¹Max Planck Institute for Intelligent Systems, Tübingen, ²Max Planck Institute for Developmental Biology, Tübingen, ³ZBIT, Eberhard Karls Universität Tübingen



MAX-PLANCK-GESELLSCHAFT

BACKGROUND

How can we find outliers efficiently in massive datasets?

- Outliers are objects located far away from the remaining objects
- Outliers appear everywhere:
 - Intrusions in network traffic, credit card fraud, defective products in ind medical diagnosis from X-ray images, ...
- Specific task: Assign an outlierness score to each point using pairwise dista
 - This distance-based approach has been successfully applied in various • Example: *k*th nearest neighbor [1,2], LOF [Breunig *et al.* SIGMOD
 - It does not require to model the underlying probability distribution, which is particularly challenging for high-dimensional data

Problem: Scalability

- Computation of all pairwise distances is needed: $O(n^2)$
- Two state-of-the-art solutions
 - 1. Partial computation to obtain only top- κ outliers
 - 2. Indexing of objects
- Unfortunately, both strategies are not sufficient
 - 1. The number of outliers often increases in direct proportion to the size which deteriorates the efficiency of partial computation
 - 2. Index structures are often not efficient enough for high-dimensional data

PROPOSAL: SAMPLING-BASED OUTLIER DETECTION

Solution: Sampling

- Given a dataset *X* (*n* data points, *m* dimensions)
- Randomly and independently sample a subset $S(X) \subset X$
- Define the score $q_{Sp}(x)$ for each object $x \in X$ as

$$q_{\rm Sp}(x) := \min_{x' \in S(X)} d(x, x')$$

- Input parameter: the number of samples S = |S(X)|
- The time complexity is $\Theta(nms)$ and the space complexity is $\Theta(ms)$



• **Related work:** Wu and Jermaine [3] proposed a sampling-based method: - Our method: one-time sampling, their method: iterative sampling for each point





Rapid Distance-Based Outlier Detection via Sampling

Mahito Sugiyama^{1,2} Karsten Borgwardt^{1,2,3}

Machine Learning and Computational Biology Research Group

			EXI	PERIMEN	TAL RESUL				
	• Compari <i>k</i> thNN (sampling based me	son partner the latest te g), iForest (r ethod) [Phar	s: chnique iOI andom fore m and Pagh	RCA [2] is est-like me , 2012], Or	used), Wu ai ethod) [Liu <i>ei</i> ne-class SVM				
ndustry,	 Parameters were set to be the same in the original parameters 								
	Datasets (*	* are synthe	tic)						
ances		# of objects	# of outliers	# of dims	~				
lances	Ionosphere	351	126	34	Sensitivity				
domains	Arrhythmia	452	207	274	0.55-				
2000]	Wdbc	569	212	30	С				
	Mfeat	600	200	649					
	Isolet	960	240	617	ອີ 0 50-				
	Pima	768	268	8					
	Gaussian*	1000	30	1000	ave –				
	Optdigits	1688	554	64					
	Spambase	4601	1813	57					
	Statlog	6435	626	36					
	Skin	245057	50859	3					
	Pamap2	373161	125953	51	0.40-				
a do	Covtype	286048	2747	10					
	Kdd1999	4898431	703067	6	5				
	Record	5734488	20887	7	<u> </u>				
	Gaussian*	1000000	30	20					
	Running ti	me (in seco kthNI	nds) N Wu's <u>(</u>	<u>Durs</u> iFore	est LOF Fas				
	lonosphe	ere							
e of the dataset,	Arrhythn	nia							
	Wdbc			_					
ata	Mifeat			_					
utu	Bima			_	_				
	Gaussian		_	_	_				
	Optdigit	ς Γ		_					
J	Spamba	se	_						
	Statlog								
	Skin								
	Pamap2								
	Covtype								
	Kdd1999								
	Record								
	Gaussiar	1							

AUPRC (area under the precision-recall curve; * are best scores)

	KTNNN	VV u's	<u>Ours</u>	IForest	LOF
Ionosphere	*				
Arrhythmia			*		
Wdbc			*		
Mfeat					*
Isolet			*		
Pima		*			
Gaussian	*	*	*		
Optdigits					*
Spambase			*		
Statlog					*
Skin			*		
Pamap2					*
Covtype					
Kdd1999	*				
Record				*	
Gaussian	*		*		
Average	0.453	0.410	0.534	0.479	0.400
Avg.rank	3.750	3.875	2.188	3.875	4.538
RMSD	0.259	0.274	0.068	0.133	0.152

- and Jermaine's method [3] (iterative t al. 2012], LOF, FastVOA (angle-[Schölkopf *et al.* 2001]
- papers or popular values

y in sample sizes



Main results

• $X(\alpha; \delta)$: the set of Knorr and Ng's DB (α, δ) -outliers:

$$x \in X(\alpha; \delta)$$
 if $\{x' \in X \mid d(x, x') > \delta\} \ge \alpha n$

- $-\delta \in \mathbb{R}$ is a distance threshold
- this should be close to 1 by definition of outliers
- NOTE: These parameters are not needed in practice
- $\overline{X}(\alpha; \delta) = X \setminus X(\alpha; \delta)$, the set of inliers
- Define β ($0 \le \beta \le \alpha$) as the minimum value s.t.

$$\forall x \in \overline{X}(\alpha; \delta), \ \left| \{ x' \in X \mid d(x,$$

• **Result 1:** For $x \in X(\alpha; \delta)$ and $x' \in \overline{X}(\alpha; \delta)$,

$$\Pr(q_{\rm Sp}(x) > q_{\rm Sp}(x')) \ge q_{\rm Sp}(x')$$

(*s* is the number of samples)

- This lower bound tends to be high in a typical setting (α is large, β is moderate)
- **Result 2:** This bound is maximized at

$$r = \log_{\beta} \frac{\log \alpha}{\log \alpha + \log \alpha}$$

- This value tends to be small

More detailed results

- For an outlier $x \in X(\alpha; \delta)$ and a cluster $C \in \mathcal{P}_{\delta}$,

$$\Pr\big(\,\forall x'\in C,\, q_{\rm Sp}(x)>q_{\rm Sp}(x')\,\big)\geq \alpha^s(1-\beta^s)\, {\rm with}\,\beta=(n-|C|)/n$$

- the multinomial distribution, and $\gamma = |I(\alpha; \delta)|/n$. Then

$$\Pr(\forall x \in X(\alpha; \delta), \forall x' \in \mathbb{R})$$

- Our method is the most effective on average

- with accuracy guarantees. KDD 2006.



Alexander von Humboldt Stiftung/Foundation

THEORETICAL ANALYSIS

 $-\alpha \in \mathbb{R} \ (0 \le \alpha \le 1)$ is the fraction of objects which locate far away from *x*;



• A δ -partition \mathcal{P}_{δ} of $\overline{X}(\alpha; \delta)$: $\forall C \in \mathcal{P}_{\delta}$, $\max_{x,y \in C} d(x, y) < \delta$ and $\bigcup_{C \in \mathcal{P}_{\delta}} C = \overline{X}(\alpha; \delta)$

• Let $I(\alpha; \delta) \subset \overline{X}(\alpha; \delta)$ s.t. $\forall x \in X(\alpha; \delta), \min_{x' \in I(\alpha; \delta)} d(x, x') > \delta, \mathcal{P}_{\delta} = \{C_1, \dots, C_l\}$ be a δ -partition of $I(\alpha; \delta)$, and $p_i = |C_i|/|I(\alpha; \delta)|$ for each $i \in \{1, ..., l\}$ • Let $\varphi(s) = \sum_{\forall i; s_i \ge 0} f(s_1, \dots, s_l; \mu, p_1, \dots, p_l)$, where *f* is the probability mass function of

 $\overline{X}(\alpha; \delta), q_{sp}(x) > q_{sp}(x') \ge \gamma^s \max_{\mathcal{D}} \varphi(s)$

CONCLUSION

• Our method is much (2 to 6 orders of magnitude) faster than exhaustive methods

REFERENCES

. Original paper on distance-based outliers: Korr, E. M., Ng, R. T., and Tucakov, V. Distancebased outliers: algorithms and applications. *The VLDB Journal*, 8(3):237–253, 2000. 2. State-of-the-art of kthNN detection: Bhaduri, K., Matthews, B. L., and Giannella, C. R. Algorithms for speeding up distance-based outlier detection. KDD 2011. 3. Related sampling-based method: Wu, M. and Jermaine, C. Outlier detection by sampling