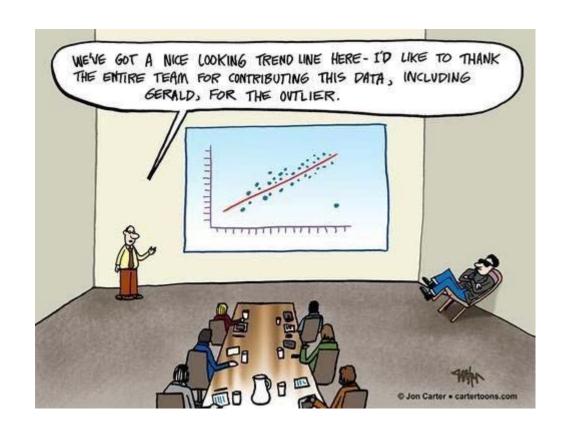
Outlier Detection

Xike Xie



What is an outlier?

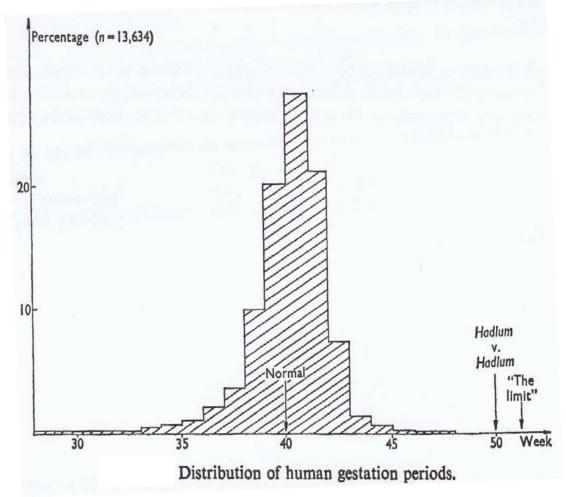
Definition of Hawkins [Hawkins 1980]:

"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"

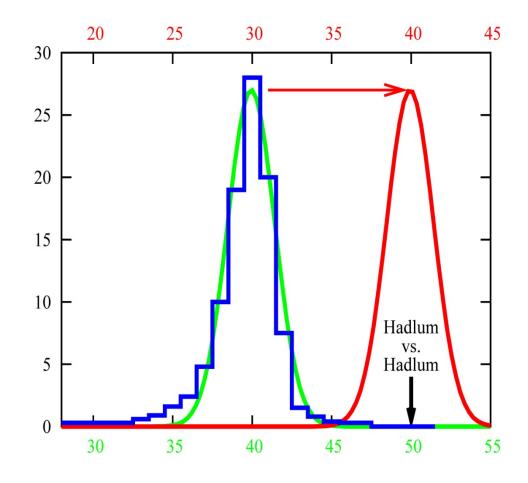
Statistics-based intuition

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

- Example: Hadlum vs. Hadlum (1949) [Barnett 1978]
- The birth of a child to Mrs.
 Hadlum happened 349 days after Mr. Hadlum left for military service.
- Average human gestation period is 280 days (40 weeks).
- Statistically, 349 days is an outlier.



- Example: Hadlum vs. Hadlum (1949) [Barnett 1978]
- blue: statistical basis (13634 observations of gestation periods)
- green: assumed underlying Gaussian process
 - Very low probability for the birth of Mrs. Hadlums child for being generated by this process
- red: assumption of Mr. Hadlum (another Gaussian process responsible for the observed birth, where the gestation period starts later)
 - Under this assumption the gestation period has an average duration and the specific birthday has highestpossible probability



Sample 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 on different aspects like frequency, spatial correlation, etc.

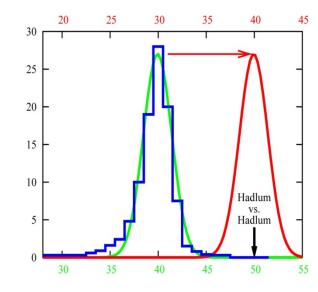
- Sample applications of outlier detection (cont.)
 - Sports statistics
 - In many sports, various parameters are recorded for players in order to evaluate the players' performances
 - Outstanding (in a positive as well as a negative sense) players may be identified as having abnormal parameter values
 - Sometimes, players show abnormal values only on a subset or a special combination of the recorded parameters, within a specific range







- Discussion of the basic intuition based on Hawking
 - Data is usually multivariate,
 - i.e., multi-dimensional
 - => basic model is univariate,
 - i.e., 1-dimensional
 - There is usually more than one generating mechanism/statistical process underlying the "normal" data
 - => basic model assumes only one "normal" generating mechanism
 - Anomalies may represent a different class (generating mechanism) of objects, so there may be a large class of similar objects that are the outliers
 - => basic model assumes that outliers are rare observations



- General application scenarios
 - Supervised scenario
 - In some applications, training data with normal and abnormal data objects are provided
 - There may be multiple normal and/or abnormal classes
 - Often, the classification problem is highly imbalanced
 - Semi-supervised Scenario
 - In some applications, only training data for the normal class(es) (or only the abnormal class(es)) are provided
 - Unsupervised Scenario
 - In most applications there are no training data available
- In this lecture, we focus on the unsupervised scenario

- 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

• 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

- We will focus on three different classification approaches
 - Global versus local outlier detection
 Considers the set of reference objects relative to which each point's "outlierness" is judged
 - Labeling versus 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 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
 - NOTE: 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

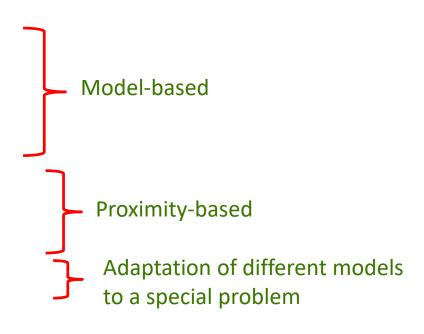
- Labeling versus scoring
 - Considers the output of an outlier detection algorithm
 - Labeling approaches
 - Binary output
 - Data objects are labeled either as normal or outlier
 - Scoring approaches
 - Continuous output
 - For each object an outlier score is computed (e.g. the probability for being 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)

- Approaches classified by the properties of the underlying modeling approach
 - Model-based Approaches
 - 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

- 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

Outline

- 1. Introduction √
- 2. Statistical Tests
- 3. Depth-based Approaches
- 4. Deviation-based Approaches
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- 7. High-dimensional Approaches
- 8. Summary



General idea

- Given 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)
- 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)
- See e.g. Barnett's discussion of Hadlum vs. Hadlum

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

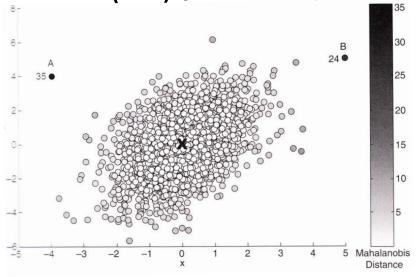
- A huge number of different tests are available differing in
 - Type of data distribution (e.g. Gaussian)
 - Number of variables, i.e., dimensions of the data objects (univariate/multivariate)
 - Number of distributions (mixture models)
 - Parametric versus non-parametric (e.g. histogram-based)
- Example on the following slides
 - Gaussian distribution
 - Multivariate
 - 1 model
 - Parametric

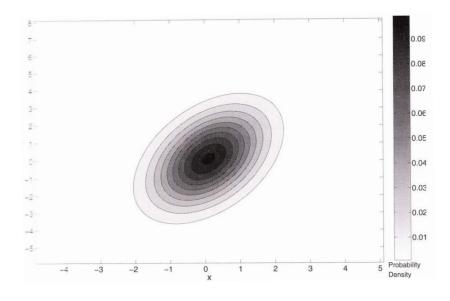
Probability density function of a multivariate normal distribution

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

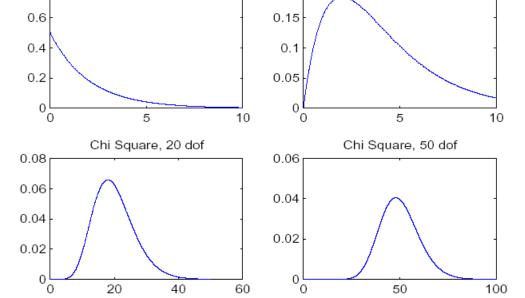
- μ is the mean value of all points (usually data is normalized such that μ =0)
- Σ is the covariance matrix from the mean
- $MDist(x, \mu) = (x \mu)^{T} \Sigma^{-1}(x \mu)$ is the Mahalanobis distance of point x to μ
- MDist follows a χ^2 -distribution with d degrees of freedom (d = data dimensionality)
- All points x, with $MDist(x,\mu) > \chi^2(0.975)$ [$\approx 3.\sigma$]

• Visualization (2D) [Tan et al. 2006]





- Problems
 - Curse of dimensionality
 Chi Square, 2 dof
 - The la



0.2

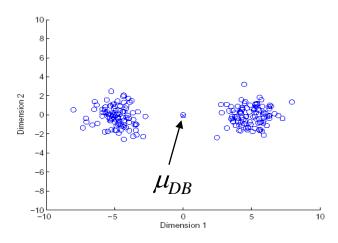
: MDist values for all points

x-axis: observed MDist values

y-axis: frequency of observation

Chi Square, 4 dof

- Problems (cont.)
 - Robustness
 - Mean and standard deviation are very sensitive to outliers
 - These values are computed for the complete data set (including potential outliers)
 - The MDist is used to determine outliers although the MDist values are influenced by these outliers
 - => Minimum Covariance Determinant [Rousseeuw and Leroy 1987]
 minimizes the influence of outliers on the Mahalanobis distance
- Discussion
 - Data distribution is fixed
 - Low flexibility (no mixture model)
 - Global method
 - Outputs a label but can also output a score



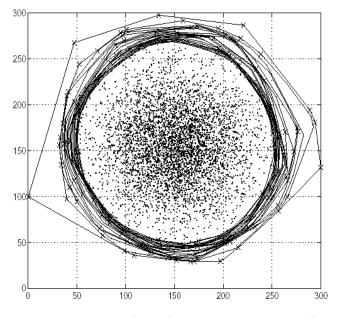
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Depth-based Approaches

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

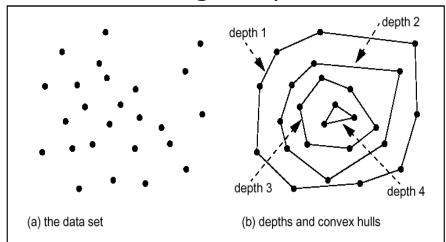


Picture taken from [Johnson et al. 1998]

- 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 $\leq k$ are reported as outliers



Depth-based Approaches

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

Discussion

- 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 (e.g. take depth as scoring value)
- Uses a global reference set for outlier detection

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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 $I \subseteq DB$ how much the variance of DB is decreased when I is removed from DB
 - If two sets have an equal *SF* value, take the smaller set
 - The outliers are the elements of the **exception set** $E \subseteq DB$ for which the following holds:

$$SF(E) \ge SF(I)$$
 for all $I \subseteq DB$

Discussion:

- Similar idea like classical statistical approaches (k = 1 distributions) but independent from the chosen kind of distribution
- Naïve solution is in $O(2^n)$ 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

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General Idea

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

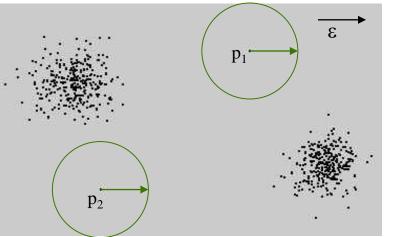
Basic Assumption

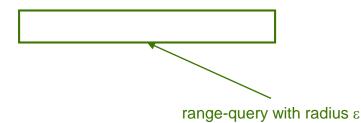
- Normal data objects have a dense neighborhood
- Outliers are far apart from their neighbors, i.e., have a less dense neighborhood

- 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

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





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 *k*NN 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

- Sample Algorithms (computing top-n outliers)
 - Nested-Loop [Ramaswamy et al 2000]
 - Simple NL algorithm with index support for kNN queries
 - Partition-based algorithm (based on a clustering algorithm that has linear time complexity)
 - Algorithm for the simple kNN-distance model
 - Linearization [Angiulli and Pizzuti 2002]
 - Linearization of a multi-dimensional data set using space-fill curves
 - 1D representation is partitioned into micro clusters
 - Algorithm for the average kNN-distance model
 - ORCA [Bay and Schwabacher 2003]
 - NL algorithm with randomization and simple pruning
 - Pruning: if a point has a score greater than the top-n outlier so far (cut-off), remove this point from further consideration
 - => non-outliers are pruned
 - => works good on randomized data (can be done in linear time)
 - => worst-case: naïve NL algorithm
 - Algorithm for both kNN-distance models and the DB(ε,π)-outlier model

- Sample Algorithms (cont.)
 - RBRP [Ghoting et al. 2006],
 - Idea: try to increase the cut-off as quick as possible => increase the pruning power
 - Compute approximate kNNs for each point to get a better cut-off
 - For approximate kNN search, the data points are partitioned into micro clusters and kNNs are only searched within each micro cluster
 - Algorithm for both *k*NN-distance models
 - Further approaches
 - Also apply partitioning-based algorithms using micro clusters [McCallum et al 2000], [Tao et al. 2006]
 - Approximate solution based on reference points [Pei et al. 2006]

Discussion

- Output can be a scoring (kNN-distance models) or a labeling (kNN-distance models and the DB(ε,π)-outlier model)
- Approaches are local (resolution can be adjusted by the user via ε or k)

Variant

- Outlier Detection using In-degree Number [Hautamaki et al. 2004]
 - Idea
 - Construct the *k*NN 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 defined 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)

Distance-based Approaches

- Resolution-based outlier factor (ROF) [Fan et al. 2006]
 - Model
 - Depending on the resolution of applied distance thresholds, points are outliers or within a cluster
 - With the maximal resolution *Rmax* (minimal distance threshold) all points are outliers
 - With the minimal resolution *Rmin* (maximal distance threshold) all points are within a cluster
 - Change resolution from *Rmax* to *Rmin* so that at each step at least one point changes from being outlier to being a member of a cluster
 - Cluster is defined similar as in DBSCAN [Ester et al 1996] as a transitive closure of r-neighborhoods (where r is the current resolution)
 - ROF value
 - Discussion
 Outputs a score (the ROF value) $ROF(p) = \sum_{R \min \le r \le R \max} \frac{clusterSize_{r-1}(p) 1}{clusterSize_r(p)}$
 - Resolution is varied automatically from local to global

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- 7. High-dimensional Approaches
- 8. Summary

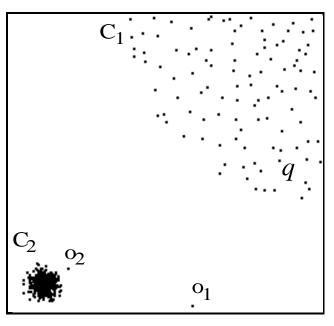
General idea

- 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 essentially 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

- 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 C₁ (e.g. q)
 are larger than the kNN-distance of o₂
 - Solution: consider relative density



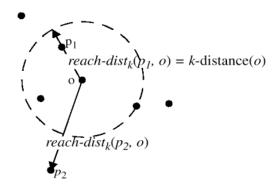
- Model
 - Reachability distance
 - Introduces a smoothing factor

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

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

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

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

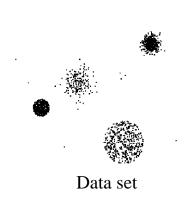


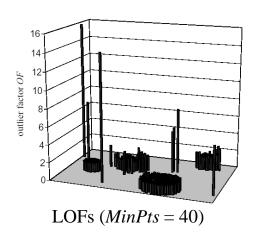
$$LOF_{k}(p) = \frac{\sum_{o \in kNN(p)} \frac{Ird_{k}(o)}{Ird_{k}(p)}}{Card(kNN(p))}$$

Properties

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







Discussion

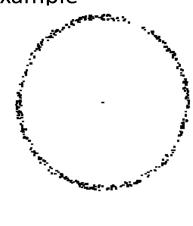
- Choice of *k* (*MinPts* in the original paper) specifies the reference set
- Originally implements a local approach (resolution depends on the user's choice for k)
- Outputs a scoring (assigns an LOF value to each point)

Variants of LOF

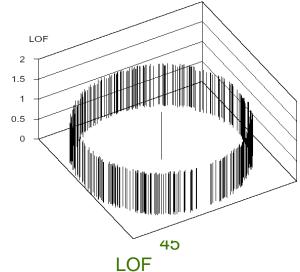
- Mining top-n local outliers [Jin et al. 2001]
 - Idea:
 - Usually, a user is only interested in the top-*n* outliers
 - Do not compute the LOF for all data objects => save runtime
 - Method
 - Compress data points into micro clusters using the CFs of BIRCH [Zhang et al. 1996]
 - Derive upper and lower bounds of the reachability distances, Ird-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

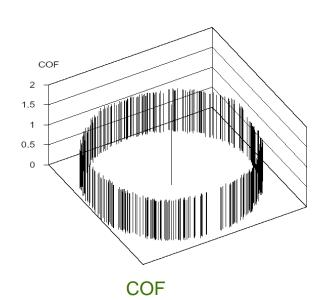
- Variants of LOF (cont.)
 - Connectivity-based outlier factor (COF) [Tang et al. 2002]
 - Motivation
 - In regions of low density, it may be hard to detect outliers
 - Choose a low value for *k* is often not appropriate
 - Solution
 - Treat "low density" and "isolation" differently



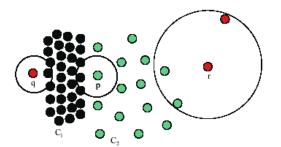


Data set





- 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

k=3

• Influence space (klS(p)) of a point p includes its kNNs (kNN(p)) and its reverse kNNs

(RkNN(p))

$$kIS(p) = kNN(p) \cup RkNN(p)$$

= $\{q_1, q_2, q_3\} \cup \{q_1, q_2, q_4\}$
= $\{q_1, q_2, q_3, q_4\}$

- 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

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

$$den(p)$$

- INFLO takes the ratio of the average density of objects in the neighborhood of a point p (i.e., in $kNN(p) \cup RkNN(p)$) to p's density
- Proposed algorithms for mining top-n outliers
 - Index-based
 - Two-way approach
 - Micro cluster based approach

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)

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Motivation

- One sample class of adaptions of existing models to a specific problem (high dimensional data)
- Why is that problem important?
 - Some (ten) years ago:
 - Data recording was expensive
 - Variables (attributes) where carefully evaluated if they are relevant for the analysis task
 - Data sets usually contain only a few number of relevant dimensions
 - Nowadays:
 - Data recording is easy and cheap
 - "Everyone measures everything", attributes are not evaluated just measured
 - Data sets usually contain a large number of features
 - Molecular biology: gene expression data with >1,000 of genes per patient
 - Customer recommendation: ratings of 10-100 of products per person
 - ...

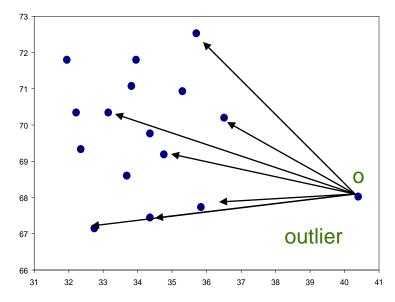
Challenges

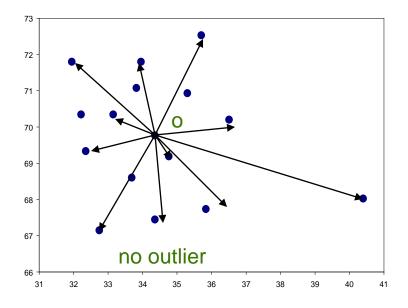
- Curse of dimensionality
 - Relative contrast between distances decreases with increasing dimensionality
 - Data are very sparse, almost all points are outliers
 - Concept of neighborhood becomes meaningless

Solutions

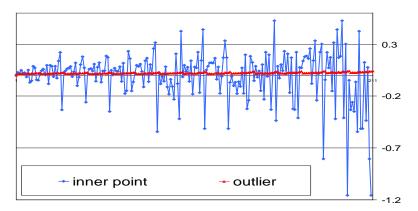
- Use more robust distance functions and find full-dimensional outliers
- Find outliers in projections (subspaces) of the original feature space

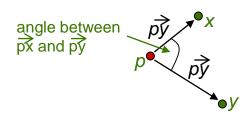
- ABOD angle-based outlier degree [Kriegel et al. 2008]
 - Rational
 - Angles are more stable than distances in high dimensional spaces (cf. e.g. the popularity of cosine-based similarity measures for text data)
 - Object o is an outlier if most other objects are located in similar directions
 - Object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





- 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 px and py for any two x,y from the database
 - Consider the spectrum of all these angles
 - The broadness of this spectrum is a score for the outlierness of a point





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

$$ABOD(p) = VAR \left(\frac{\left\langle xp, yp \right\rangle}{\left\| xp \right\|^{2} \cdot \left\| yp \right\|^{2}} \right)$$

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

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 (inversely scaled: high ABOD => inlier, low ABOD => outlier)

Outline

- 1. Introduction √
- 2. Statistical Tests √
- 3. Depth-based Approaches √
- 4. Deviation-based Approaches √
- 5. Distance-based Approaches √
- 6. Density-based Approaches √
- 7. High-dimensional Approaches √
- 8. Summary

Summary

- Summary
 - Historical evolution of outlier detection methods
 - Statistical tests
 - Limited (univariate, no mixture model, outliers are rare)
 - No emphasis on computational time
 - Extensions to these tests
 - Multivariate, mixture models, ...
 - Still no emphasis on computational time
 - Database-driven approaches
 - First, still statistically driven intuition of outliers
 - Emphasis on computational complexity
 - Database and data mining approaches
 - Spatial intuition of outliers
 - Even stronger focus on computational complexity
 (e.g. invention of top-k problem to propose new efficient algorithms)

Summary

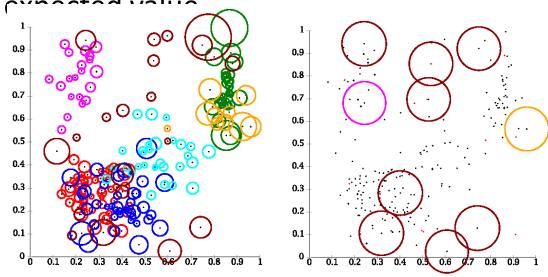
- Consequence
 - Different models are based on different assumptions to model outliers
 - Different models provide different types of output (labeling/scoring)
 - Different models consider outlier at different resolutions (global/local)
 - Thus, different models will produce different results
 - A thorough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

Summary

Outlook

- Experimental evaluation of different approaches to understand and compare differences and common properties
- A first step towards unification of the diverse approaches: providing density-based outlier scores as probability values [Kriegel et al. 2009a]: judging the deviation of the outlier score from the concepted value.
- Visualization [Achtert et al. 2010]
- New models
- Performance issues
- Complex data types
- High-dimensional data

• ...



Outline

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- 7. High-dimensional Approaches **v**
- 8. Summary √