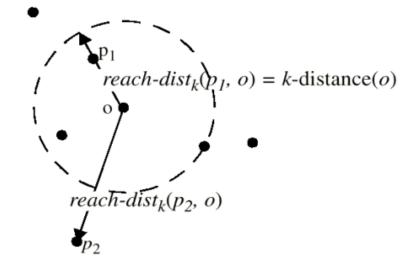
LOF(Local Outlier Factor): Reachability distance

Reachability distance of an object p w.r.t. an object o

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

- \neg k-distance(o) is the distance of o to its k-th nearest neighbor
- \Box dist(p,o) is the actual distance between p and o

- Note that the set of the k nearest neighbors includes all objects at this distance, which can in the case of a "tie" be more than k objects
- This is not symmetric!



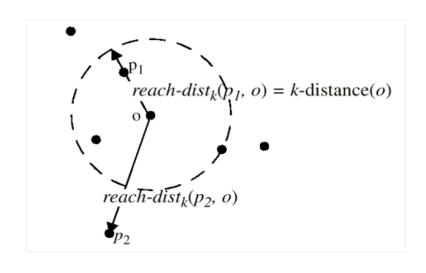
LOF(Local Outlier Factor)

Reachability distance of an object p w.r.t. an object o

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

Average reachability distance in the kNN of a point p

$$\frac{\sum_{o \in kNN(p)} reach - dist_k(p, o)}{|kNN(p)|}$$



• We turn this into "density" using the <u>inverse</u> of the average reachability distance in the KNN of $p \rightarrow$ Local reachability density (*Ird*) of point p

$$lrd_{k}(p) = 1 / \left(\frac{\sum_{o \in kNN(p)} reach - dist_{k}(p, o)}{|kNN(p)|} \right) \Rightarrow \frac{1}{lrd_{k}(p)} = \frac{\sum_{o \in kNN(p)} reach - dist_{k}(p, o)}{|kNN(p)|}$$

LOF(Local Outlier Factor)

Reachability distance of an object p w.r.t. an object o

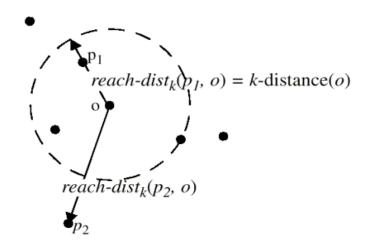
$$reach-dist_k(p,o) = \max\{k-\text{distance}(o), dist(p,o)\}$$

Local reachability density (Ird) of point p

$$lrd_{k}(p) = 1 / \left(\frac{\sum_{o \in kNN(p)} reach - dist_{k}(p, o)}{|kNN(p)|} \right)$$

- Local outlier factor (LOF) of point p
 - Average ratio of Irds of neighbors of p and Ird of p

$$LOF_{k}(p) = \frac{1}{|kNN(p)|} * \sum_{o \in kNN(p)} \frac{lrd_{k}(o)}{lrd_{k}(p)}$$
 relative density average



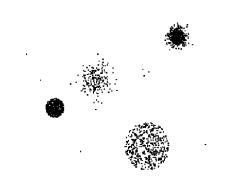
LOF(Local Outlier Factor): Discussion

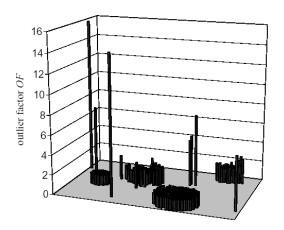
Properties

- LOF ≈ 1: point is in a cluster (region with homogeneous density around the point and its neighbors)
- □ LOF >> 1: point is an outlier
- So, outliers are points with the largest LOF values

Discussion

- □ Choice of *k* (*MinPts* in the original paper) specifies the reference set
- Implements a local approach (resolution depends on the user's choice for k)
- Outputs a scoring (assigns a LOF value to each point)





LOFs (MinPts = 40)

LOF(Local Outlier Factor): Another example

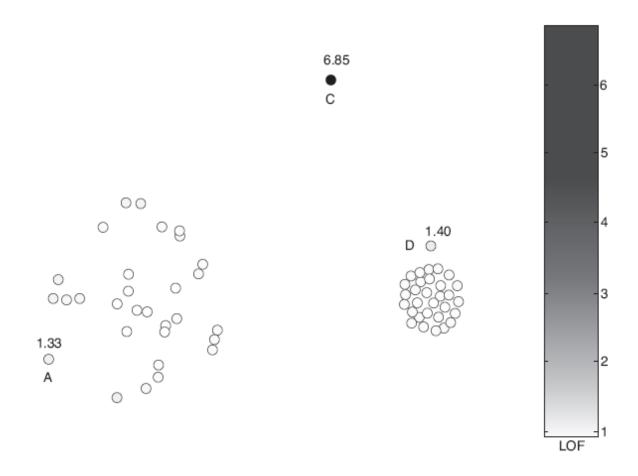


Figure 10.8. Relative density (LOF) outlier scores for two-dimensional points of Figure 10.7.

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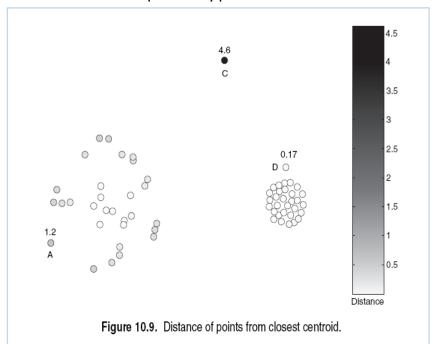
Clustering-based approaches

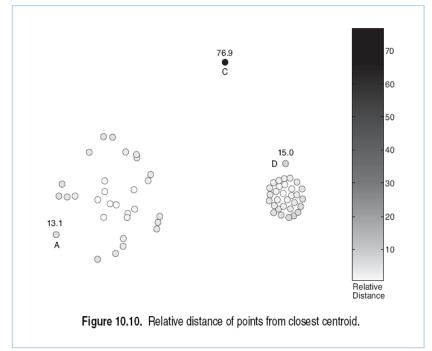
ullet Intuition: An object is a cluster-based outlier if it does not strongly belong to any clusullet

- Basic idea:
 - Cluster the data into groups
 - Choose points in small clusters as candidate outliers. Compute the distance between candidate points and non-candidate clusters.
 - If candidate points are far from all other non-candidate points, they are outliers
- A more systematic approach
 - □ Find clusters and then assess the degree to which a point belongs to any cluster
 - e.g. for k-Means distance to the centroid
 - In case of k-Means (or in general, clustering algorithms with some objective function), if the elimination of a point results in substantial improvement of the objective function, we could classify it as an outlier
 - i.e., clustering creates a model of the data and the outliers distort that model.

Prototype-based clusters

- Methods like k-Means, k-Medoids
- Several ways to assess the extent to which a point belongs to a cluster
 - Measure the distance of the object to the cluster prototype and take this as the outlier score
 - Or, if the clusters are of different densities, the outlier score could be the relative distance of an object from the cluster prototype w.r.t. the distances of the other objects in the cluster.





Outlier evaluation

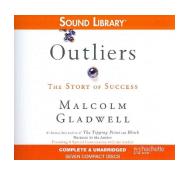
- If there are class labels
 - Similar to classifier evaluation, but outlier class is typically smaller than the normal class
 - Measures such as precision and recall are more appropriate than e.g., accuracy or error rate
- In the absence of class labels
 - More difficult
 - For model-based approaches, one could check model improvement after outlier removal
- Outlier evaluation is a topic of its own ©

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Overview and Reading

- Basics
- Statistical-based approaches
- Distance-based approaches
- Density-based approaches
- Clustering-based approaches
- Reading
 - □ Tan P.-N., Steinbach M., Kumar V book, Chapter 10.
 - "Outlier Detection Techniques" tutorial by H.-P. Kriegel, P. Kröger, A. Zimek at KDD'10.
 - An interesting book on outliers



Hands on experience

- Use the ELKI tool to experiment with different outlier detection approaches
 - https://elki-project.github.io/
- You can find several datasets for experimentation here
 - https://www.dbs.ifi.lmu.de/research/outlier-evaluation/



Thank you

Questions/Feedback/Wishes?

Acknowledgements

- The slides are based on
 - □ KDD I lecture at LMU Munich (Johannes Aßfalg, Christian Böhm, Karsten Borgwardt, Martin Ester, Eshref Januzaj, Karin Kailing, Peer Kröger, Eirini Ntoutsi, Jörg Sander, Matthias Schubert, Arthur Zimek, Andreas Züfle)
 - □ Introduction to Data Mining book slides at http://www-users.cs.umn.edu/~kumar/dmbook/
 - Thank you to all TAs contributing to their improvement, namely Vasileios Iosifidis, Damianos Melidis, Tai Le Quy, Han Tran.

Gaussian Mixture Models

Probability of a cluster c

$$P(c_l) = \frac{1}{N} \sum_{i=1}^{N} P(c_l|x_i)$$

Probability of observing an object xi

$$P(x_i) = \sum_{l=1}^k P(c_l)P(x_i|c_l)$$

□ where P(xi|cl) is given by the probability density function of the Gaussian distribution

Outline

- Hierarchical clustering basics
- Hierarchical clustering methods
- Bisecting k-Means
- Things you should know from this lecture & reading material

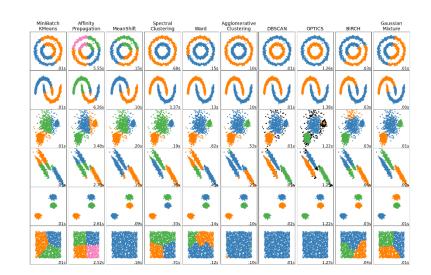
Overview and Reading

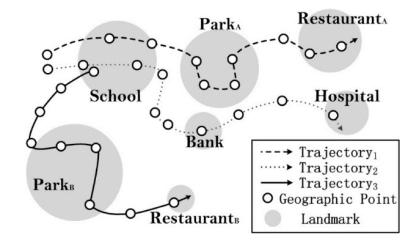
- Overview
 - Density-based clustering
 - DBSCAN
 - Core, border, noisy points
 - Grid-based clustering basics
- Reading
 - Tan P.-N., Steinbach M., Kumar V book, Chapter 8.
 - Data Clustering: A Review, https://www.cs.rutgers.edu/~mlittman/courses/lightai03/jain99data.pdf
 - □ The original DBSCAN paper at KDD96, https://www.aaai.org/Papers/KDD/1996/KDD96-037.pdf
 - □ Nando de Freitas youtube video: https://www.youtube.com/watch?v=voN8omBe2r4

Hands on experience



- Try density-based clustering on mobility data (you can use your own mobility data)
 - Do you recognize any clusters in your activities?
 - E.g., going to University, out and about
- Or, analysis existing GPS trajectory data
 - E.g., Geolife GPS trajectory dataset
- Or, try toy datasets from scikit-learn





Source: https://www.mdpi.com/2220-9964/6/7/212/htm

Thank you

Questions/Feedback/Wishes?

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