Reverse Nearest Neighbors in Unsupervised Distance-Based Outlier Detection*

* Article accepted in IEEE TKDE

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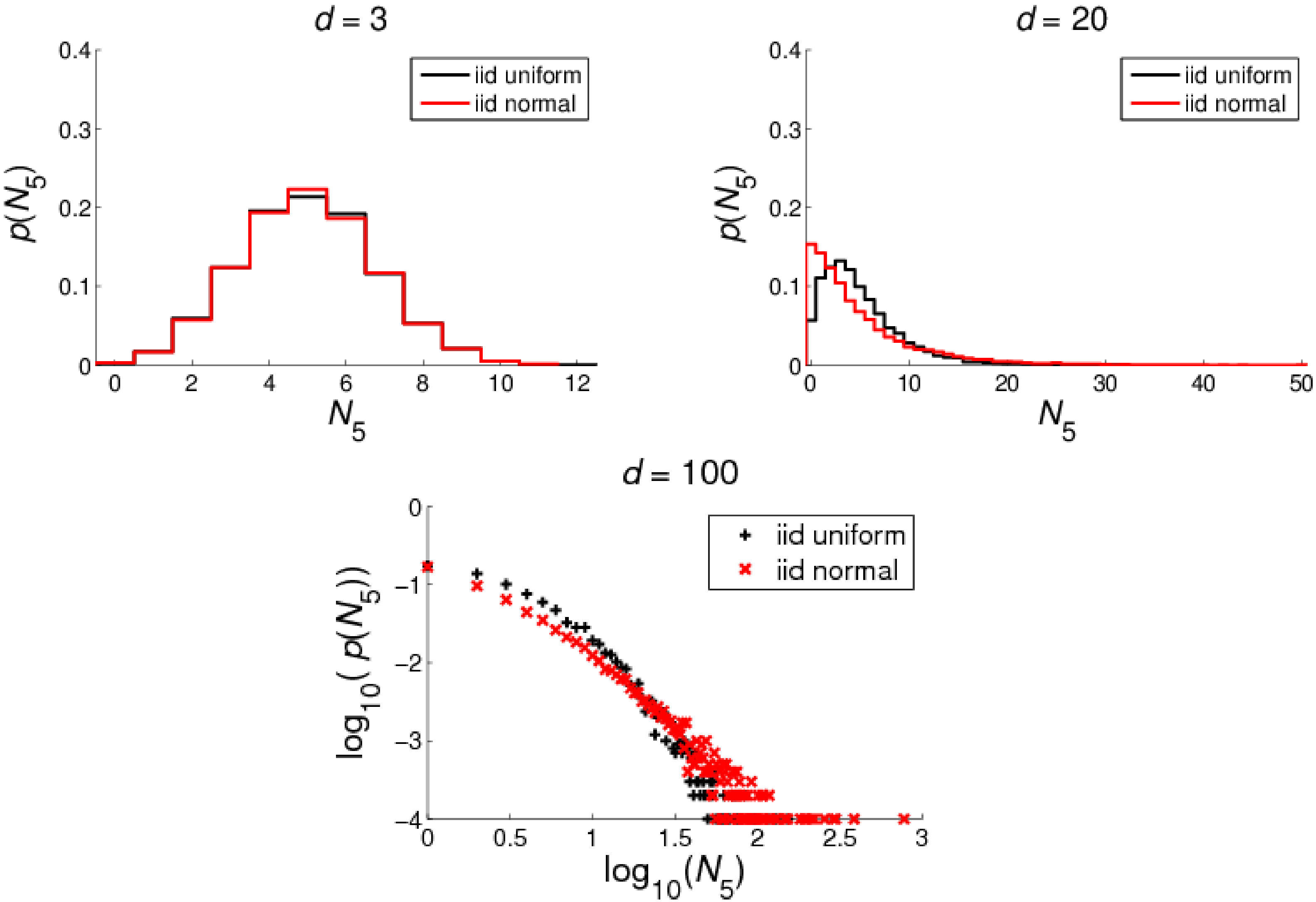
The Hubness Phenomenon

[Radovanović et al. ICML'09, Radovanović et al. JMLR'10]

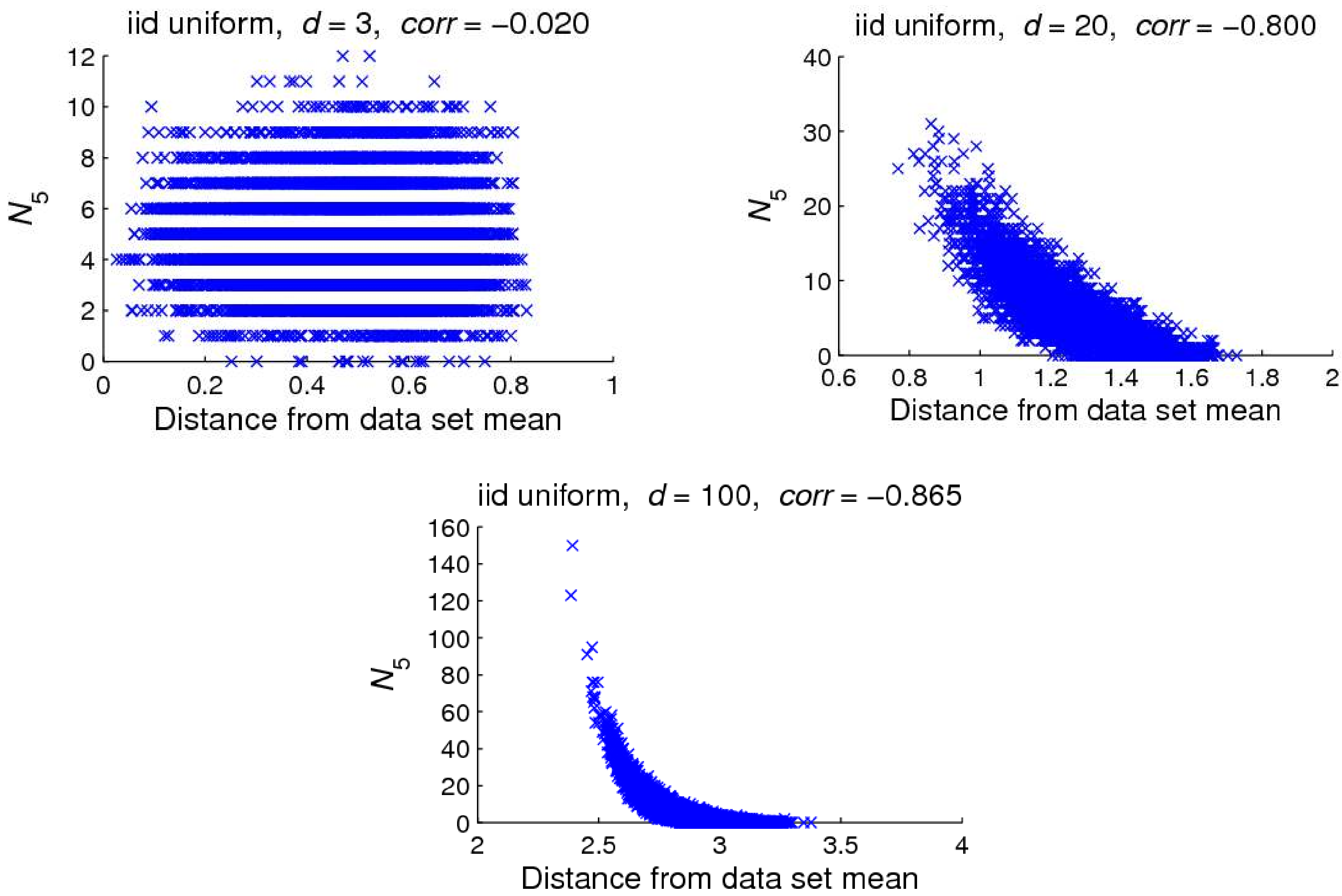
- $N_k(x)$, the number of ***k*-occurrences** of point $x \in \mathbf{R}^d$, is the number of times x occurs among k nearest neighbors of all other points in a data set. In other words:
  - $N_k(x)$ is the reverse k-nearest neighbor count of x
  - $N_k(x)$ is the in-degree of node x in the kNN digraph

- Observed that the distribution of N_k can become skewed, and have high variance, resulting in **hubs – points with high N_k values**, and **anti-hubs – points with low N_k**
  - Music retrieval [Aucouturier & Pachet PR'07]
  - Speaker verification ("Doddington zoo") [Doddington et al. ICSLP'98]
  - Fingerprint identification [Hicklin et al. NIST'05]

- Cause remained unknown, attributed to the specifics of data or algorithms



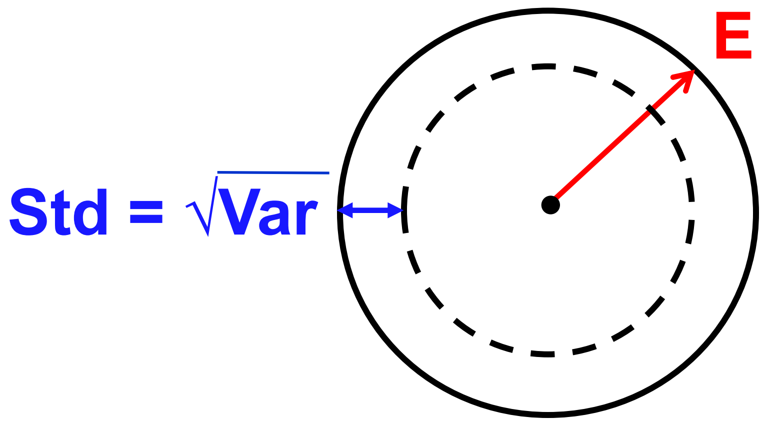
d = 3
0.4
0.3
0.2
0.1
0
p(N5)
iid uniform
iid normal
0
2
4
6
8
10
12
N5
d = 20
0.4
0.3
0.2
0.1
0
p(N5)
iid uniform
iid normal
0
10
20
30
40
50
N5
d = 100
0
−1
−2
−3
−4
log10(p(N5))
iid uniform
iid normal
0
0.5
1
1.5
2
2.5
3
log10(N5)



iid uniform, d = 3, corr = −0.020
N5
Distance from data set mean
iid uniform, d = 20, corr = −0.800
N5
Distance from data set mean
iid uniform, d = 100, corr = −0.865
N5
Distance from data set mean

Causes of Hubness

- **Related phenomenon: concentration of distance / similarity**
  - High-dimensional data points approximately lie on a **sphere** centered at any fixed point [Beyer et al. ICDT'99, Aggarwal & Yu SIGMOD'01]
  - The distribution of distances to a fixed point always has non-negligible variance [François et al. TKDE'07]
  - As the fixed point we observe the data set **center**



- **Centrality:** points closer to the data set center tend to be closer to all other points (regardless of dimensionality)

Centrality is amplified by high dimensionality

Important to Emphasize

- Generally speaking, **concentration does not CAUSE hubness**
- "Causation" might be possible to derive under certain assumptions. My preferred view: they are both manifestations of underlying mechanisms triggered by high dimensionality
- Example settings with(out) concentration and with(out) hubness:
  - C+, H+: iid uniform data, Euclidean dist.
  - C–, H+: iid uniform data, squared Euclidean dist.
  - C+, H–: iid normal data (centered at 0), cosine sim.
  - C–, H–: spatial Poisson process data, Euclidean dist.
- **Two "ingredients" needed for hubness:**
  1) **High dimensionality**
  2) **Centrality** (existence of **centers** / **borders**)

Hubness in Real Data

- Important factors for real data
  1) **Dependent attributes**
  2) **Grouping (clustering)**

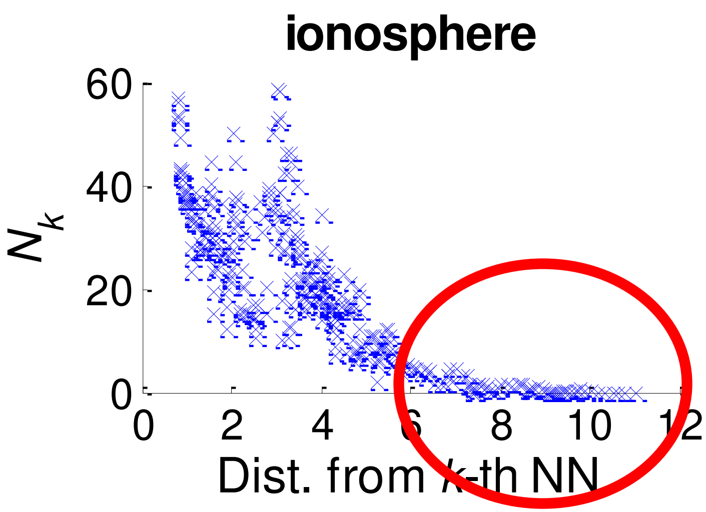
- 50 data sets
  - From well known repositories (UCI, Kent Ridge)
  - Euclidean and cosine, as appropriate

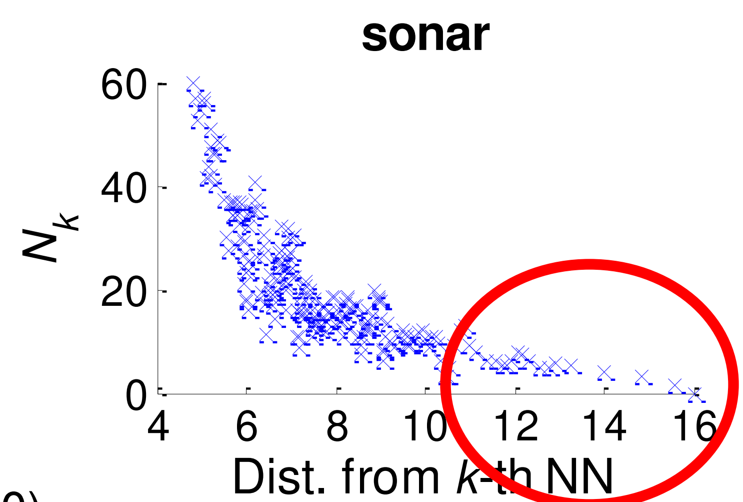
- **Conclusions** [Radovanović et al. JMLR'10]**:**
  1) Hubness depends on **intrinsic dimensionality**
  2) Hubs are in proximity of **cluster centers**

Anti-Hubs in Outlier Detection

[Radovanović et al. JMLR'10]

- In high dimensions, **points with low N_k** – the **anti-hubs** can be considered **distance-based outliers**
  - They are far away from other points in the data set / their cluster
  - High dimensionality contributes to their existence





(k = 20)

Anti-Hubs in Outlier Detection

[Aggarwal and Yu SIGMOD'01]

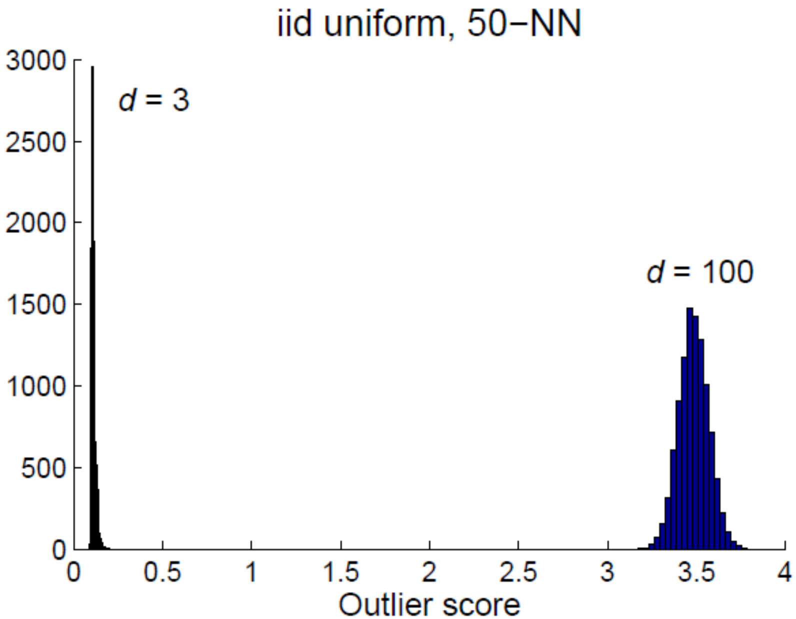
- In high-dimensional space unsupervised methods detect every point as an almost equally good outlier, since distances become indiscernible as dimensionality increases

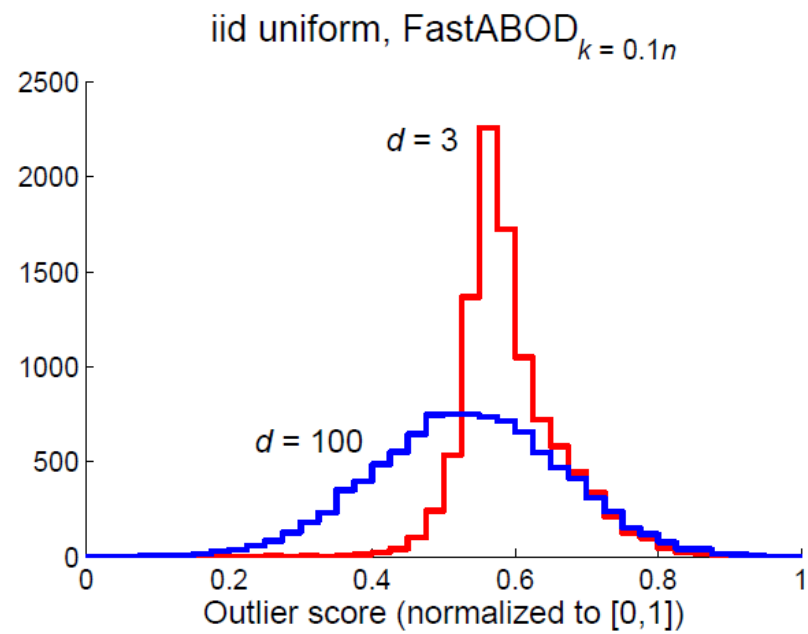
[Zimek et al. SADM'12]

- The above view was challenged by showing that the exact **opposite** may take place
- As dimensionality increases, outliers generated by a different mechanism from the data tend to be detected as more prominent by unsupervised methods
  - Assuming all dimensions carry useful information

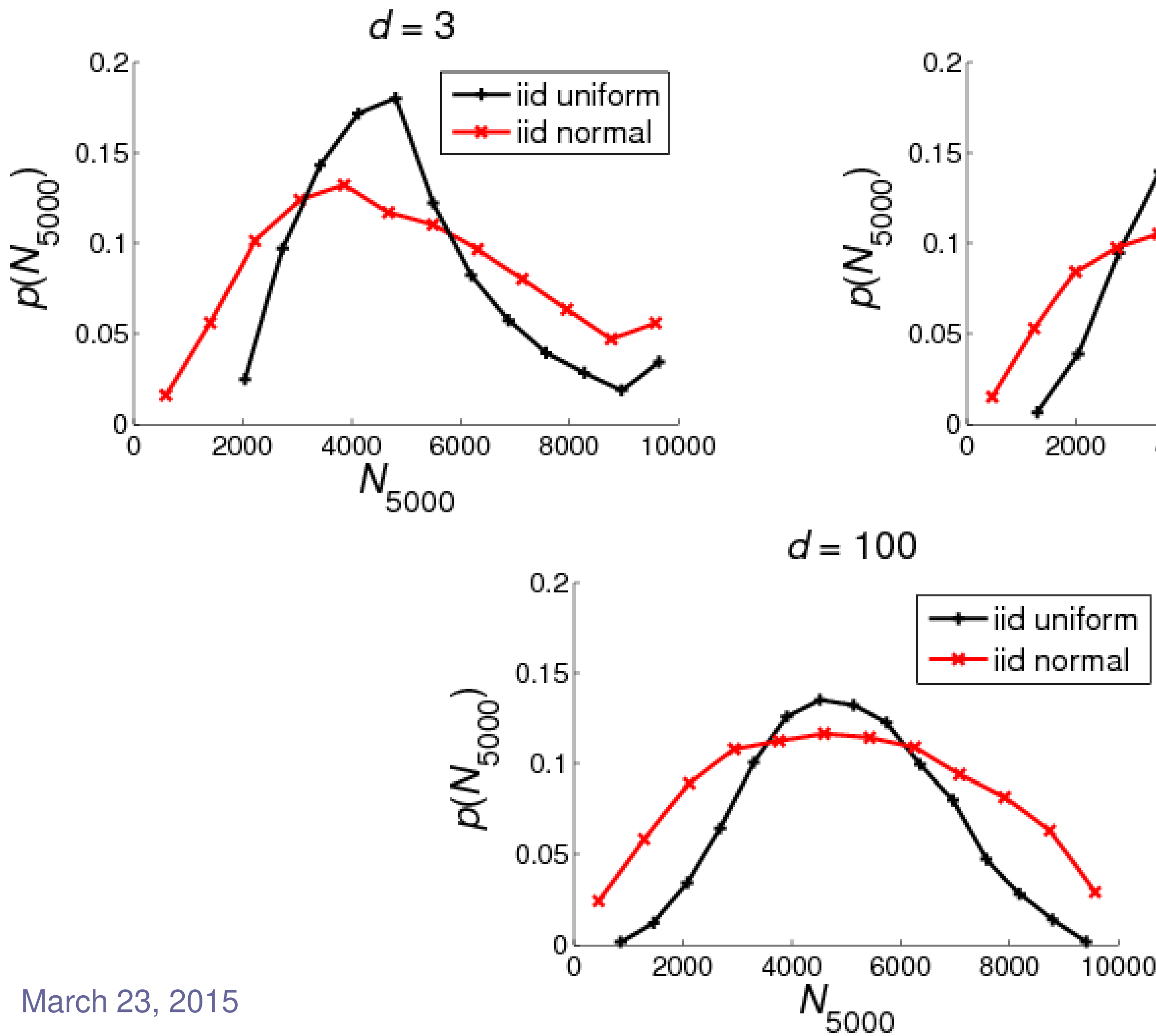
Anti-Hubs in Outlier Detection

- We show that the opposite can take place even when no true outliers exist, in the sense of originating from a different distribution
- This suggests that high dimensionality affects outlier scores and (anti-)hubness in similar ways

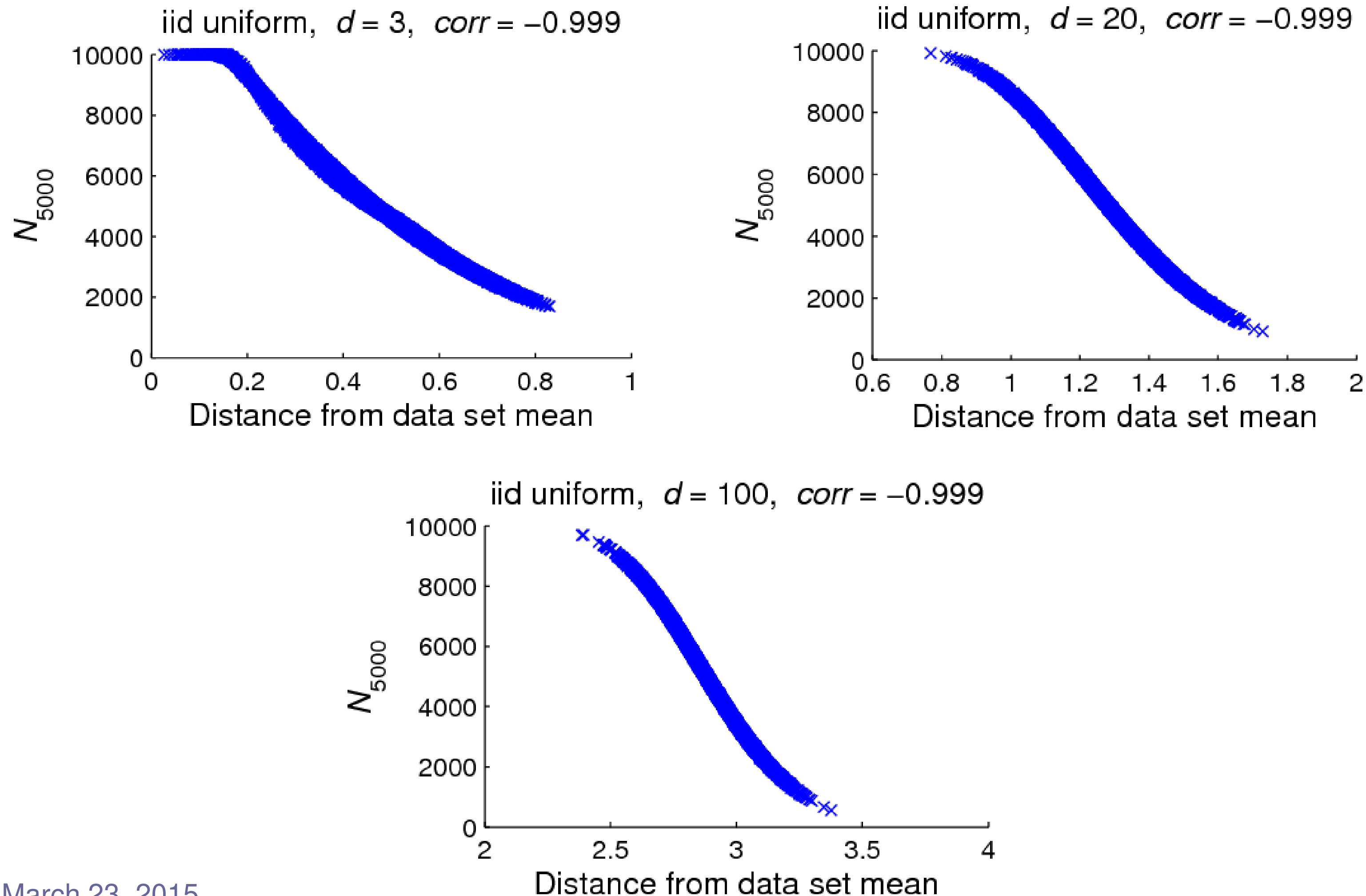




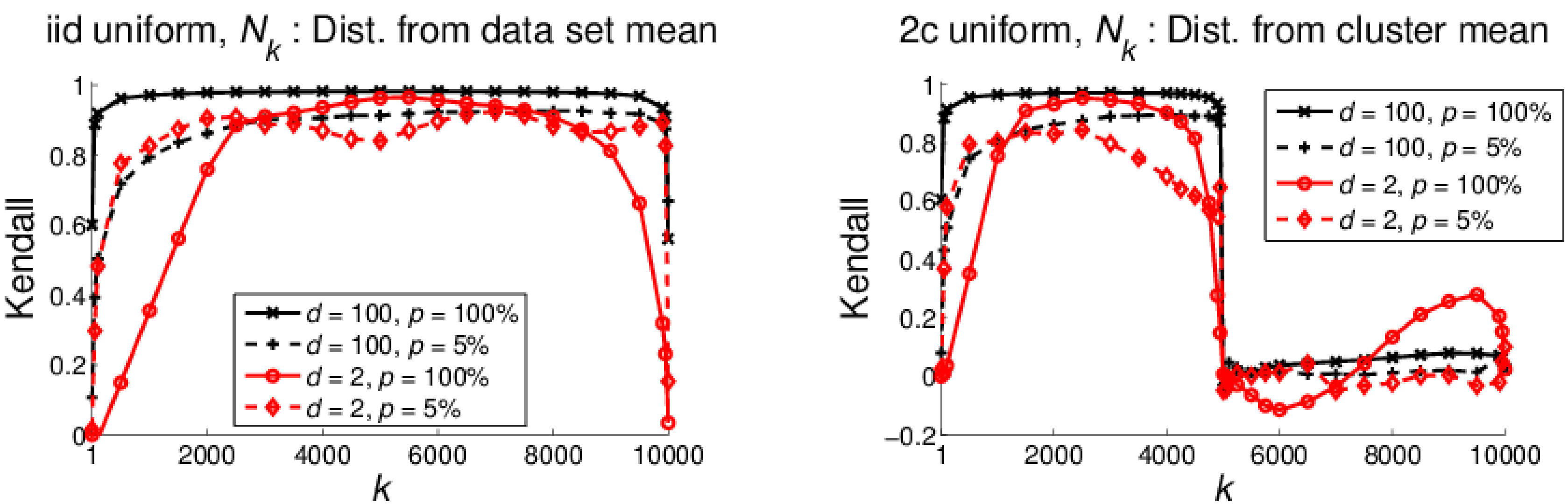
Hubness and Large Neighborhoods



Hubness and Large Neighborhoods



Hubness and Large Neighborhoods



- p = percentage of points with lowest N_k scores
- High dimensionality (d): N_k strong indicator of centrality overall (p = 100%), but weaker for anti-hubs (p = 5%)
- Low d: the opposite, especially w.r.t low k values
- Raising k strengthens correlation, but not when cluster boundary is crossed

The AntiHub Method

[Hautamäki et al. ICPR’04]

- Proposed method ODIN (Outlier Detection using Indegree Number), which selects as outliers points with N_k below or equal to a user-specified threshold
- Experiments on 5 data sets showed it can work better than various *k*NN distance methods
- Not aware of the hubness phenomenon, little insight into reasons why ODIN should work, its strengths, weaknesses…
- In method AntiHub, we use $N_k(x)$ as the outlier score of x (same as ODIN, without the threshold)

The AntiHub Method

Algorithm 1 AntiHub$_{dist}(D, k)$ (based on ODIN [11])

Input:

- Distance measure *dist*
- Ordered data set $D = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$, where $\mathbf{x}_i \in \mathbb{R}^d$, for $i \in \{1, 2, \ldots, n\}$
- No. of neighbors $k \in \{1, 2, \ldots\}$

Output:

- Vector $\mathbf{s} = (s_1, s_2, \ldots, s_n) \in \mathbb{R}^n$, where s_i is the outlier score of $\mathbf{x}_i$, for $i \in \{1, 2, \ldots, n\}$

Temporary variables:

- $t \in \mathbb{R}$

Steps:

1) For each $i \in (1, 2, \ldots, n)$
2) $t := N_k(\mathbf{x}_i)$ computed w.r.t. *dist* and data set $D \backslash \mathbf{x}_i$
3) $s_i := f(t)$, where $f : \mathbb{R} \to \mathbb{R}$ is a monotone function

The AntiHub Method

- We experimentally identified strengths and weaknesses of AntiHub with respect to different properties (factors):

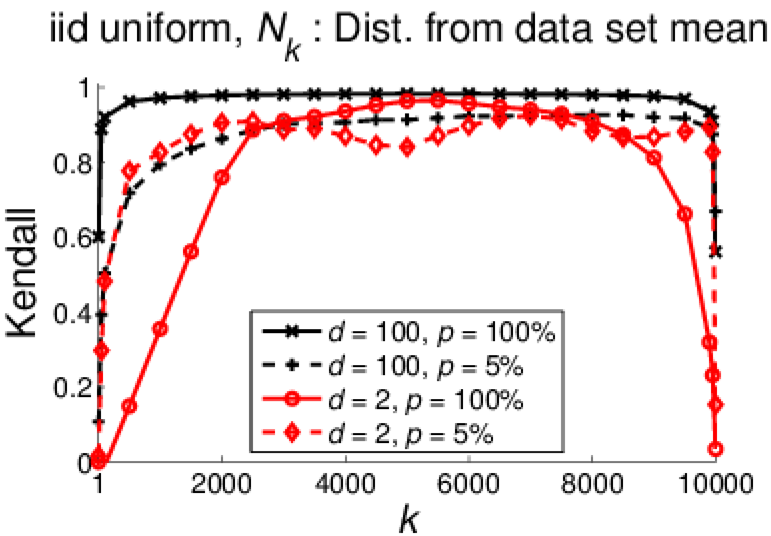
    1. Hubness
    2. Locality vs. globality
    3. Discreteness of scores
    4. Varying density
    5. Computational complexity

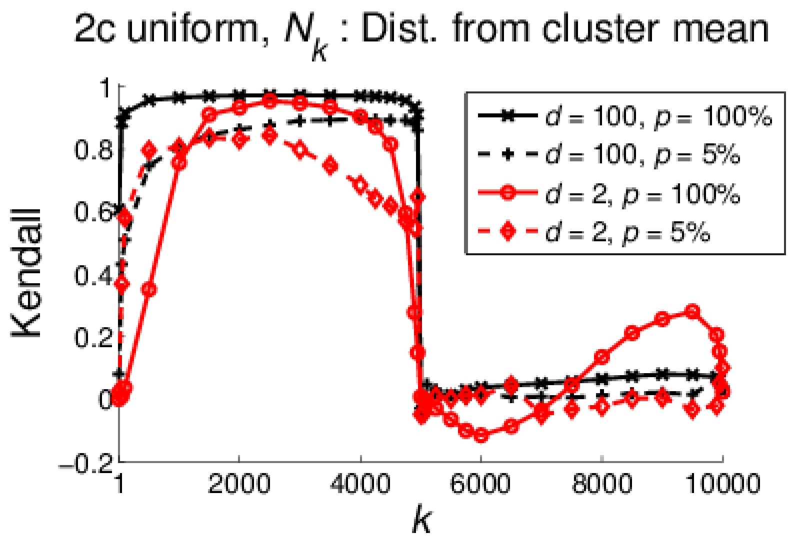
The AntiHub Method

Property 1: Hubness

- High (intrinsic) dimensionality, $k << n$:
  - Good overall correlation between N_k and distance to a center, but
  - Many N_k values of 0 – problem with discrimination
- Low dimensionality, $k << n$
  - Low correlation between N_k and distance to a center, but
  - For a small number of points with low N_k, this correlation is better, so AntiHub/ODIN can be meaningful

The AntiHub Method





The AntiHub Method

Property 2: Locality vs. globality

- For AntiHub and other methods based on *k*NN:
  - $k << n$: notion of outlierness is local
  - $k \sim n$: notion of outlierness is global
- AntiHub in “local mode” may have problems with discrimination
- Raising *k* can address this, but the notion of outlierness goes global
  - This can be problematic if we are interested in local outliers, but *k* crosses cluster boundaries

Property 3: Discreteness of scores

- Regardless of all of the above, N_k scores are integers, hence inherently discrete, which can also cause discrimination problems

The AntiHub Method

Property 4: Varying density

- AntiHub is not sensitive to the scale of distances in the data
- Can effectively detect (local) outliers in clusters of different densities without explicitly modeling density

Property 5: Computational complexity

- Using high k values can be useful
- However, approximate kNN search/indexing methods typically assume $k = O(1)$

The AntiHub^2 Method

- Notable weakness of AntiHub, discrimination of scores, contributed to by two factors:
  - Hubness
  - Discreteness of scores
- Therefore, we proposed method AntiHub^2, which combines the N_k score of a point with N_k scores of it's k nearest neighbors, in order to maximize discrimination
- AntiHub^2 improves discrimination of scores compared to the AntiHub method

The AntiHub^2 Method

Algorithm 2 AntiHub$^2_{dist}(D, k, p, step)$

Input:

- Distance measure $dist$
- Ordered data set $D = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$, where $\mathbf{x}_i \in \mathbb{R}^d$, for $i \in \{1, 2, \dots, n\}$
- No. of neighbors $k \in \{1, 2, \dots\}$
- Ratio of outliers to maximize discrimination $p \in (0, 1]$
- Search parameter $step \in (0, 1]$

Output:

- Vector $\mathbf{s} = (s_1, s_2, \dots, s_n) \in \mathbb{R}^n$, where s_i is the outlier score of $\mathbf{x}_i$, for $i \in \{1, 2, \dots, n\}$

Temporary variables:

- AntiHub scores $\mathbf{a} \in \mathbb{R}^n$
- Sums of nearest neighbors' AntiHub scores $\mathbf{ann} \in \mathbb{R}^n$
- Proportion $\alpha \in [0, 1]$
- (Current) discrimination score $cdisc, disc \in \mathbb{R}$
- (Current) raw outlier scores $\mathbf{ct}, \mathbf{t} \in \mathbb{R}^n$

The AntiHub^2 Method

Local functions:

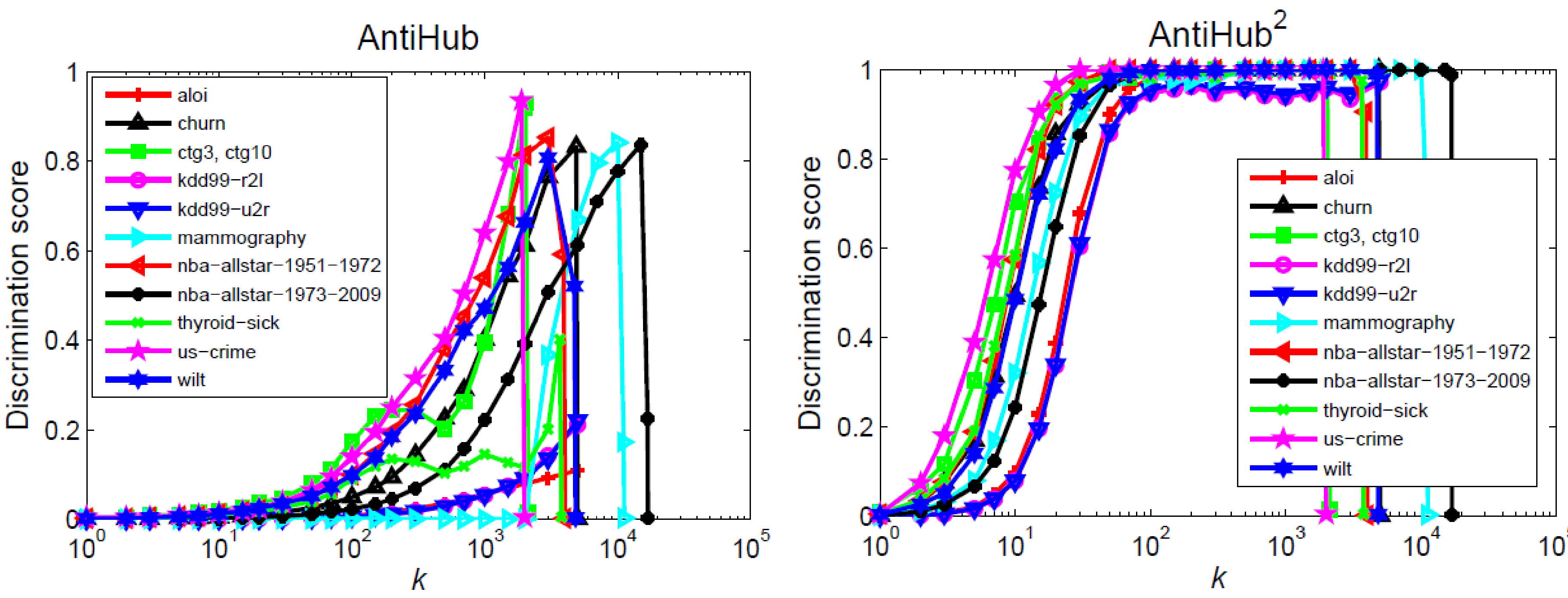
- discScore($\mathbf{y}, p$): for $\mathbf{y} \in \mathbb{R}^n$ and $p \in (0, 1]$ outputs the number of unique items among $\lceil np \rceil$ smallest members of $\mathbf{y}$, divided by $\lceil np \rceil$

Steps:

1) $\mathbf{a} :=$ AntiHub$_{dist}(D, k)$
2) For each $i \in (1, 2, \ldots, n)$
3) $\quad ann_i := \sum_{j \in \mathrm{NN}_{dist}(k,i)} a_j$, where $\mathrm{NN}_{dist}(k, i)$ is the set of indices of k nearest neighbors of $\mathbf{x}_i$
4) $disc := 0$
5) For each $\alpha \in (0, step, 2 \cdot step, \ldots, 1)$
5) $\quad$ For each $i \in (1, 2, \ldots, n)$
6) $\quad\quad ct_i := (1 - \alpha) \cdot a_i + \alpha \cdot ann_i$
7) $\quad cdisc :=$ discScore($\mathbf{ct}, p$)
8) $\quad$ If $cdisc > disc$
9) $\quad\quad \mathbf{t} := \mathbf{ct}$, $disc := cdisc$
10) For each $i \in (1, 2, \ldots, n)$
11) $\quad s_i := f(t_i)$, where $f : \mathbb{R} \to \mathbb{R}$ is a monotone function

Discrimination Improvement

discScore values for real data (p = 10%, $step$ = 0.01)



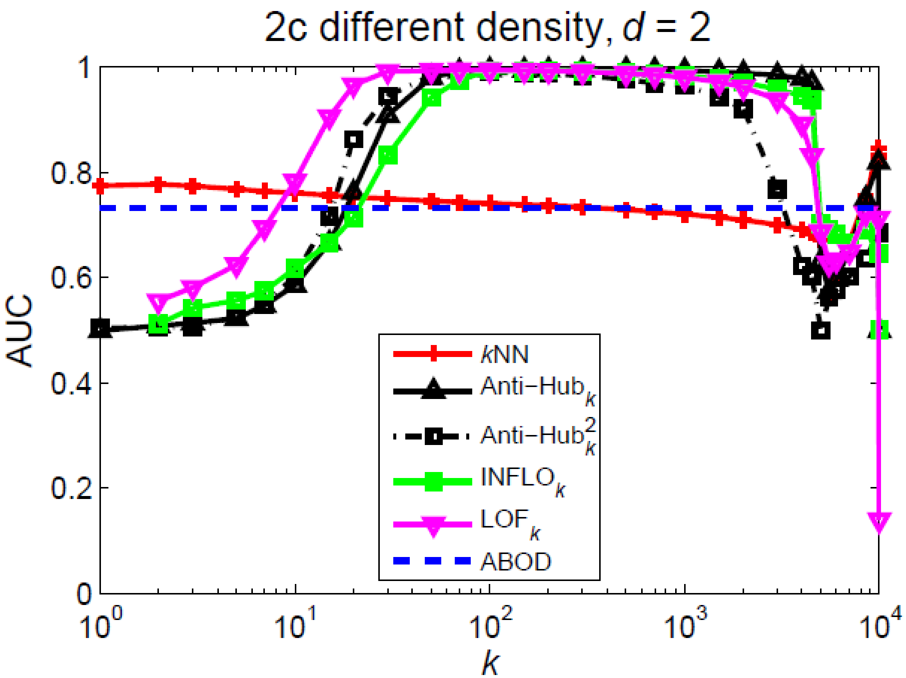
Performance Evaluation

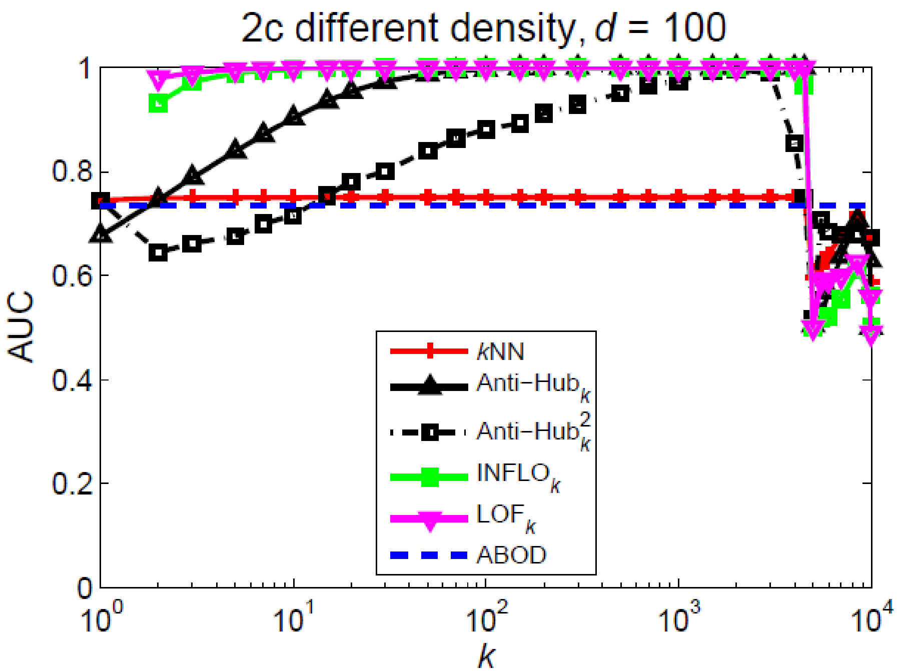
Methods for comparison:

- *k*NN: distance to the *k*th nearest neighbor
  [Ramaswamy et al. SIGMOD Rec'00]
- ABOD: Angle Based Outlier Detection
  [Kriegel et al. KDD'08]
- LOF: Local Outlier Factor
  [Breunig et al. SIGMOD Rec'00]
- INFLO: INFLuenced Outlierness
  [Jin et al. PAKDD'06]

Performance Evaluation

- Synthetic data: two well-separated Gaussian clusters of the same size, std of one 10 times larger than other, outliers 5% of points from each cluster projected 20% farther from respective cluster center

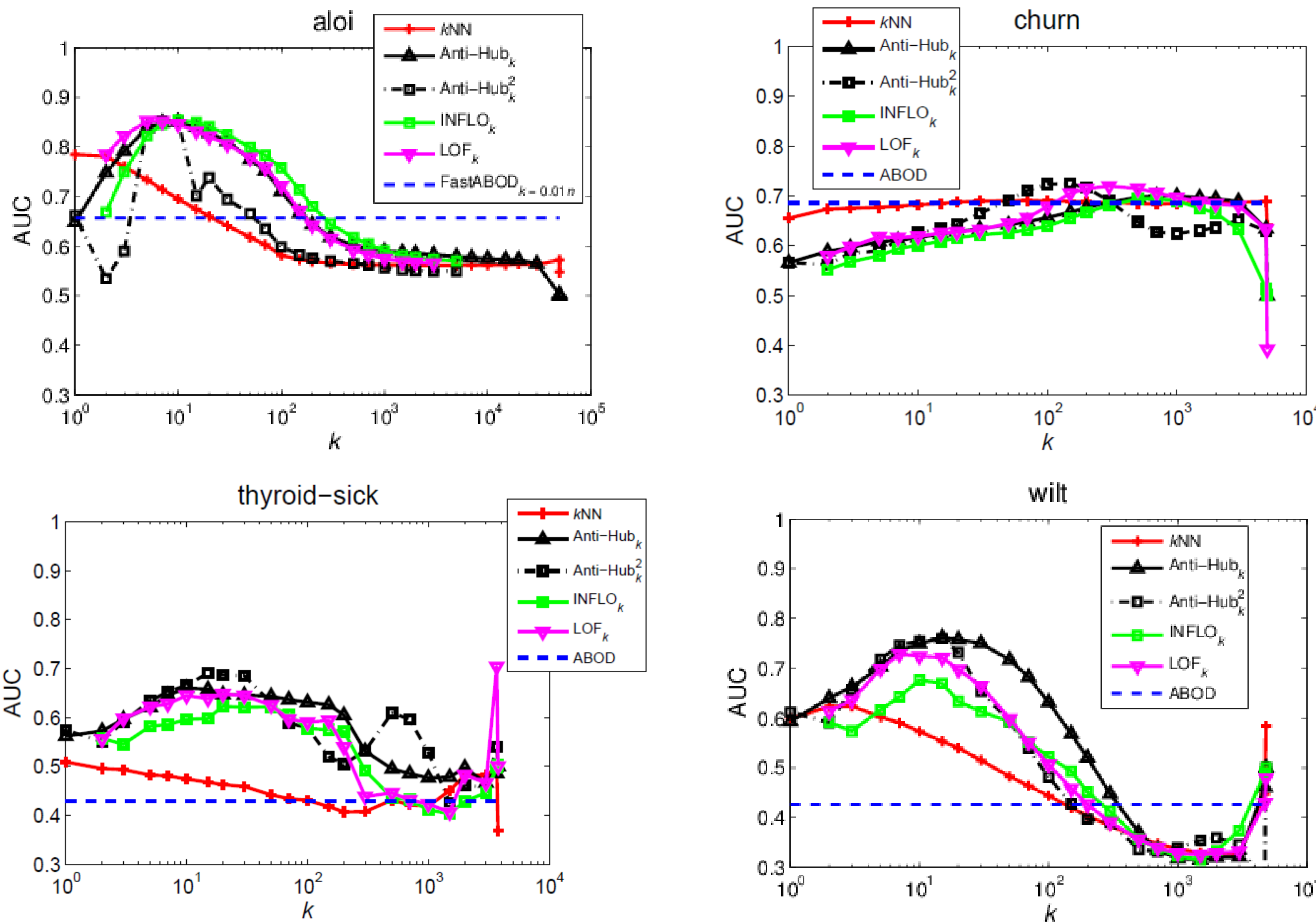


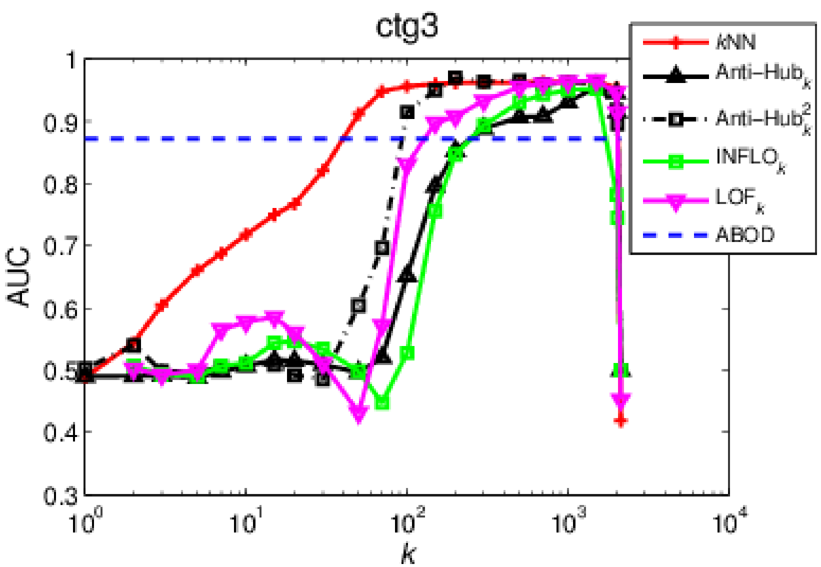


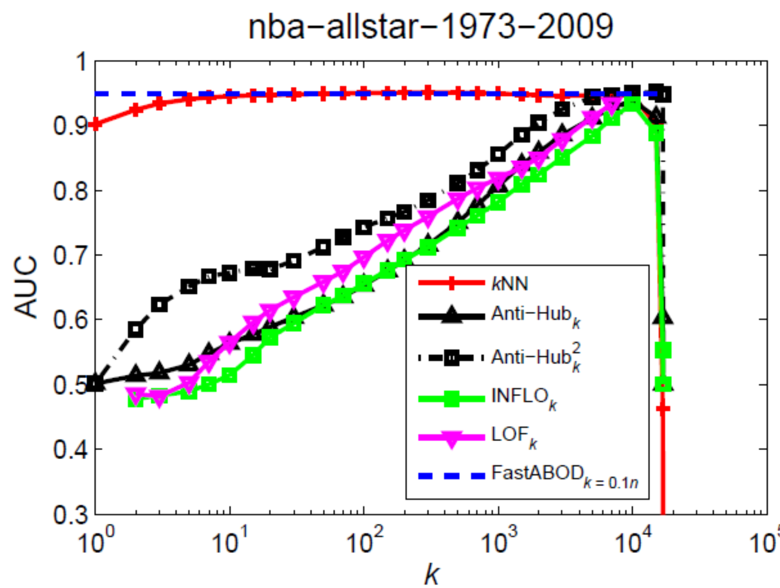
Performance Evaluation

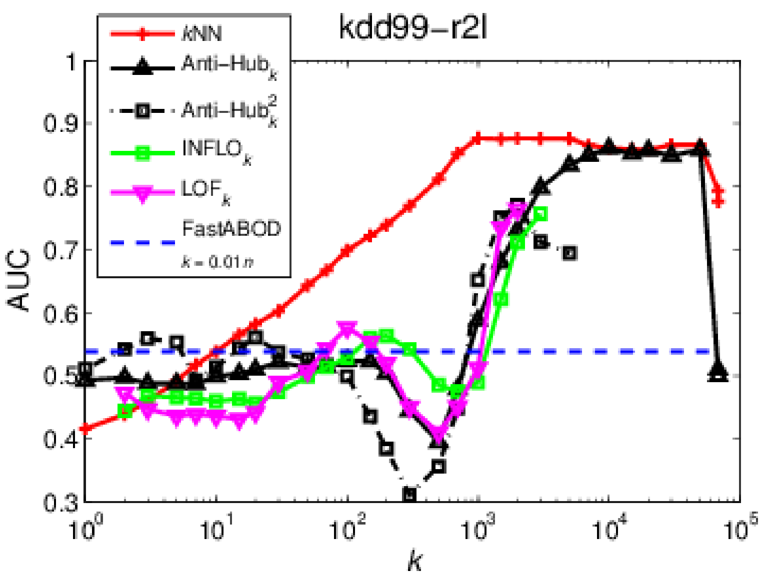
- Real data: mostly natural labeled outliers from various domains

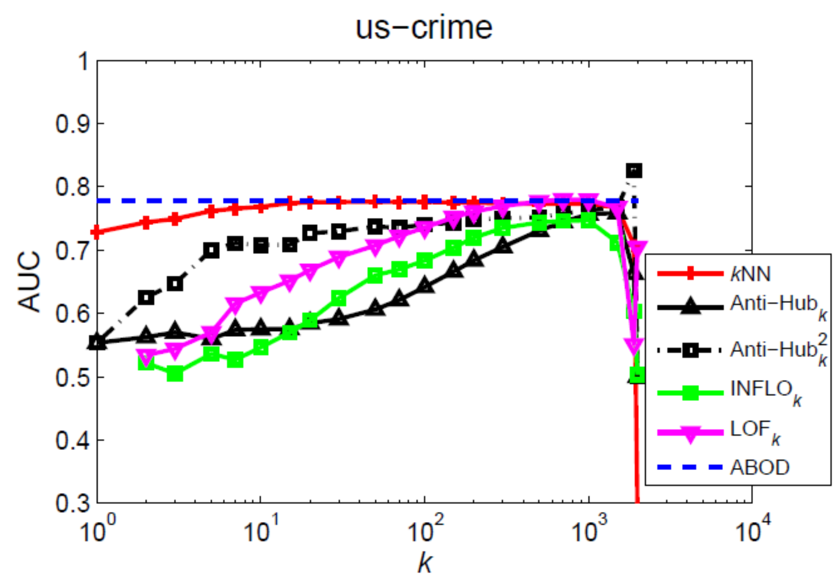
Name	n	d	$S_{N_{10}}$	Outlier%
aloi	50,000	64	0.260	3.016
churn	5,000	17	0.849	14.140
ctg3	2,126	35	0.652	8.279
ctg10	2,126	35	0.652	2.493
kdd99-r2l	68,338	38	0.018	1.456
kdd99-u2r	67,395	38	0.031	0.077
mammography	11,183	6	0.103	2.325
nba-allstar-1951-1972	4,018	15	0.483	15.903
nba-allstar-1973-2009	16,916	17	0.730	5.669
thyroid-sick	3,772	52	0.371	6.124
us-crime	1,994	100	1.327	7.523
wilt	4,839	5	-0.075	5.394


aloi
kNN
Anti–Hub$_k$
Anti–Hub$_k^2$
INFLO$_k$
LOF$_k$
FastABOD$_{k=0.01n}$
AUC
k
churn
ABOD
thyroid–sick
wilt


ctg3
AUC
k
kNN
Anti-Hub$_k$
Anti-Hub^2_k
INFLO$_k$
LOF$_k$
ABOD


nba-allstar-1973-2009
AUC
k
kNN
Anti-Hub$_k$
Anti-Hub^2_k
INFLO$_k$
LOF$_k$
FastABOD$_{k=0.1n}$


kdd99-r2l
AUC
k
kNN
Anti-Hub$_k$
Anti-Hub^2_k
INFLO$_k$
LOF$_k$
FastABOD $k = 0.01n$


us-crime
AUC
k
kNN
Anti-Hub$_k$
Anti-Hub^2_k
INFLO$_k$
LOF$_k$
ABOD

Performance Evaluation

- Two types of data sets: mostly local and mostly global outliers
- With respect to different *k* values, AUC of AntiHub and AntiHub^2 behaves similarly to density-based methods (LOF, INFLO)
- Very high *k* values can be useful for all methods, especially LOF, INFLO, AntiHub and AntiHub^2, suggesting there may be a relationship between "global" density-based and distance-based outliers
- AntiHub^2 can improve AUC of AntiHub, but not always, thus discrimination is not the only factor that should be addressed

Conclusions

- We provided a unifying view of the role of reverse nearest neighbor counts in unsupervised outlier detection:
  - Effects of high dimensionality on unsupervised outlier-detection methods and hubness
  - Extension of previous examinations of (anti-)hubness to large values of k
  - The article also explores the relationship between hubness and data sparsity
- We formulated the AntiHub method, discussed its properties, and improved it in AntiHub^2 by focusing on discrimination of scores
- Our main hope: clearing the picture of the interplay between types of outliers and properties of data, filling a gap in understanding which may have so far hindered the widespread use of reverse neighbor methods in unsupervised outlier detection

Future Possibilities

- High values of *k* can be useful, but:
  - Cluster boundaries can be crossed, producing meaningless results of local outlier detection. How to determine optimal neighborhood size(s)?
  - Computational complexity is raised; approximate NN search/indexing methods do not work any more. Is it possible to solve this for large *k*?
- AntiHub and AntiHub^2 are no "rock star" methods
  - Can N_k scores be applied to outlier detection in a better way? Through outlier ensembles?
- Extend to (semi-)supervised outlier detection methods

Future Possibilities

- Explore relationships between intrinsic dimensionality, distance concentration, (anti-)hubness, and their impact on subspace methods for outlier detection

- Investigate secondary measures of distance/similarity, such as shared-neighbor distances

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