



Lecture 8

Outlier Detection

Zhou Shuigeng

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Outline

- What is Outlier?
- Methods for Outliers Detection
- LOF: A Density Based Algorithm
- Variants of LOF Algorithm
- Summary



Outline

- **What is Outlier?**
- Methods for Outliers Detection
- LOF: A Density Based Algorithm
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- Summary



What is Outlier Detection?

- Outlier Definition by Hawkins

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

— D. Hawkins. *Identification of Outliers*. Chapman and Hall, London, 1980

- Another term: **anomaly detection**
- Examples: The Beatles, Michael Schumacher



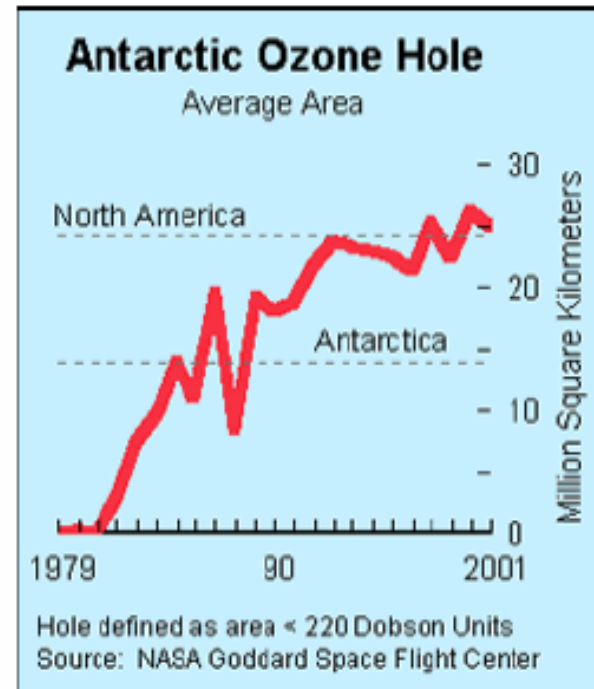
What is Outlier Detection?

- The goal of outlier detection is to uncover the “different mechanism”
- If samples of the “different mechanism” exist, then build a classifier to learn from samples
- Often called the “Imbalanced Classification Problem” -size of outlier sample is small vis-à-vis normal samples.
- In most practical real-life settings, samples of the outlier generating mechanism are non-existent

Importance of Outlier 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!



Sources:

<http://exploringdata.cqu.edu.au/ozone.html>

<http://www.epa.gov/ozone/science/hole/size.html>



Outlier Detection Applications

- Credit card fraud detection
- Telecom fraud detection
- Customer segmentation
- Medical analysis
- Counter-terrorism
-



Outlier Detection: Challenges & Assumption

- Challenges

- How many outliers are there in the data?
- Method is unsupervised
- Validation can be quite challenging (just like for clustering)
- Finding needle in a haystack

- Working assumption:

- There are considerably more “normal” observations than “abnormal” observations (outliers/anomalies) in the data



Detection Schemes

- From normal to abnormal
 - Build a profile of the “normal” behavior
 - Profile can be 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
- Build profile of abnormal behavior
 - Find these conforming to the profile



Outline

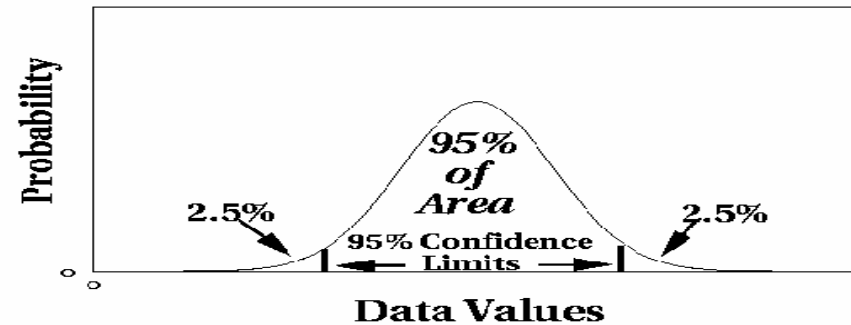
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Outliers Detection Methods

- Statistical method
- Distance based method
- Graphical method
- Depth-based outlier detection
- Density based method
- ...

Statistical Approaches



- Assume a model underlying distribution that generates data set (e.g. normal distribution)
- Use discordancy tests depending on
 - data distribution
 - distribution parameter (e.g., mean, variance)
 - number of expected outliers
- Drawbacks
 - most tests are for single attribute
 - In many cases, data distribution may not be known



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:

$$G = \frac{\max |X - \bar{X}|}{s}$$

\bar{X} -: mean
 s : standard deviation

- Reject H_0 if:

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



Likelihood Approach (1)

- 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, $D = L_t(D) - L_{t+1}(D)$
 - If $D > c$ (some threshold), then x_t is declared as an anomaly and moved permanently from M to A



Likelihood Approach (2)

- Data distribution, $D = (1 - \lambda) M + \lambda A$
- 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 :

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



Distance-Based Approach

- Introduced to counter the main limitations imposed by statistical methods
 - We need multi-dimensional analysis without knowing data distribution.
- Distance-based outlier: A $DB(p, D)$ -outlier is an object O in a dataset T such that at least a fraction p of the objects in T lies at a distance greater than D from O
 - First introduced by Knorr and Ng



Other Distance-based Outlier Definitions

- **Kollios et al Definition**

- An object o in a dataset T is a $DB(k,d)$ outlier if at most k objects in T lie at distance at most d from o

- **Ramaswamy et al Definition**

- Outliers are the top n data elements whose distance to the k -th nearest neighbor is greatest



The Nested Loop Algorithm

- Simple Nested Loop Algorithm: $O(N^2)$
 - For each object $o \in T$, compute distance to each $q \neq o \in T$, until $k + 1$ neighbors are found with distance less than or equal to d .
 - If $|\text{Neighbors}(o)| \leq k$, Report o as DB(k, d) outlier
- Nested Loop with Randomization and Pruning
 - The fastest known distance-based algorithm for DB(k, d) proposed by Bay and Schwabacher, its expected running time is $O(N)$



Outlier and Dimension

- In high-dimensional space, data is sparse and notion of proximity becomes meaningless
 - Every point is an almost equally good outlier from the perspective of proximity-based definitions
- Lower-dimensional projection methods
 - A point is an outlier if in some lower dimensional projection, it is present in a local region of abnormally low density



Subspace Outlier Detection

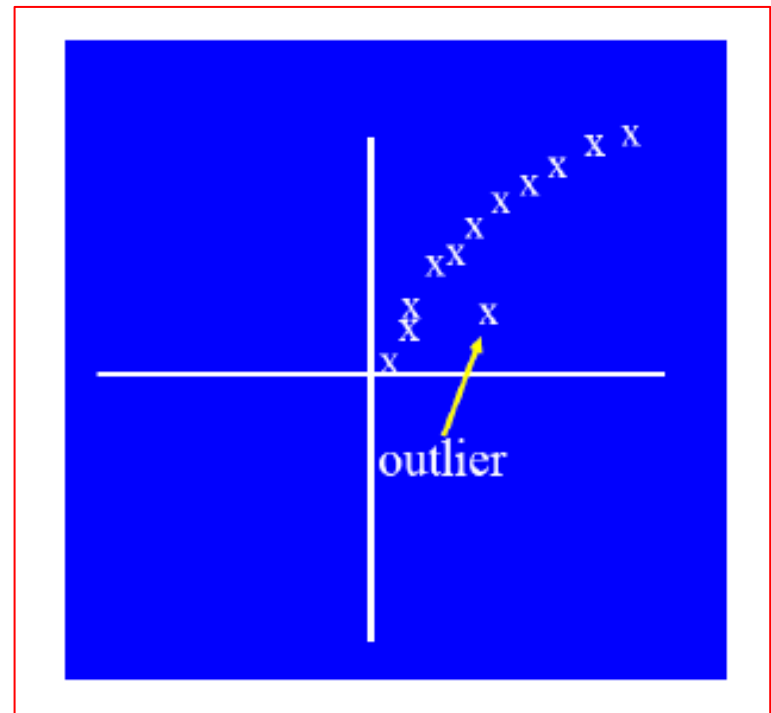
- Divide each attribute into ϕ equal-depth intervals
 - Each interval contains a fraction $f = 1/\phi$ of the records
- Consider a k -dimensional cube created by picking grid ranges from k different dimensions
 - If attributes are independent, we expect region to contain a fraction f^k of the records
 - If there are N points, we can measure sparsity of a cube D as:

$$S(D) = \frac{n(D) - N \cdot f^k}{\sqrt{N \cdot f^k \cdot (1 - f^k)}}$$

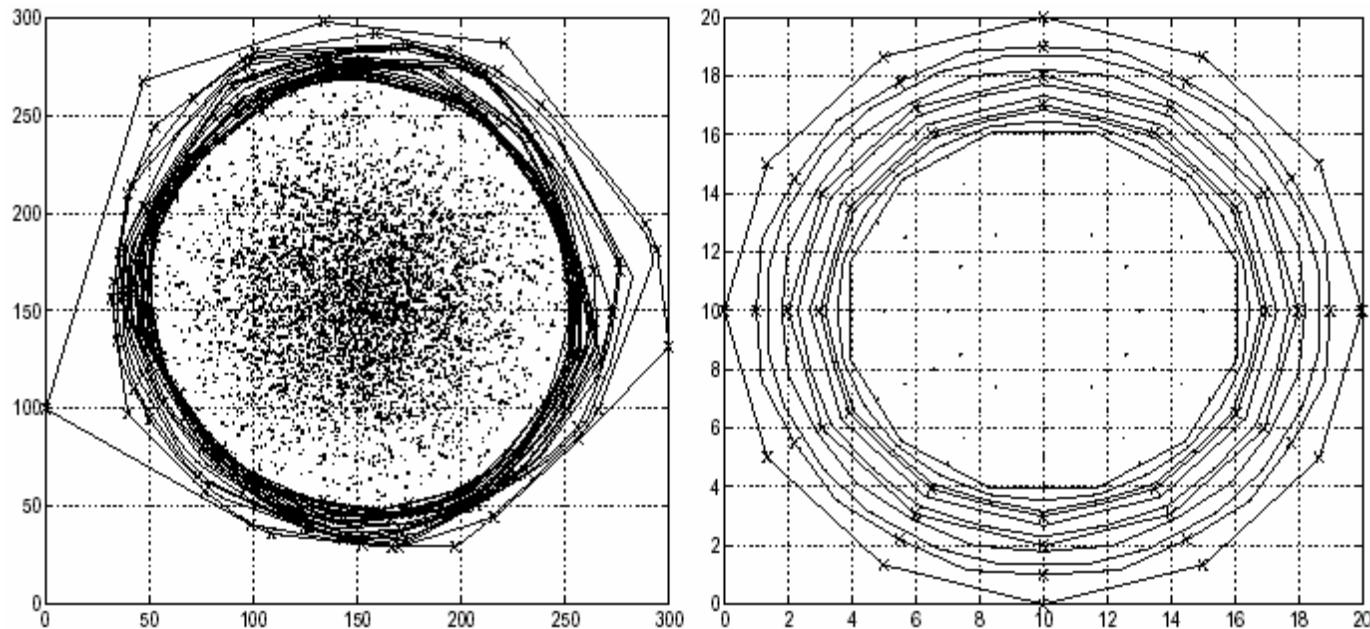
- Negative sparsity indicates cube contains smaller number of points than expected

Graphical Approaches

- Boxplot (1-D), Scatter plot (2-D), Spin plot (3-D)
- Limitations
 - Time consuming
 - Subjective



Depth based Method

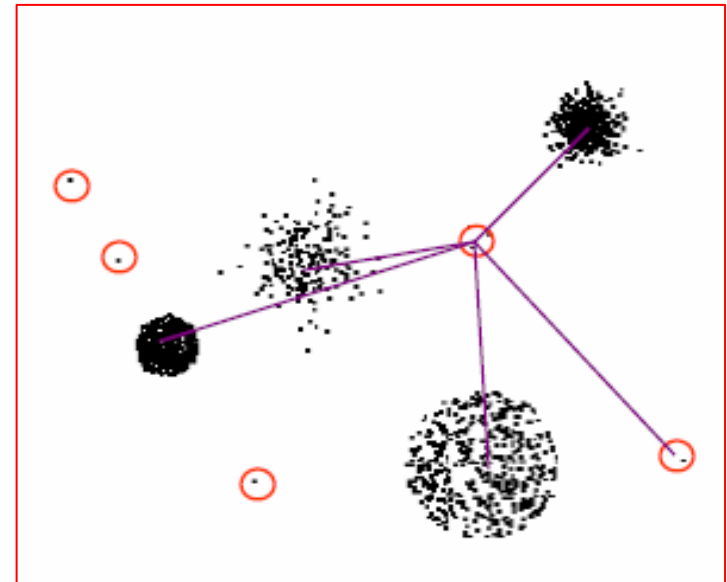


- Based on some definition of *depth*, objects are organized in layers in the data space
- Shallow layer are more likely to contain outliers

Clustering-based Outlier Detection

- Basic idea:

- Cluster the data into groups of different density
- Choose points in small cluster 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





Spatial Outliers

- Outlier detection techniques are often used in GIS, climate studies, public health, etc. The spread and detection of “bird flu” can be cast as an outlier detection problem
- The distinguishing characteristics of spatial data is the presence of “spatial attributes” and the neighborhood relationship
- Spatial Outlier Definition by Shekhar et al.
 - A spatial outlier is a spatial referenced object whose non-spatial attribute values are significantly different from those of other spatially referenced objects in its spatial neighborhood



Finding Spatial Outliers

- Let O be a set of spatially-referenced objects and $N \subset O \times O$ a neighborhood relationship. $N(o)$ are all the neighbors of o .
- A Theorem (Shekhar et. al.)
 - Let f be function which takes values from a Normally distributed rv on O . Let $g(x) = \frac{1}{|N(x)|} \sum_{y \in N(x)} f(y)$
 - Then $h = f - g$ is Normally distributed.
- h effectively captures the deviation in the neighborhood, Because of spatial autocorrelation, a large value of $|h|$ would be considered unusual.
- For multivariate f , use the Chi-Square test to determine outliers



Sequential Outliers

- In many applications, data is presented as a set of symbolic sequences
 - **Proteomics:** Sequence of amino acids
 - **Computer Virus:** Sequence of register calls
 - **Climate Data:** Sequence of discretized SOI readings
 - **Surveillance:** Airline travel patterns of individuals
 - **Health:** Sequence of diagnosis codes



Example Sequence Data

- Examples
 - SRHPAZBGKPBFLBCYVSGFHPXZIZIBLLKB
 - IXCXNCXKEGHSARQFRA
 - MGVRNSVLSGKKADELEKIRLRPGGKKKYYML
- How to determine sequence outlier?
- Properties of Sequence Data
 - Not of same length; Sequence of symbols.
 - Unknown distribution; No standard notion of similarity



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LOF: Identifying Density-based Local Outliers

(Appeared in SIGMOD'00)

M. M. Breunig, H. Kriegel, R. T. Ng, and J. Sander



Outline

- Problems of Existing Approaches
- Local Outlier Factor (LOF)
- Properties of Local Outliers
- How to Choose *MinPts*
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Non-local Approaches (1)

- Some Notations

- $d(p, q)$: distance between objects p & q
- $D(p, C) = \min\{ d(p, q) \mid q \in C \}$, where C is an object set

- $DB(pct, dmin)$ -Outlier

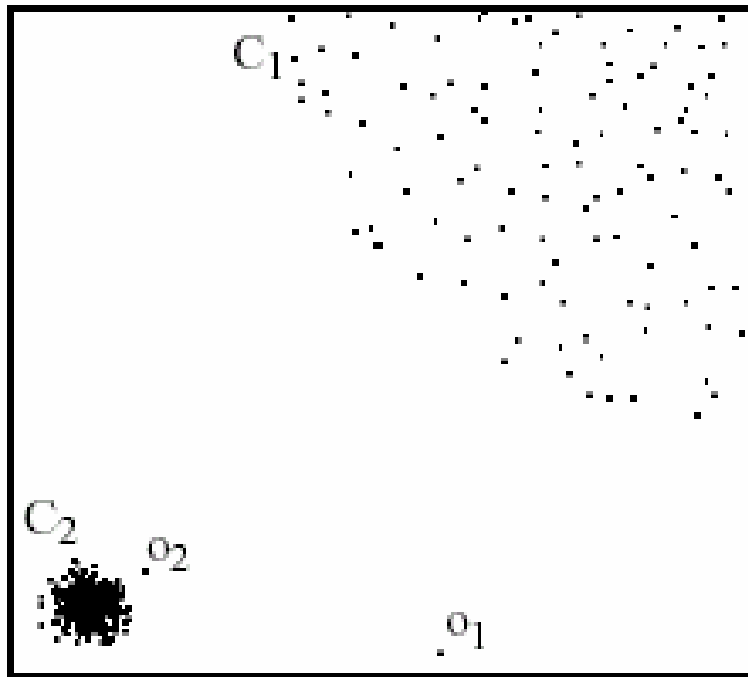
An object p in a dataset D is a $DB(pct, dmin)$ -outlier if at least percentage of pct of the objects in D lies greater than distance $dmin$ from p , i.e., the cardinality of the set $\{q \in D \mid d(p, q) \leq dmin\}$ is less than or equal to $(100 - pct)\%$ of the size of D .



Non-local Approaches (2)

- $DB(pct, dmin)$ -Outlier takes a “global” view
- Many real world data exhibit complex structure, and other kinds of outlier are needed
- Say, objects outlying relative to their local neighborhoods, particularly to densities → “local” outliers

Non-local Approaches (3)



- C_1 : 400 objects
- C_2 : 100 objects
- o_1, o_2 : outliers

If every object q in C_1 , the distance between q and its nearest neighbor is greater than $d(o_2, C_2)$, there's no appropriate value of pct and $dmin$ such that o_2 is identified as outlier, but the objects in C_1 are not.



Non-local Approaches (4)

- Why?
 - If $d_{min} < d(o_2, C_2)$, o_2 and all the objects in C_1 are DB-outliers
 - Otherwise, that o_2 is a not DB-outlier



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Definitions (1)

- k -distance of an object p : $k\text{-distance}(p)$

For any positive integer k , the k -distance of object p , denoted as $k\text{-distance}(p)$, is defined as the distance $d(p, o)$ between p and an object $o \in D$ such that:

- (i) for at least k objects $o' \in D \setminus \{p\}$ it holds that $d(p, o') \leq d(p, o)$, and
- (ii) for at most $k-1$ objects $o' \in D \setminus \{p\}$ it holds that $d(p, o') < d(p, o)$.

- k -distance neighborhood of p : $N_{k\text{-distance}(p)}(p)$

Given the k -distance of p , the k -distance neighborhood of p contains every object whose distance from p is not greater than the k -distance, i.e. $N_{k\text{-distance}(p)}(p) = \{ q \in D \setminus \{p\} \mid d(p, q) \leq k\text{-distance}(p) \}$.

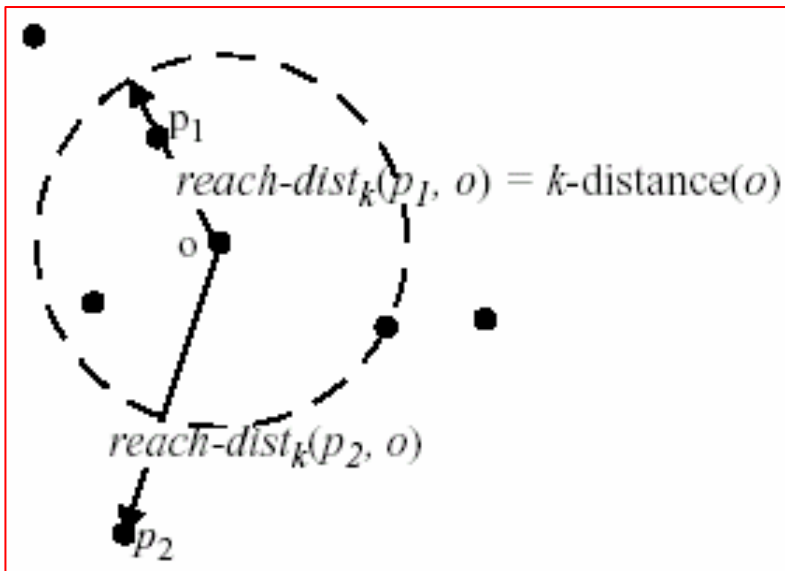
These objects q are called the k -nearest neighbors of p .

Definitions (2)

- Reachability distance of p w.r.t. o : $\text{reach-dist}_k(p, o)$

Let k be a natural number. The *reachability distance* of object p with respect to object o is defined as

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



- Reachability distance aims to reduce the statistical fluctuation of $d(p, o)$ for all the p 's close to o .
- The strength of such smoothing effect can be controlled by the value of k



Definitions (3)

- *Local reachability density*

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

- The inverse of the average reachability distance based on the *MinPts*-NN of p .
- lrd relies on only one parameter, *MinPts*, different from the traditional clustering cases where *MinPts* and a parameter of volume are needed



LOF: Local Outlier Factor

- *local outlier factor*

$$LOF_{MinPts}(p) = \frac{\sum_{o \in N_{MinPts}(p)} \frac{lrd_{MinPts}(o)}{lrd_{MinPts}(p)}}{|N_{MinPts}(p)|}$$

- The average of the ratio of the local reachability density of p and those of p 's *MinPts*-NNs.



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LOF for Outliers Deep in a Cluster

Lemma 1: Let C be a collection of objects. Let *reach-dist-min* denote the minimum reachability distance of objects in C , i.e., $reach-dist-min = \min \{reach-dist(p, q) \mid p, q \in C\}$. Similarly, let *reach-dist-max* denote the maximum reachability distance of objects in C . Let ϵ be defined as $(reach-dist-max/reach-dist-min - 1)$.

Then for all objects $p \in C$, such that:

- (i) all the *MinPts*-nearest neighbors q of p are in C , and
- (ii) all the *MinPts*-nearest neighbors o of q are also in C ,

it holds that $1/(1 + \epsilon) \leq LOF(p) \leq (1 + \epsilon)$.

For “tight” cluster, ϵ will be quite small, thus forcing the lof of p to be quite close to 1.



Upper and Lower Bound

- What's the behavior of lof on the objects near the periphery of a cluster, or those out of a cluster?
- Theorem 1 gives a more general and better bound on LOF
- Some notations first:)



Notations (1)

- *direct_{min}(p)*: the minimum reachability distance between p and a *MinPts*-NN of p .

$$direct_{min}(p) = \min \{ reach-dist(p, q) \mid q \in N_{MinPts}(p) \}.$$

- Similarly,

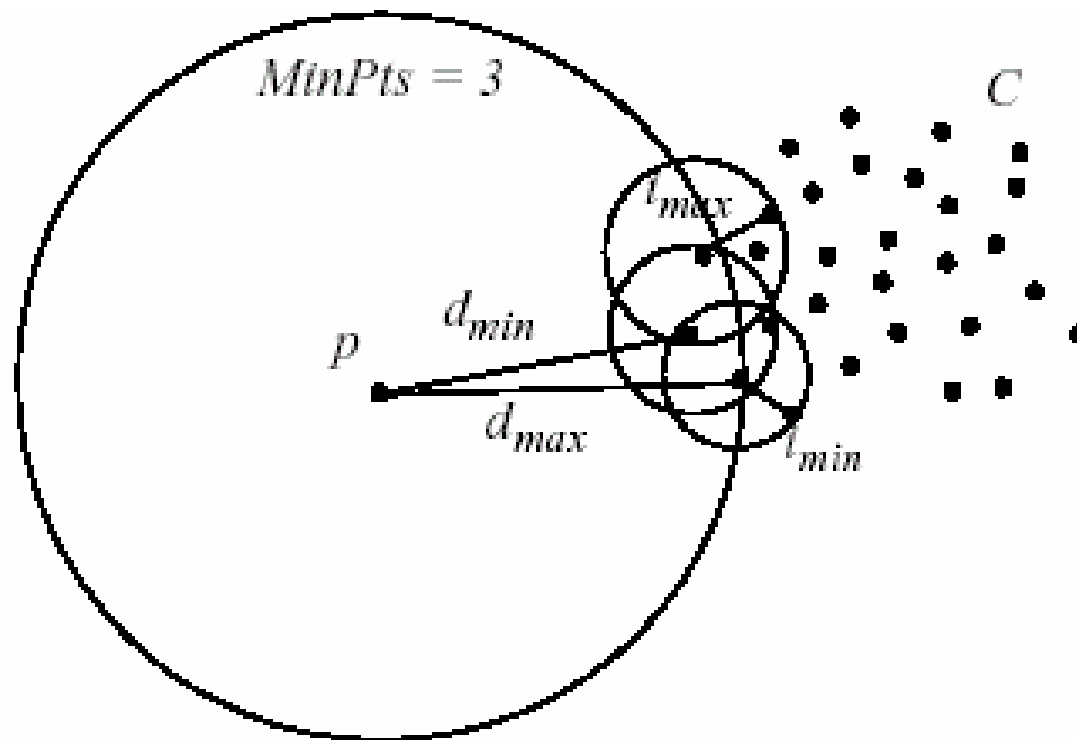
$$direct_{max}(p) = \max \{ reach-dist(p, q) \mid q \in N_{MinPts}(p) \}.$$

- *indirect_{min}(p)*: the minimum reachability distance between q and a *MinPts*-NN of q

$$indirect_{min}(p) = \min \{ reach-dist(q, o) \mid q \in N_{MinPts}(p) \text{ and } o \in N_{MinPts}(q) \}.$$

- Similarly we can define *indirect_{max}(p)*

Notations (2)



$$d_{min} = 4 * l_{max}$$

$$\Rightarrow LOF_{MinPts}(p) \geq 4$$

$$d_{max} = 6 * l_{min}$$

$$\Rightarrow LOF_{MinPts}(p) \leq 6$$



Theorem 1

Theorem 1: Let p be an object from the database D , and $1 \leq MinPts \leq |D|$.

Then, it is the case that

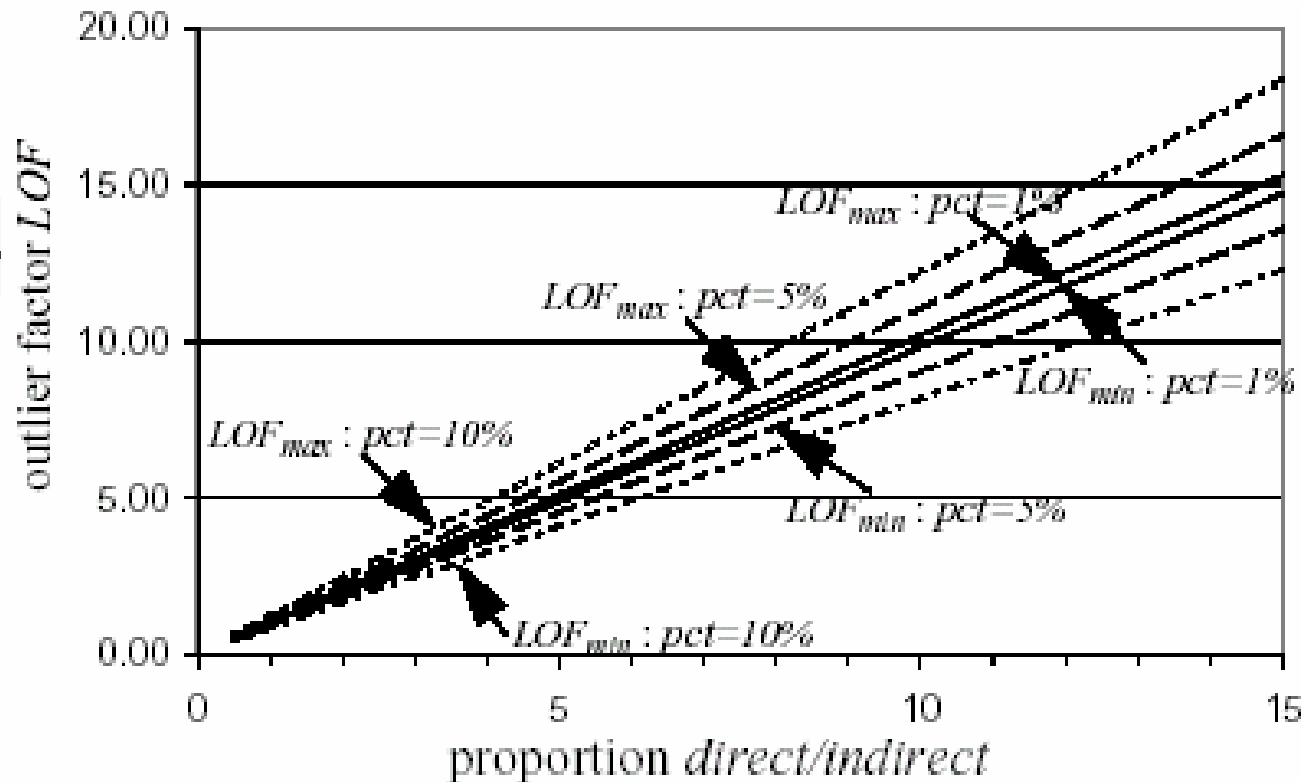
$$\frac{direct_{min}(p)}{indirect_{max}(p)} \leq LOF(p) \leq \frac{direct_{max}(p)}{indirect_{min}(p)}$$

We can see from Theorem 1, that LOF is just a function of the reachability distances in p 's **direct** neighborhood relative to those in p 's **indirect** neighborhood.



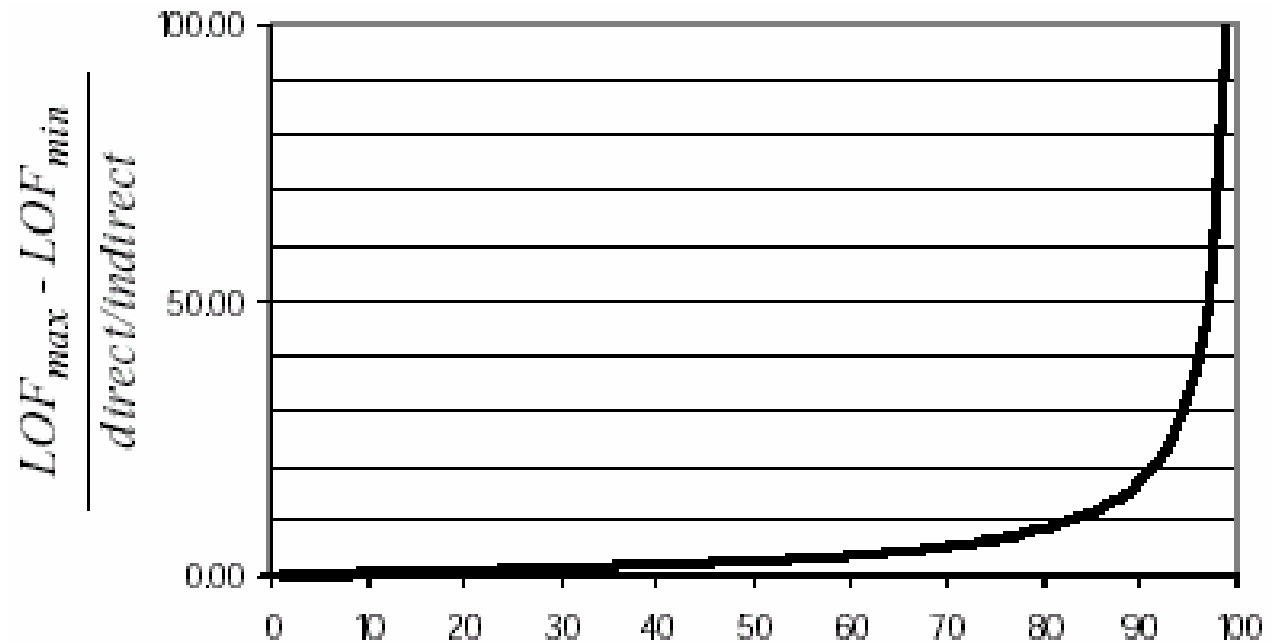
Tightness of the Bounds

- $direct(p)$: the mean of $direct_{min}(p)$ & $direct_{max}(p)$
- $indirect(p)$: the mean of $indirect_{min}(p)$ & $indirect_{max}(p)$
- Assumption:
$$(direct_{max} - direct_{min})/direct = (indirect_{max} - indirect_{min})/indirect.$$
- Let $pct = x\% = (direct_{max} - direct_{min})/2 = (indirect_{max} - indirect_{min})/2$



- The relative span $(LOF_{max} - LOF_{min}) / (\text{direct/indirect})$ is constant
- In other words, the relative fluctuation of LOF relies only on the ratios of distances, not on *absolute* values

$(LOF_{max} - LOF_{min}),$
 $(direct/indirect), pct$



$$\frac{LOF_{max} - LOF_{min}}{\frac{direct}{indirect}} = \frac{4 \times \frac{pct}{100}}{1 - \left(\frac{pct}{100}\right)^2}$$

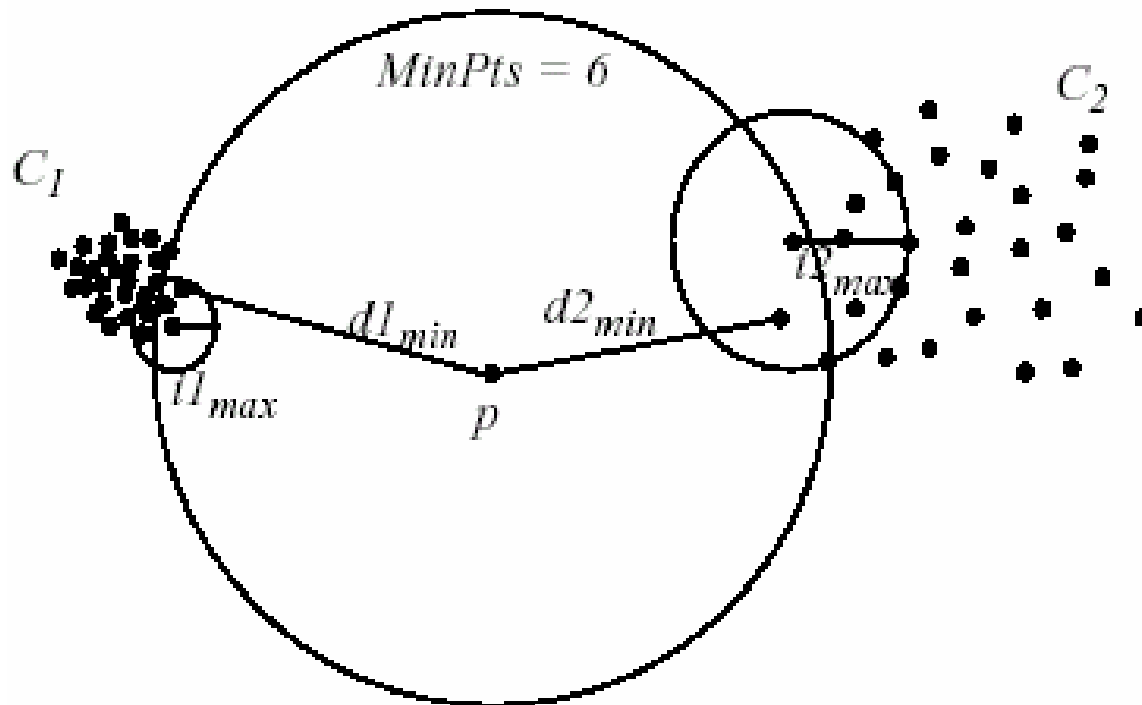
percentage of fluctuation pct



Some Conclusions on Bounds

- If pct is small, theorem 1 estimates the LOF very well, as the bounds are "tight".
 - For the instance deep in a cluster...
 - For those not deep inside a cluster, but whose MinPts-NN belong to the same cluster...

Theorem 2 (1)



- P 's MinPts-NNs do not belong to the same cluster, which makes pct very large...

Theorem 2 (2)

Theorem 2: Let p be an object from the database D , $1 \leq MinPts \leq |D|$, and C_1, C_2, \dots, C_n be a partition of $N_{MinPts}(p)$, i.e. $N_{MinPts}(p) = C_1 \cup C_2 \cup \dots \cup C_n \cup \{p\}$ with $C_i \cap C_j = \emptyset$, $C_i \neq \emptyset$ for $1 \leq i, j \leq n, i \neq j$.

$$LOF(p) \geq \left(\sum_{i=1}^n \xi_i \cdot direct_{min}^l(p) \right) \left(\sum_{i=1}^n \frac{\xi_i}{indirect_{max}^l(p)} \right)$$

$$LOF(p) \leq \left(\sum_{i=1}^n \xi_i \cdot direct_{max}^l(p) \right) \left(\sum_{i=1}^n \frac{\xi_i}{indirect_{min}^l(p)} \right)$$

Where $\xi_i = |C_i| / |N_{MinPts}(p)|$

For p in the figure of the last slide, we get $LOF_{min} =$

$$(0.5 \cdot d1_{min} + 0.5 \cdot d2_{min}) / (0.5/i1_{max} + 0.5/i2_{max})$$



Outline

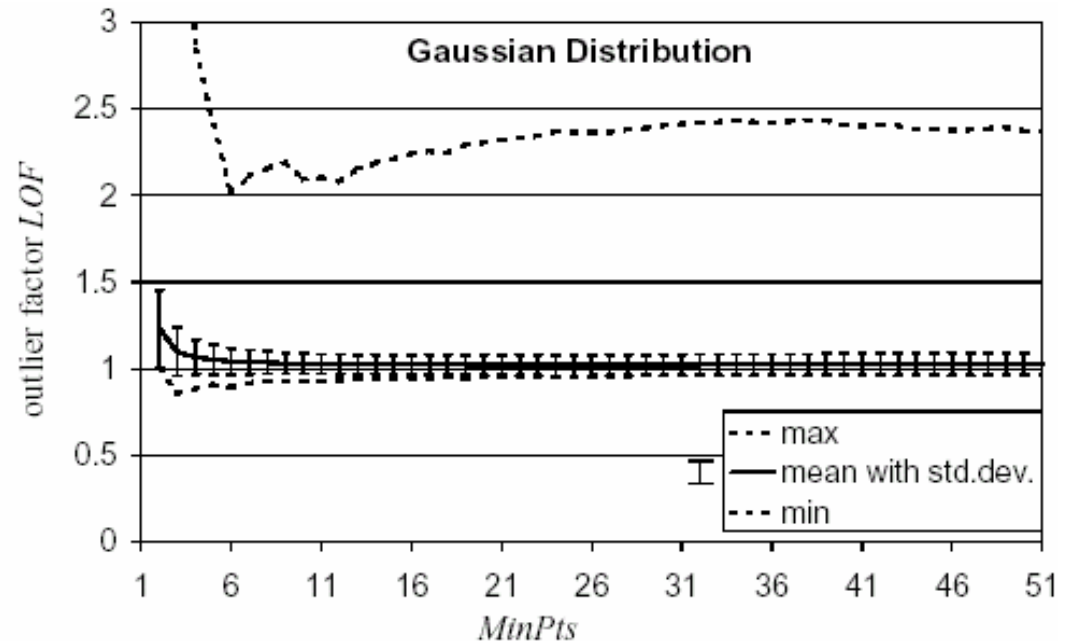
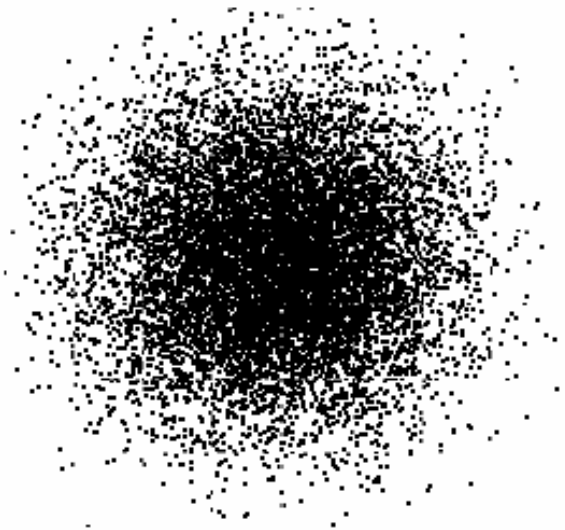
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LOF, MinPts

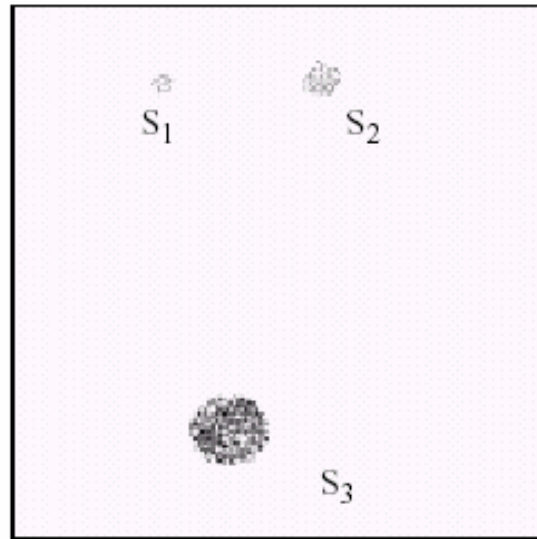
- How *LOF* changes according to changing *MinPts* values?
 - Increase monotonic w.r.t *MinPts*,
 - Or decrease monotonic w.r.t. *MinPts*,
 - Or ...

An Example

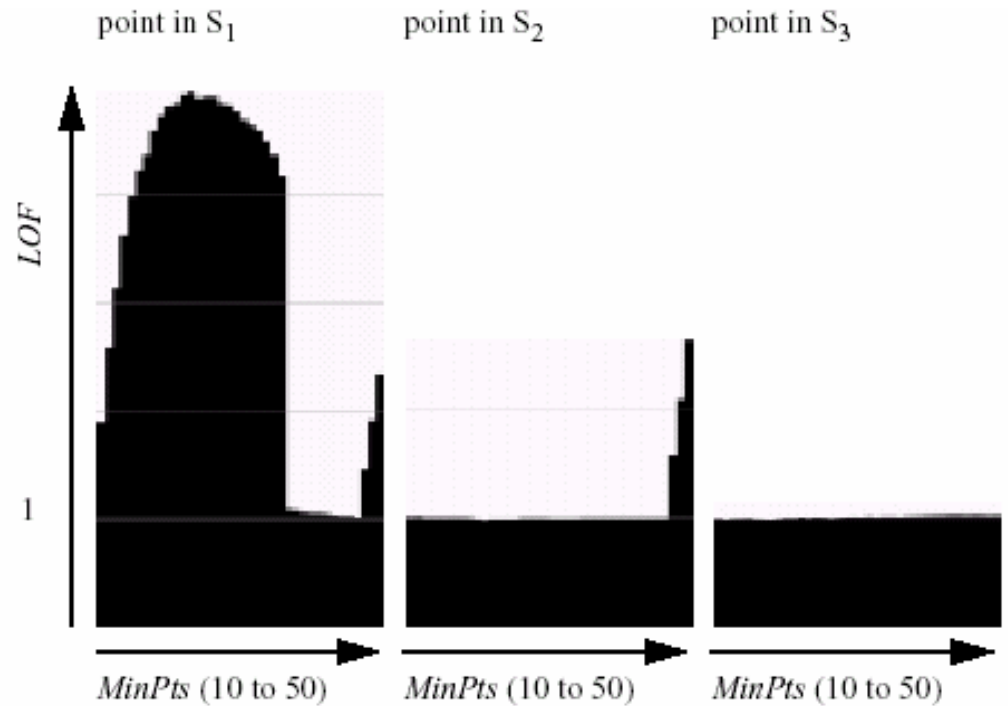


- The dataset (500 objects) follows Gaussian distribution

Another Example



Example dataset



- S_1 : 10, S_2 : 35, S_3 : 500



Determine a Range of MinPts

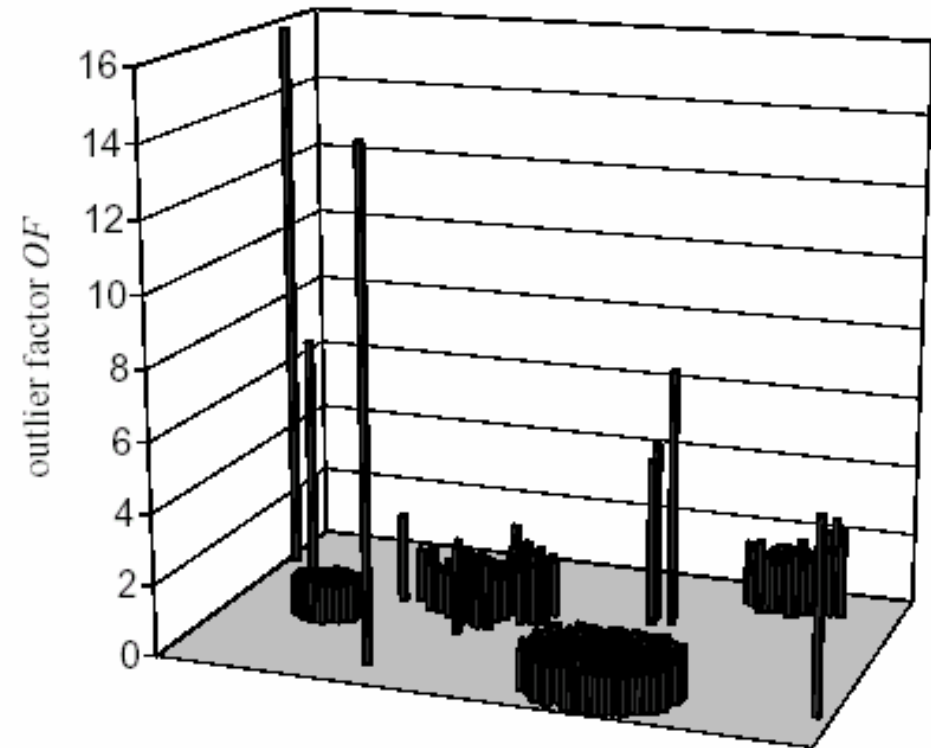
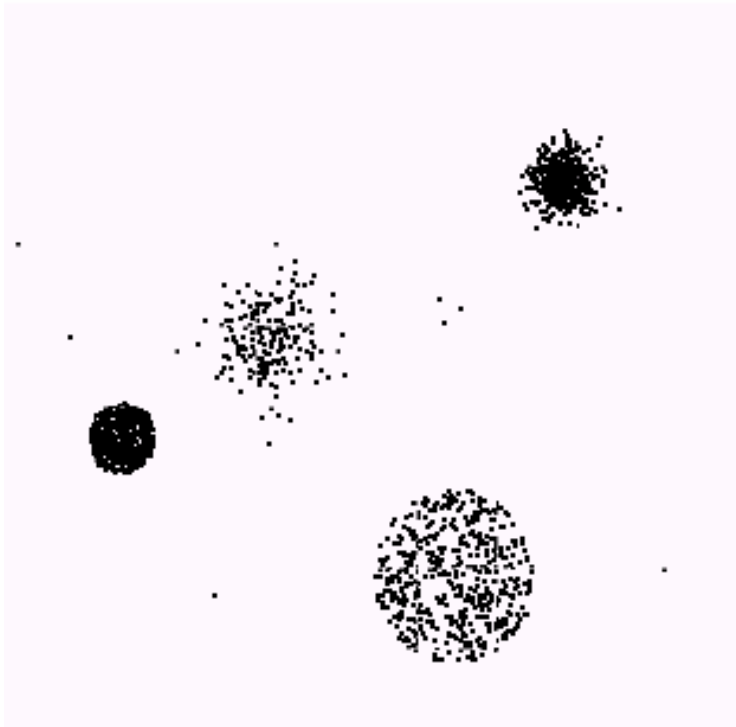
- *MinPtsLB*
 - According to the figure in slide 54, *MinPtsLB* ≥ 10
 - *MinPtsLB* can be regarded as the minimum number of objects a "cluster" has to contain
 - 10 ~ 20 ✓
- *MinPtsUB*
 - The maximum number of "close by" objects that can potentially be local outliers
- Compute *LOF* for each value of *MinPts* between *MinPtsLB* & *MinPtsUB*, and rank w.r.t. the maximum *LOF* within the range



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A Synthetic Example



MinPts = 40



Soccer Data

Rank	Outlier Factor	Player Name	Games Played	Goals Scored	Position
1	1.87	Michael Preetz	34	23	Offense
2	1.70	Michael Schjönberg	15	6	Defense
3	1.67	Hans-Jörg Butt	34	7	Goalie
4	1.63	Ulf Kirsten	31	19	Offense
5	1.55	Giovane Elber	21	13	Offense
minimum			0	0	
median			21	1	
maximum			34	23	
mean			18.0	1.9	
standard deviation			11.0	3.0	

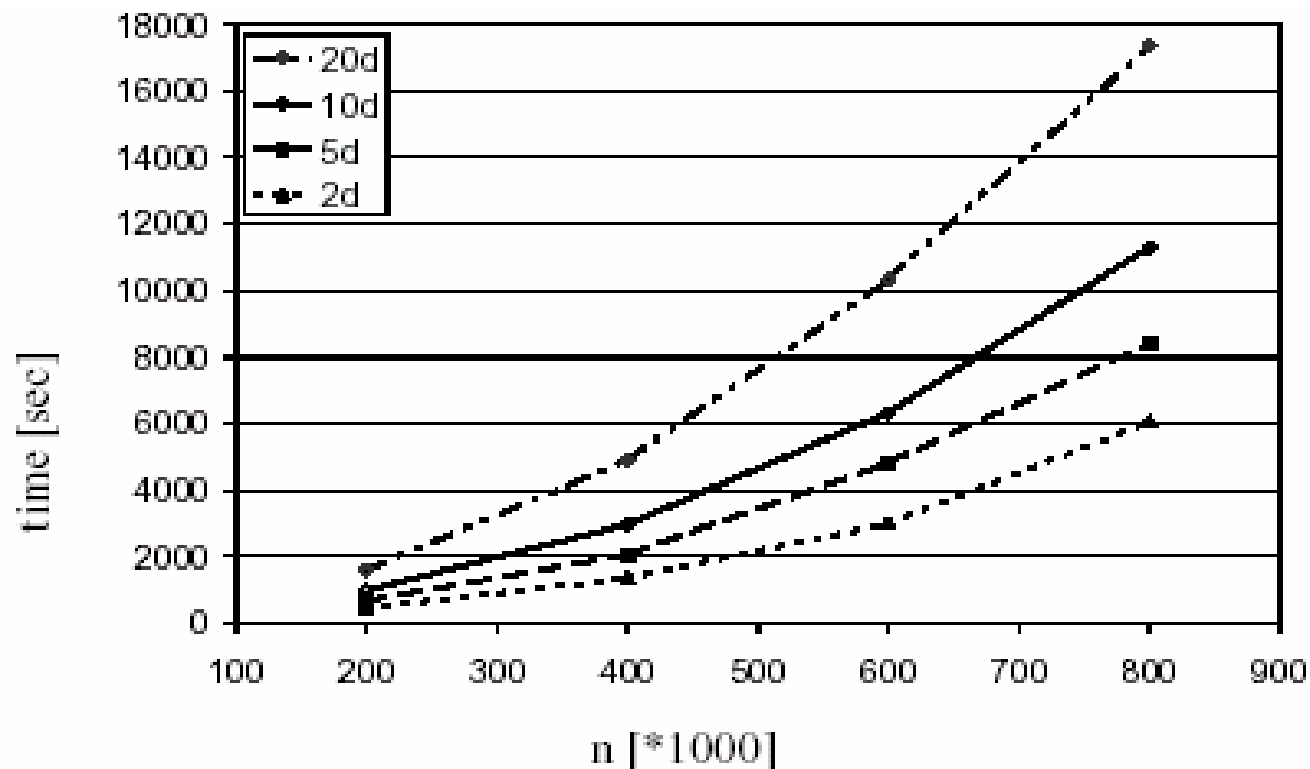
1. number of games
2. average goals per game
3. Position (coded in integer)



Performance (1)

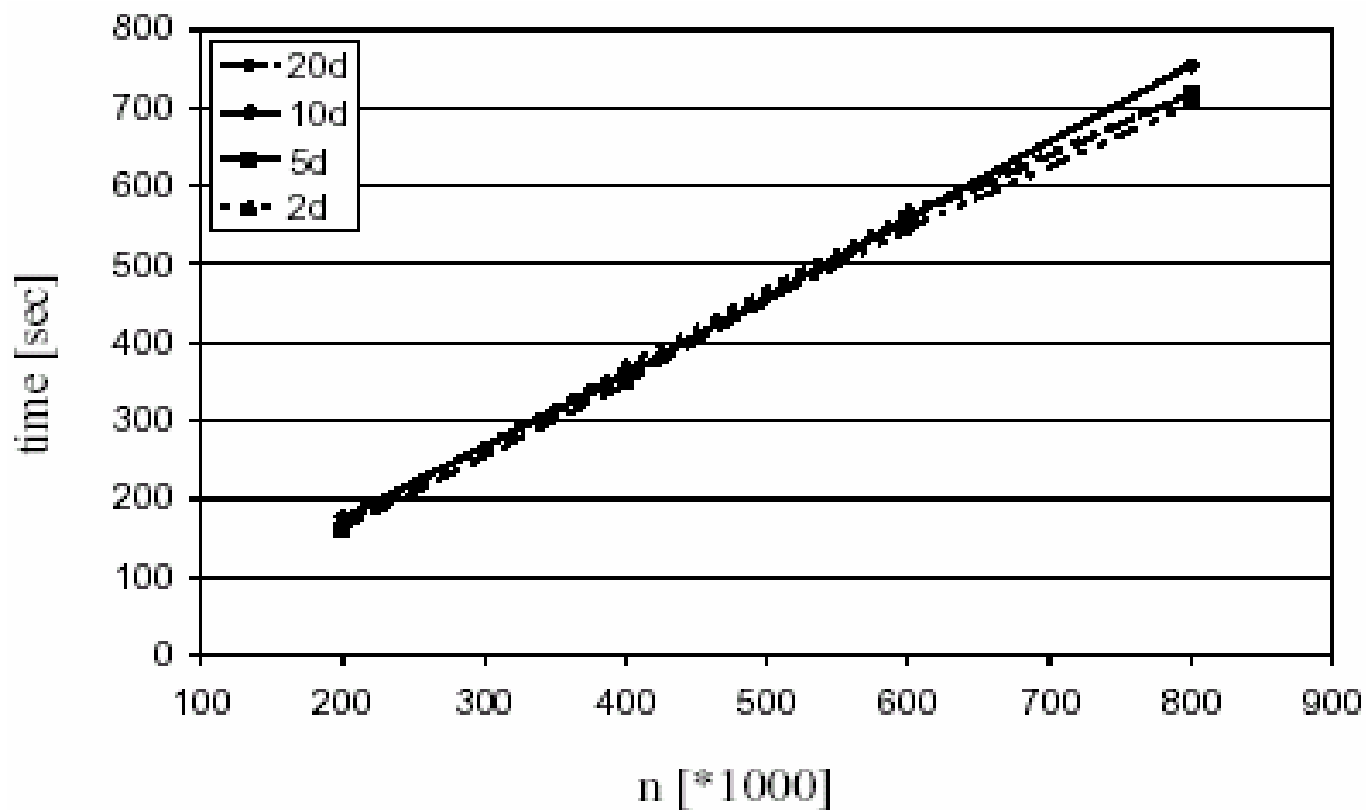
- Two steps
 - Compute and materialize MinPtsUB-NNs for each objects in the dataset to get a database of MinPtsUB-NNs ($O(n \times \text{time for } k\text{-nn query})$)
 - Based on the database, for each value between MinPtsLB & MinPtsUB, compute lrd of each object, then compute LOF of each object

Performance (2)



**Runtime of the materialization of the
50-nn queries for different dataset sizes and
different dimensions using an index**

Performance (3)



**Runtime for the computation of the LOFs
for different dataset sizes**



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Summary

- LOF, captures relative degree of isolation
- LOF enjoy many good properties
 - Close to 1 for the objects deep in cluster
 - Meaningful bounds are given
- The effect of MinPts
- Fantastic experiments



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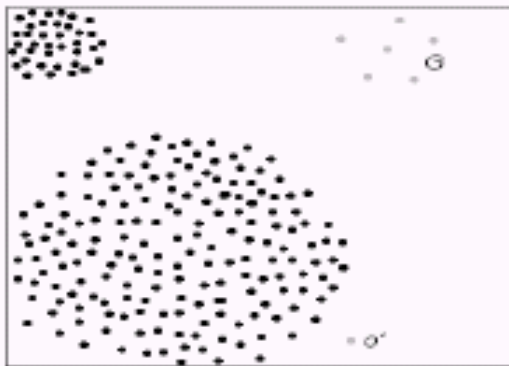
Variants of LOF (1)

- Some work done by Ada Fu
 - COF (PAKDD'02)
 - LOF', LOF'' and GridLOF (IDEAS'03)

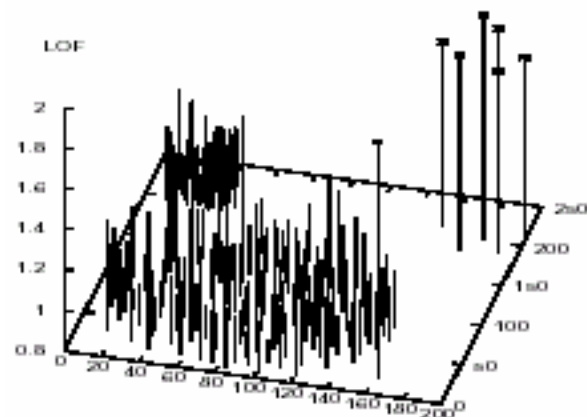
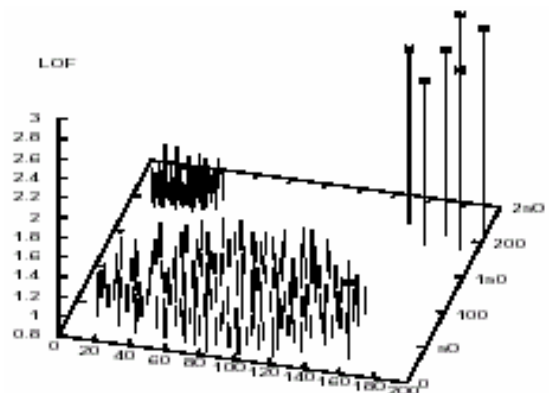
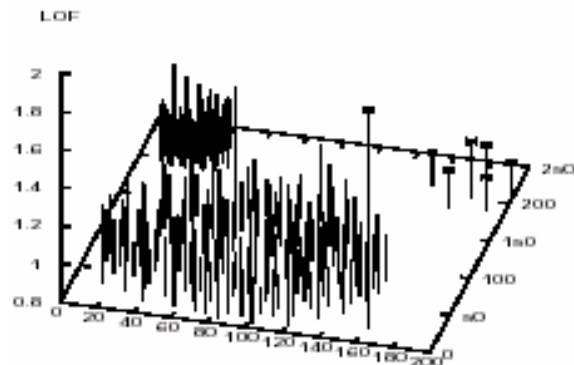
$$LOF'_{MinPts}(p) = \frac{\sum_{o \in N_{MinPts-dist}(p)} \frac{MinPts-dist(p)}{MinPts-dist(o)}}{|N_{MinPts-dist}(p)|}$$

$$LOF''_{MinPts_1, MinPts_2} = \frac{\sum_{o \in N_{MinPts_1-dist}(p)} \frac{lr_{dMinPts_2}(o)}{lr_{dMinPts_2}(p)}}{|N_{MinPts_1-dist}(p)|}$$

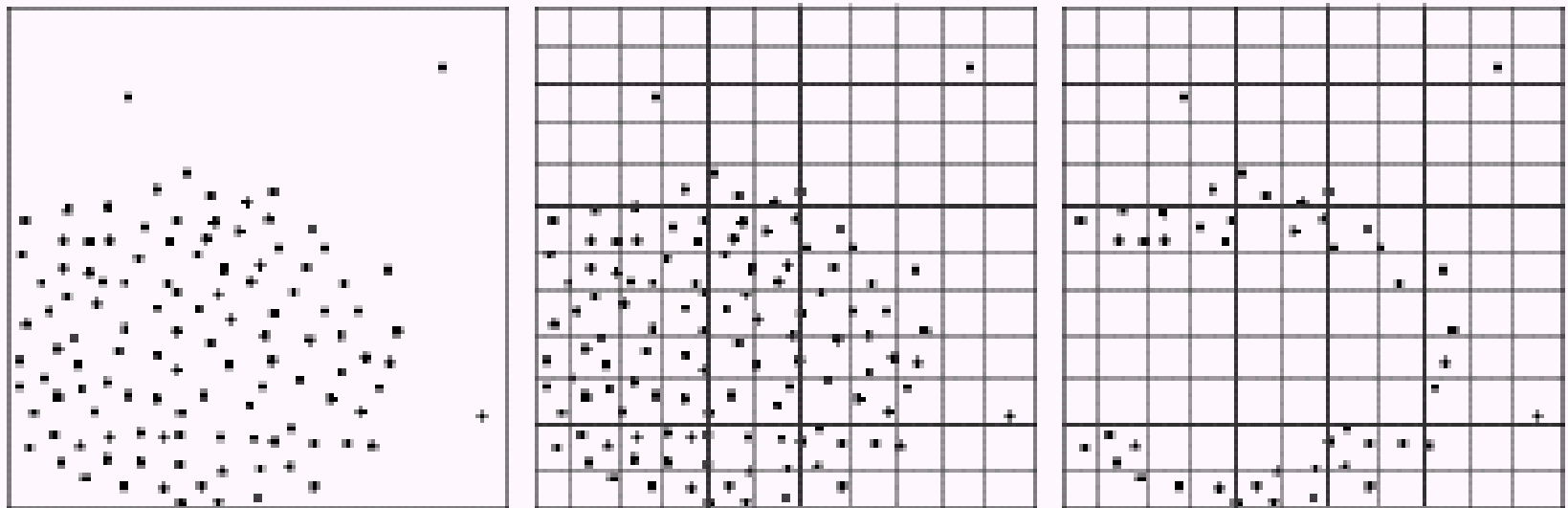
Variants of LOF (2)



(a)



Variants of LOF (3)



- GridLOF aims to save computation cost



Outline

- What's Is Outlier
- Methods for Outliers Detection
- LOF: A Density Based Algorithm
- Variants of LOF Algorithm
- Summary



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