Clustering methods: Part 7

Outlier removal

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Outlier detection methods

Distance-based methods

- Knorr & Ng

Density-based methods

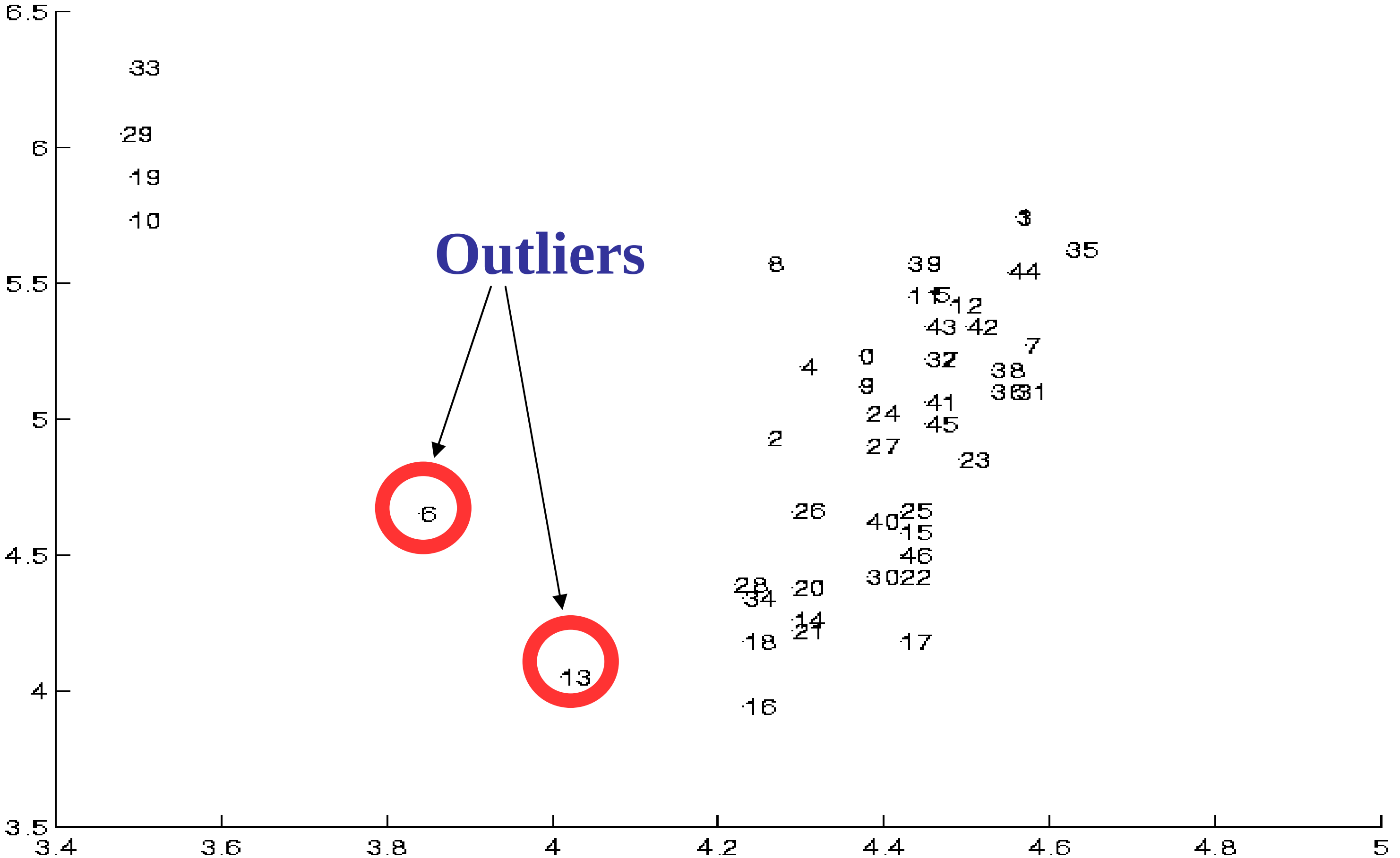
- KDIST: K^{th} nearest distance
- MeanDIST: Mean distance

Graph-based methods

- MkNN: Mutual K-nearest neighbor
- ODIN: Indegree of nodes in k-NN graph

What is outlier?

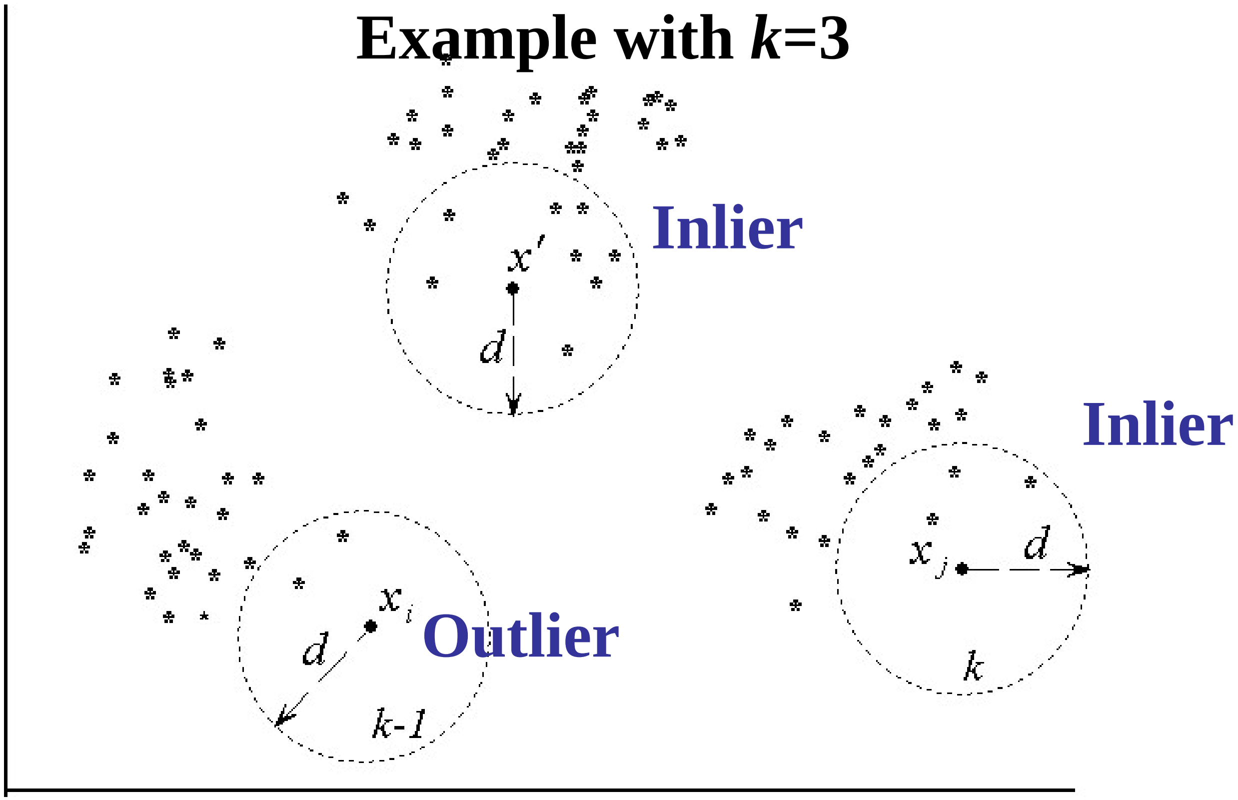
One definition: Outlier is an observation that deviates from other observations so much that it is expected to be generated by a different mechanism.



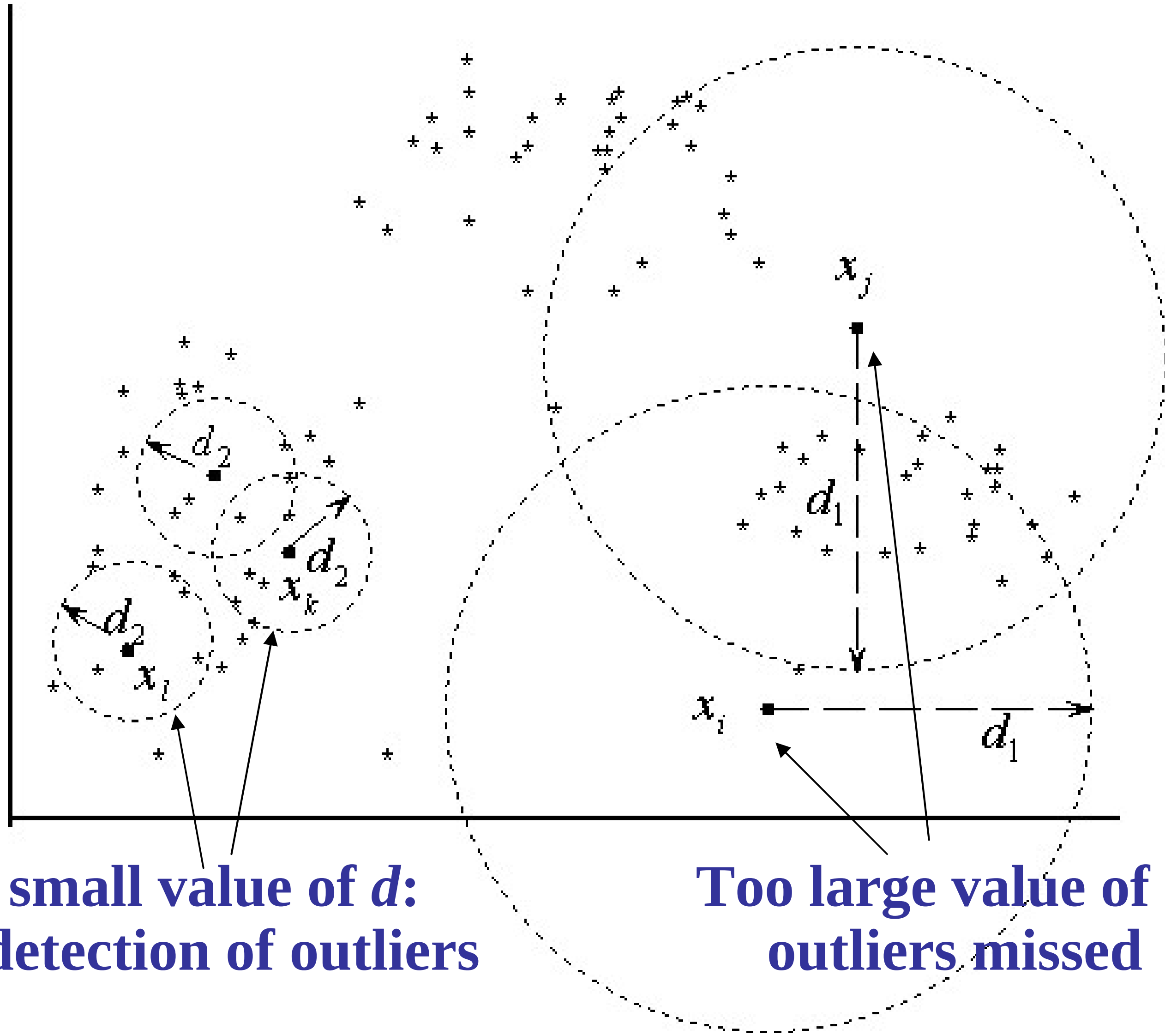
Distance-based method

[Knorr and Ng , CASCR 1997]

Definition: Data point x is an outlier if at most k points are within the distance d from x.



Selection of distance threshold



Too small value of *d*: false detection of outliers

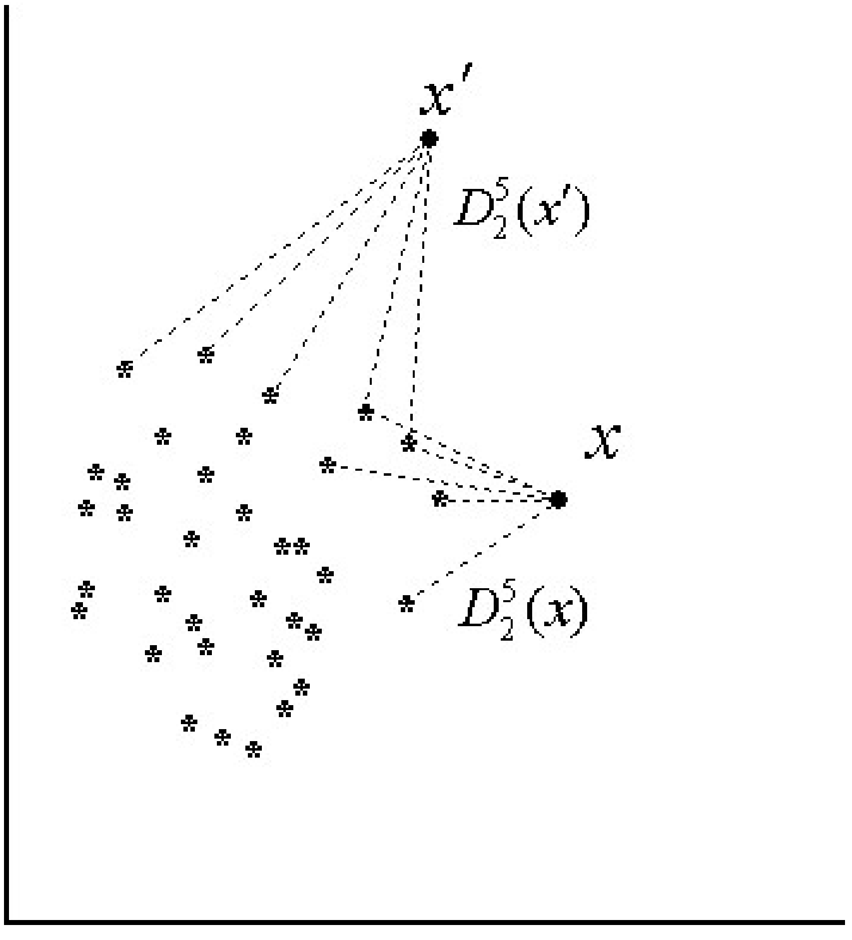
Too large value of *d*: outliers missed

Density-based method: KDIST

[Ramaswamy *et al.*, ACIM SIGMOD 2000]

• Define *KDIST* as distance to the k^{th} nearest point.

• Points are sorted by their *KDIST* distance. The last *n* points in the list are classified as outliers.



Density-based: MeanDist

[Hautamäki *et al.*, ICPR 2004]

MeanDIST = the mean of *k* nearest distances.

User parameters: Cutting point *k*, and local threshold *t:*

$$T = \max\left(L_i - L_{i-1}\right)\cdot t$$

Algorithm 2 MeanDIST

Compute T using Eq. 1 with t

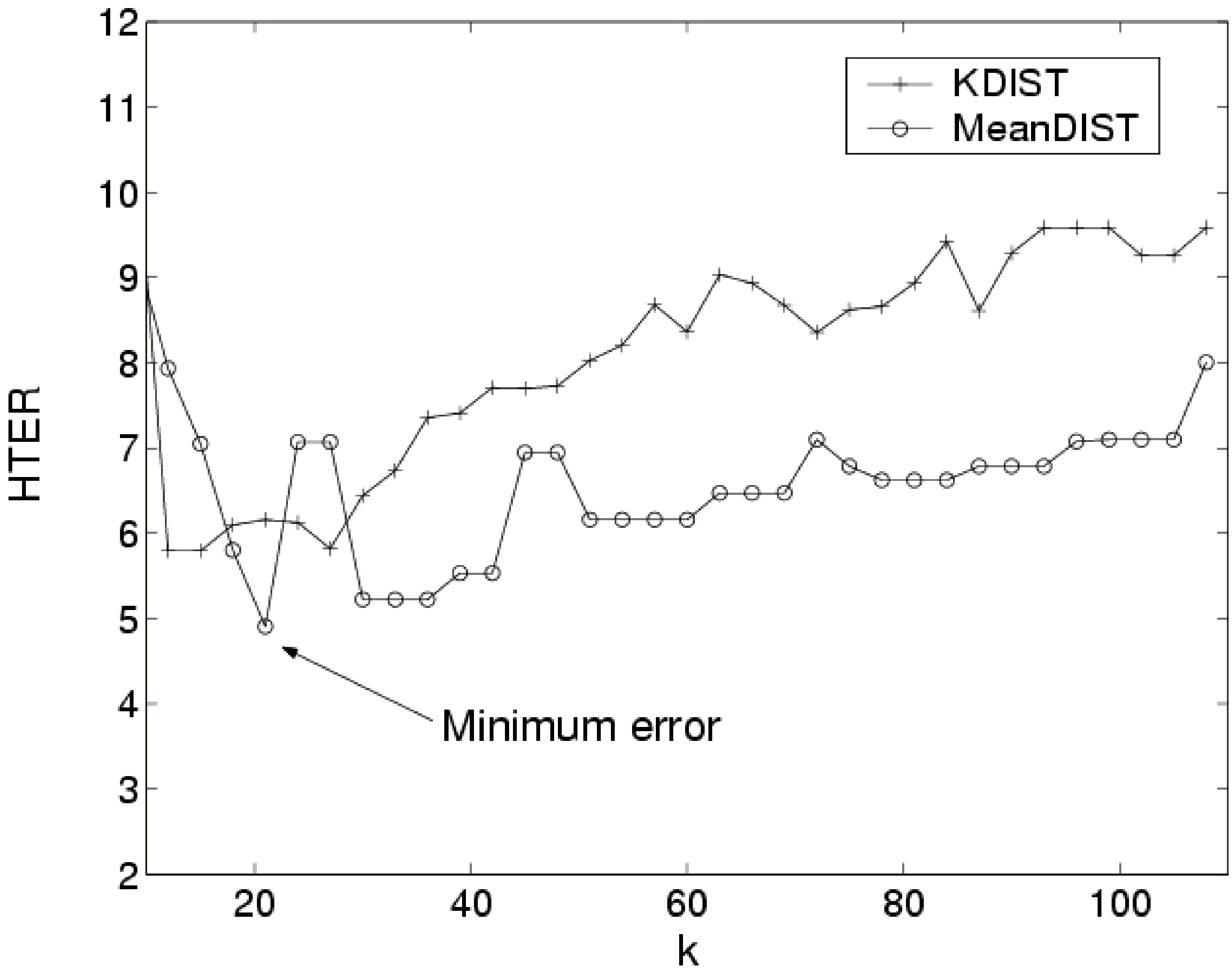
Calculate kNN graph of S

$L \leftarrow$ Sort vectors in ascending order by kNN density

Find smallest i for which $L_i - L_{i-1} \geq T$

Mark $L_i, \ldots, L_{|S|}$ as outliers

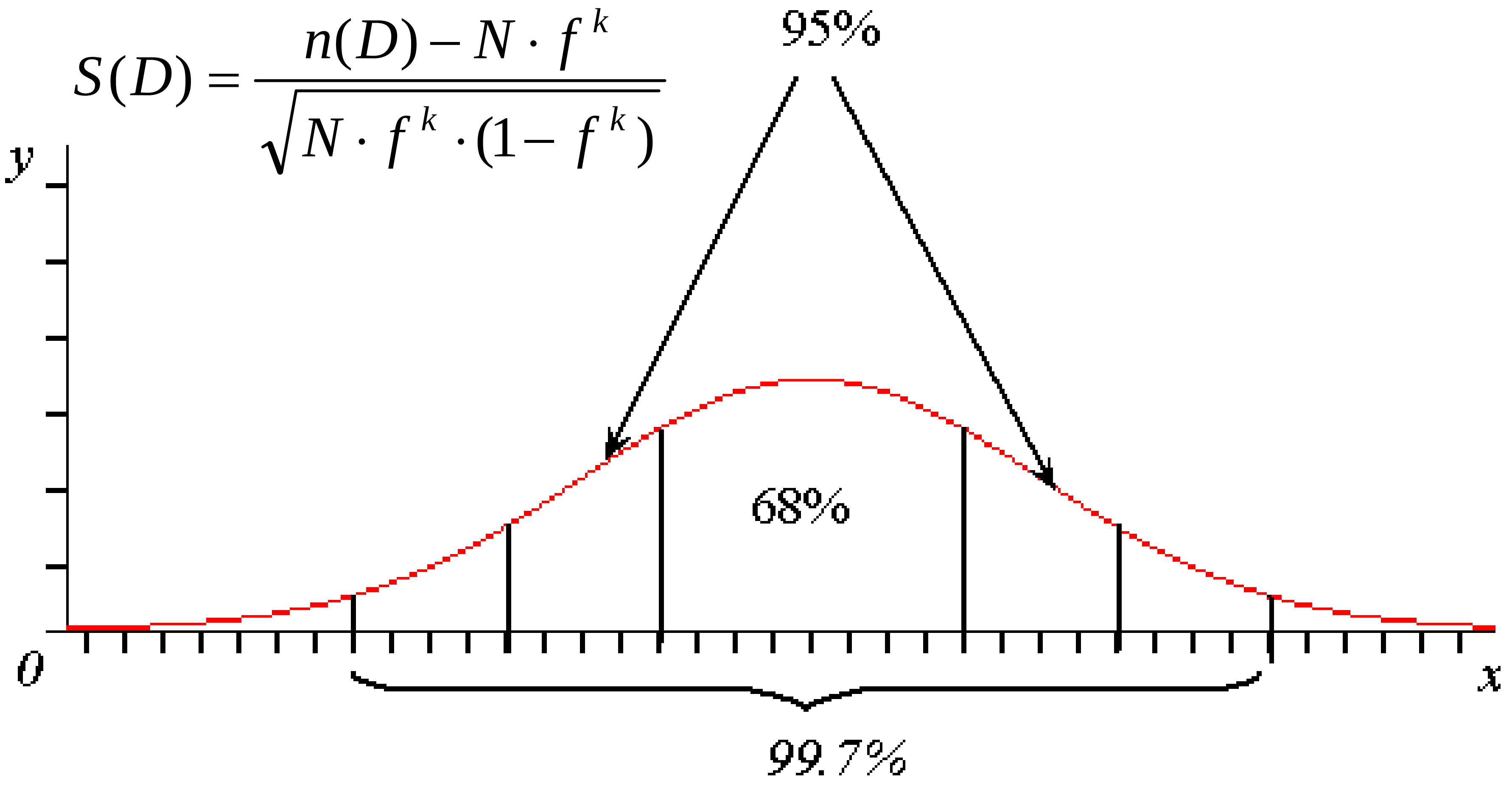
Comparison of KDIST and MeanDIST



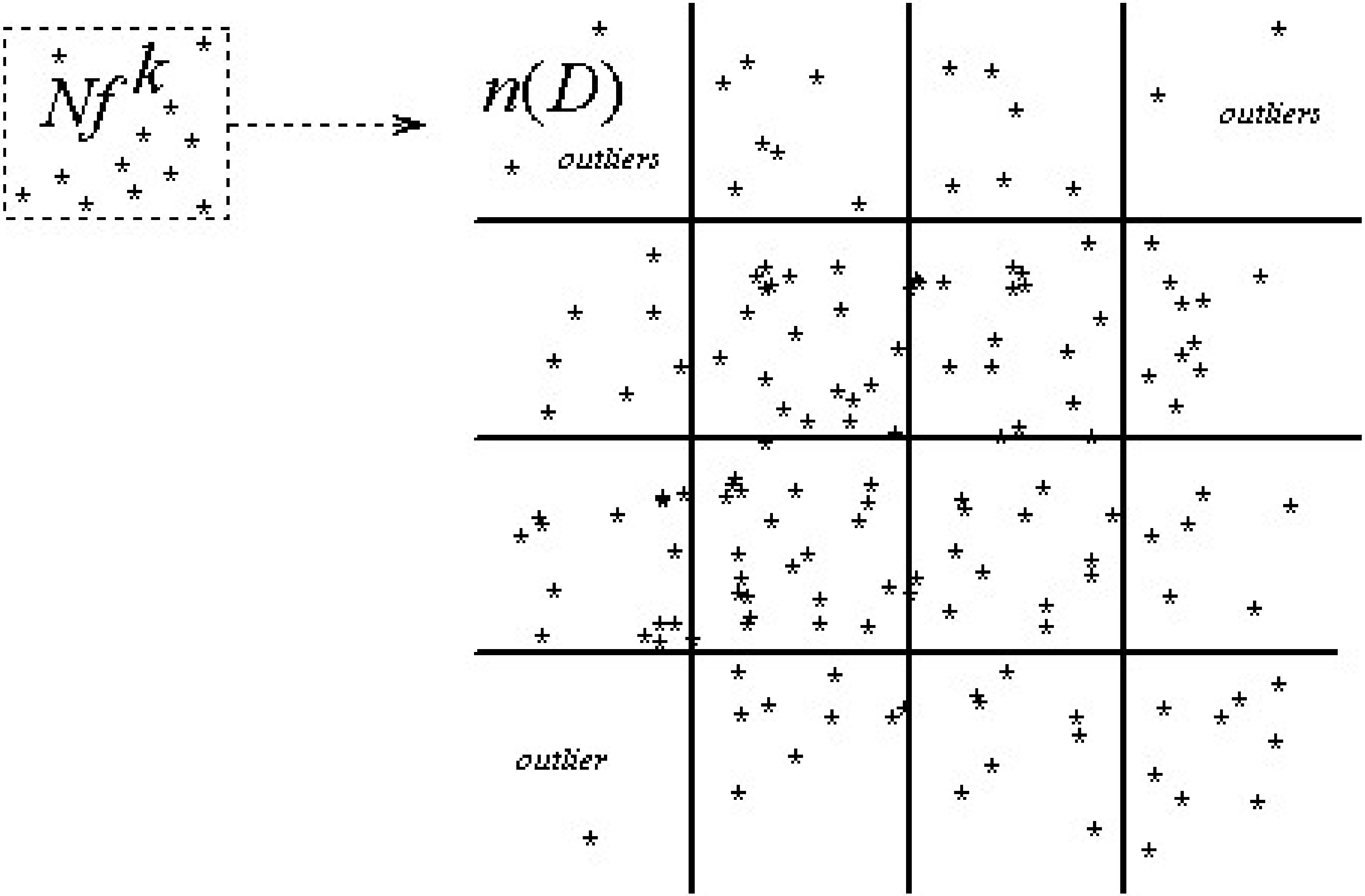
Distribution-based method

[Aggarwal and Yu, ACM SIGMOD, 2001]

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



Detection of sparse cells



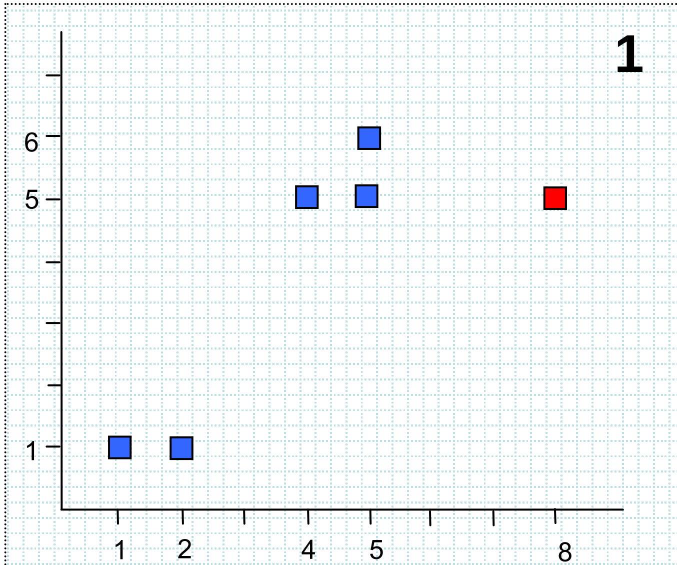
Mutual *k*-nearest neighbor

[Brito et al., *Statistics & Probability Letters*, 1997]

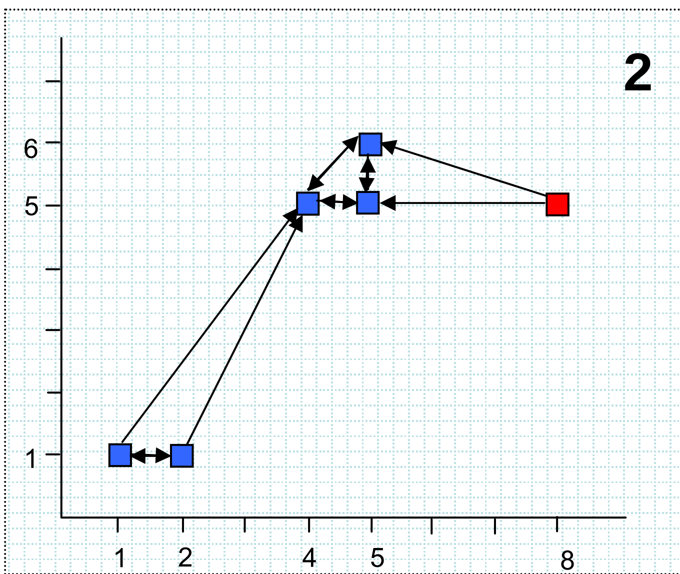
- Generate directed k-NN graph.
- Create undirected graph:
  1. Points *a* and *b* are *mutual neighbors* if both links $a \rightarrow b$ and $b \rightarrow a$ exist.
  2. Change all mutual links $a \leftrightarrow b$ to undirected link a—b.
  3. Remove the rest.
- Connected components are clusters.
- Isolated points as outliers.

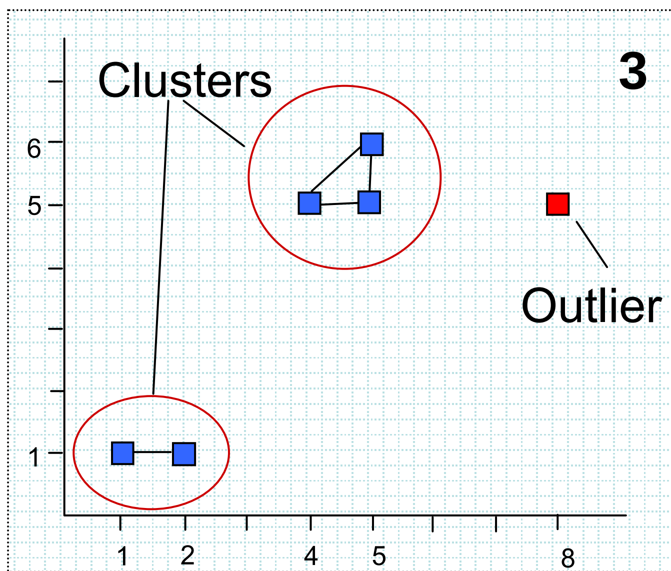
Mutual *k*-NN example

$k = 2$



1. Given a data with one outlier.
2. For each point find two nearest neighbours and create <u>*directed 2-NN*</u> graph.
3. For each pair of points, create link if both a→b and b→a exist.





ODIN: Outlier detection using indegree

[Hautamäki et al., ICPR 2004]

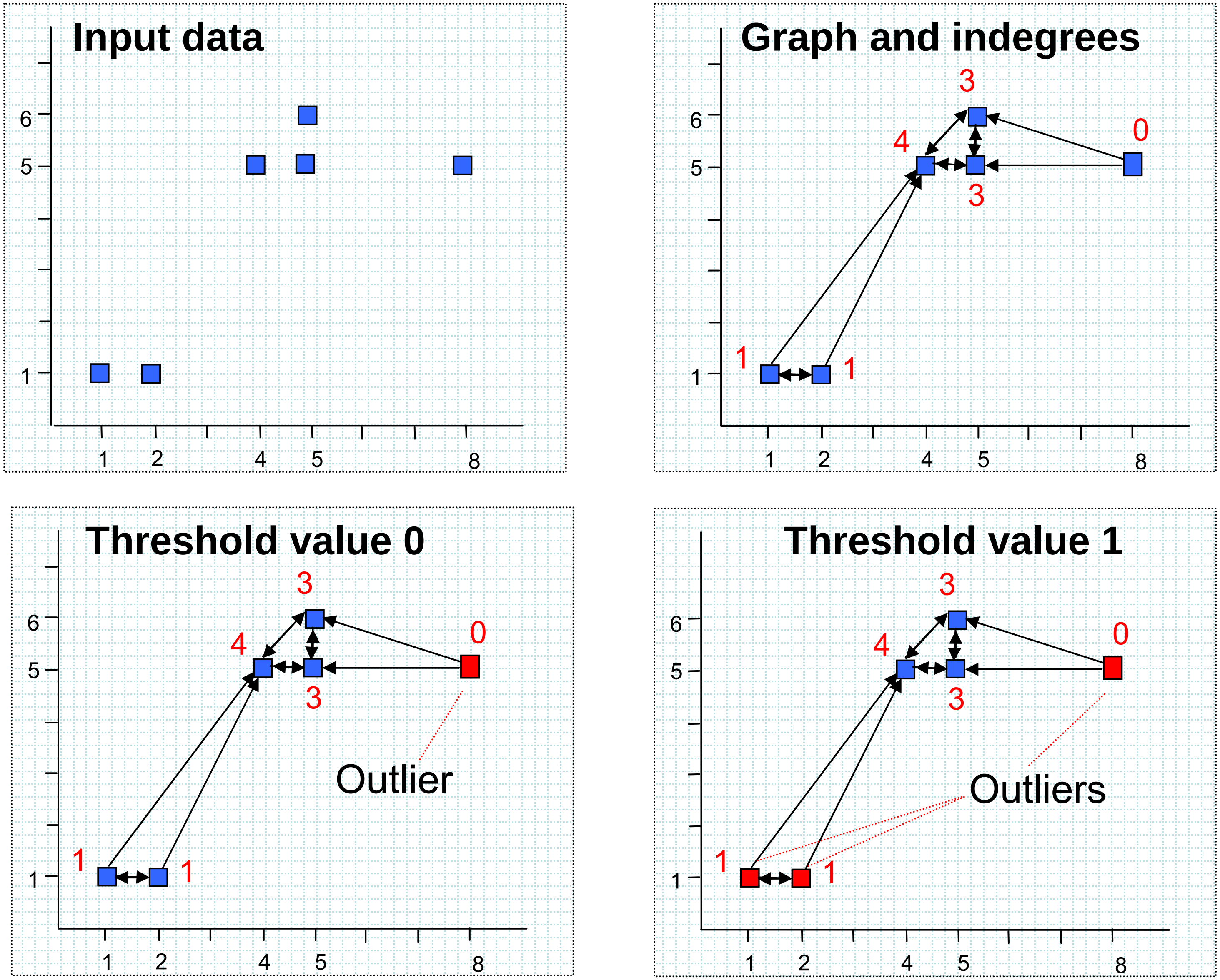
Definition: Given kNN graph, classify data point *x* as an outlier its indegree ≤ *T*.

Algorithm 1 ODIN

T is indegree threshold
Calculate kNN graph of S
for $i = 1$ to $|S|$ **do**
  if indegree of $v_i \leq T$ **then**
    Mark v_i as outlier
  end if
end for

Example of ODIN

$k = 2$

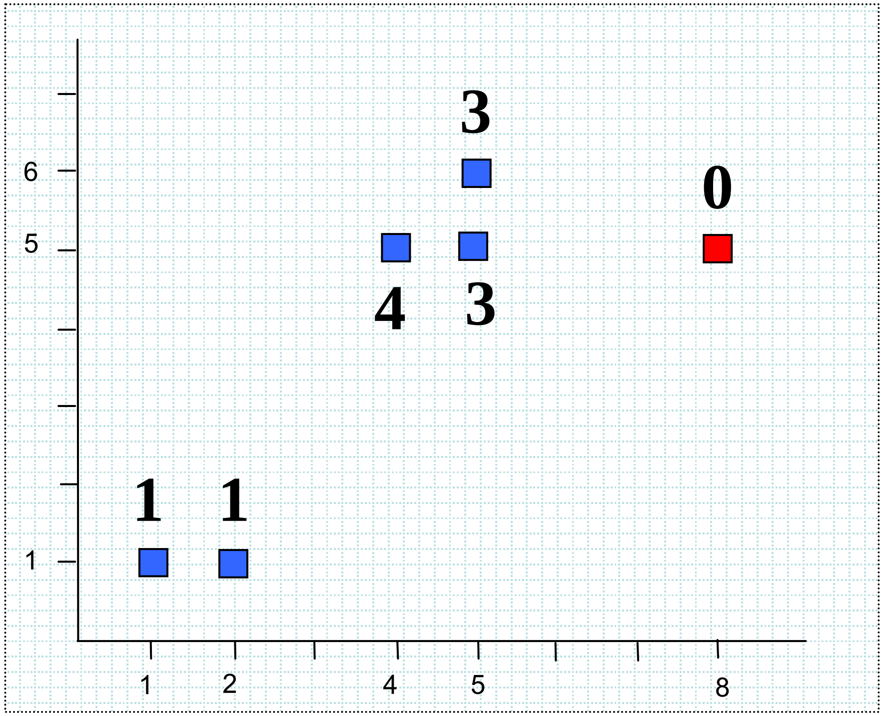


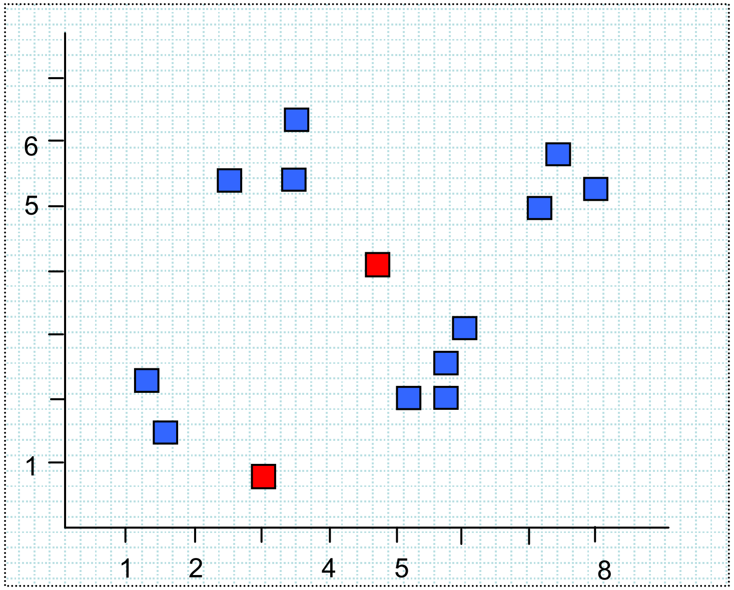
Example of FA and FR

$k = 2$

T	False Acceptance	False Rejection
0	0/1	0/5
1	0/1	2/5
2	0/1	2/5
3	0/1	4/5
4	0/1	5/5
5	0/1	5/5
6	0/1	5/5

Detected as outlier with different threshold values (*T*)





6
5
1
1
2
4
5
8

Experiments

Measures

- False acceptance (FA):
  - Number of outliers that are not detected.
- False rejection (FR):
  - Number of good points wrongly classified as outlier.
- Half total error rate:
  - HTER = (FR+FA) / 2

Comparison of graph-based methods

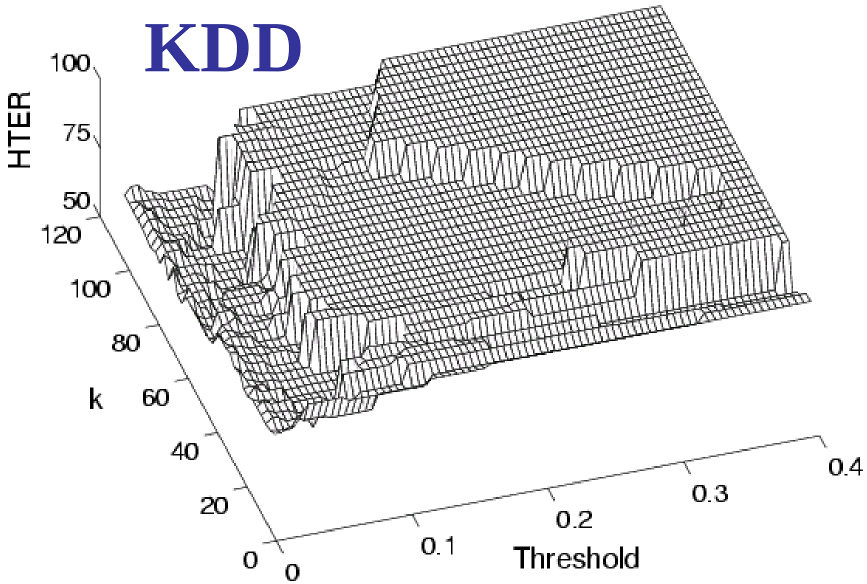
Name	N	d	Outliers
HR [12]	47	2	2
KDD [9]	60318	3	486
NHL1 [8]	681	3	2
NHL2 [8]	731	3	1
synthetic	5165	2	165

Method	synthetic	KDD	HR	NHL1	NHL2
MkNN [1]	50.0 (13)	77.0 (1)	25.0 (5)	25.0 (29)	44.4 (28)
ODIN	9.0 (190,26)	49.6 (1,2)	**0.0** (7, 1)	**0.0** (87, 9)	**0.0** (36, 2)
MeanDIST	**4.9** (21, 0.05)	49.6 (232, 0.19)	30.0 (1, 0.15)	16.7 (20, 0.05)	43.8 (1, 0.57)
KDIST [11]	5.7 (12, 0.06)	**48.6** (72, 0.40)	30.0 (1, 0.15)	30.0 (1, 0.02)	41.7 (7, 0.75)

Difficulty of parameter setup

MeanDIST:

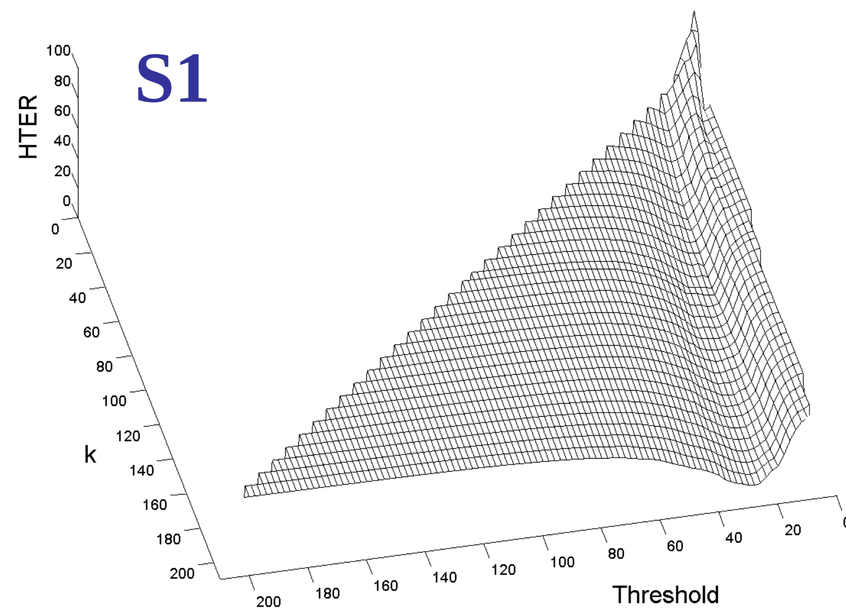
KDD



Value of *k* is not important as long as threshold below 0.1.

ODIN:

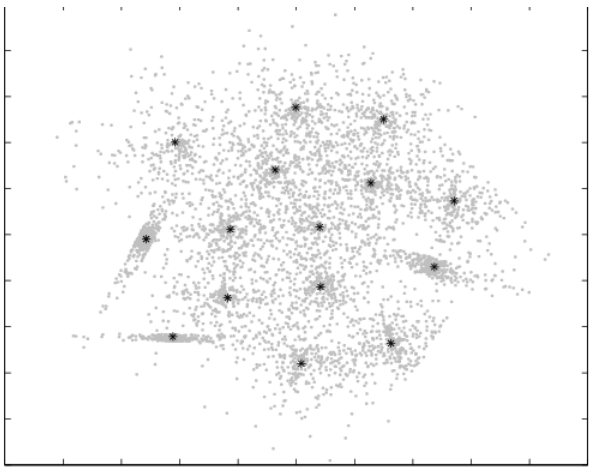
S1



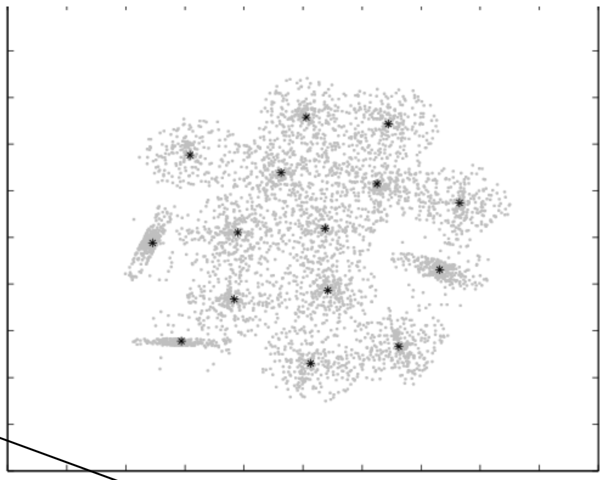
A clear valley in error surface between 20-50.

Improved k-means using outlier removal

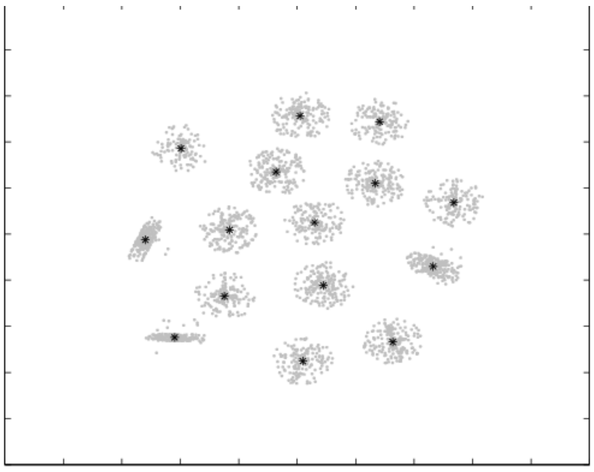
Original



After 40 iterations



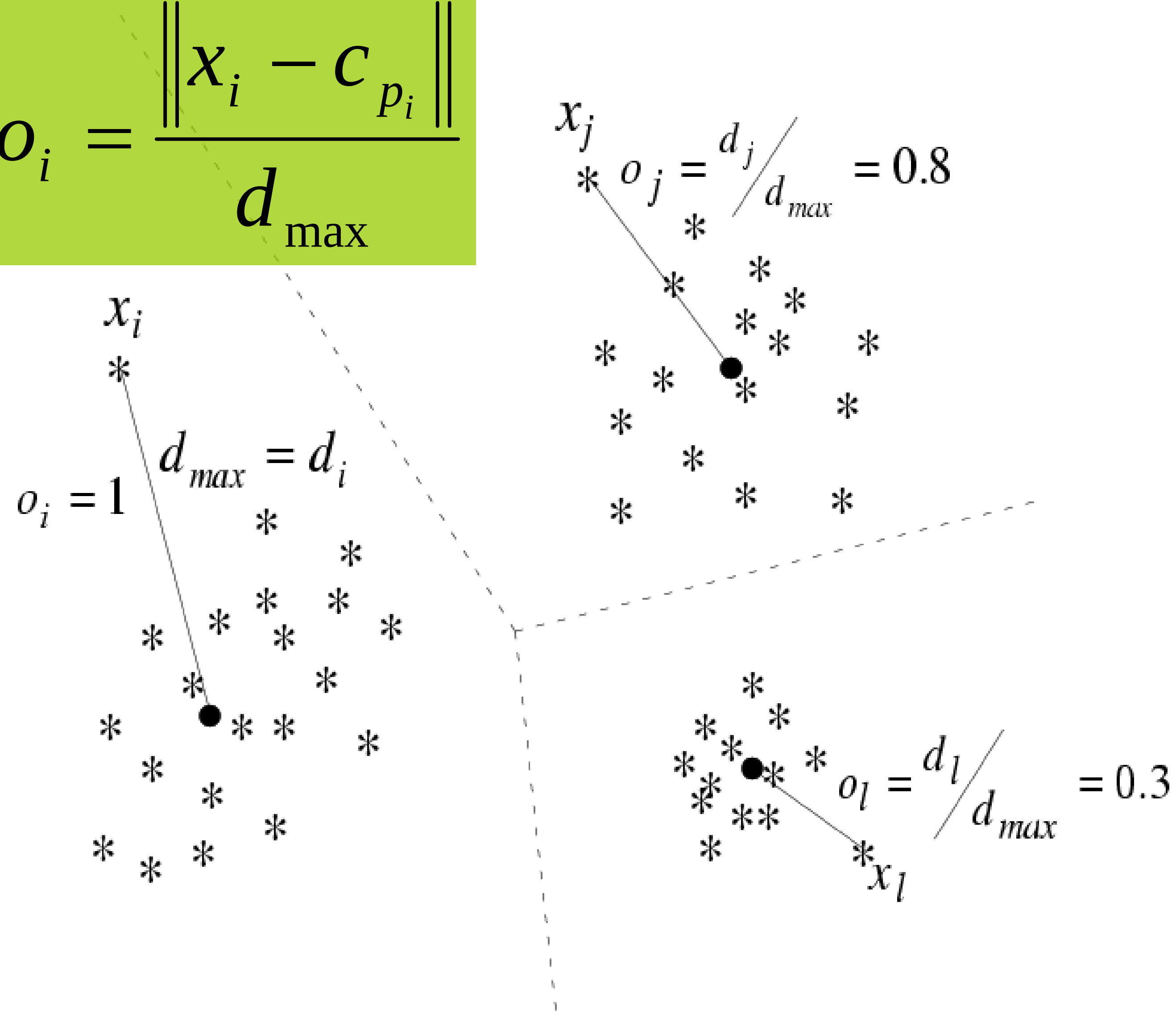
After 70 iterations



At each step, remove most diverging data objects and construct new clustering.

Example of removal factor

$$o_i = \frac{\left\| x_i - c_{p_i} \right\|}{d_{\max}}$$



CERES algorithm

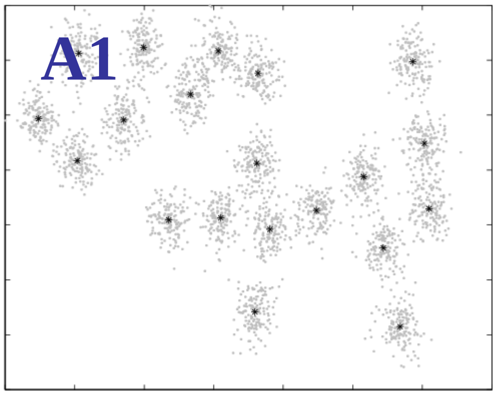
[Hautamäki et al., SCIA 2005]

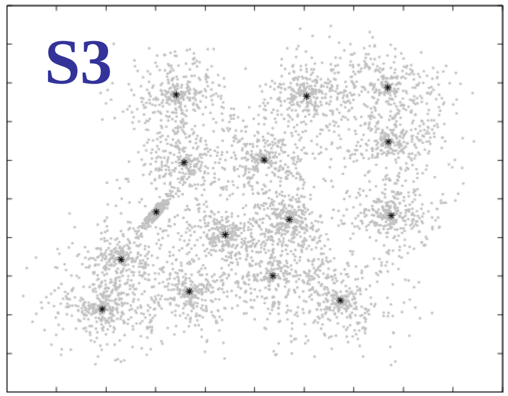
Algorithm 1 CERES(I, T)

$C \leftarrow$ Initialize codebook
for $j \leftarrow 1, \ldots, I$ **do**
  $d_{\max} \leftarrow \max_i\{\|\vec{x}_i - \vec{c}_{p_i}\|\}$
  for $i \leftarrow 1, \ldots, N$ **do**
    $o_i = \|\vec{x}_i - \vec{c}_{p_i}\|/d_{\max}$
    if $o_i > T$ **then**
      $X \leftarrow X \setminus \{\vec{x}_i\}$
    end if
  end for
  $(C, P) \leftarrow$ K-means(X, C)
end for

Experiments

Artificial data sets





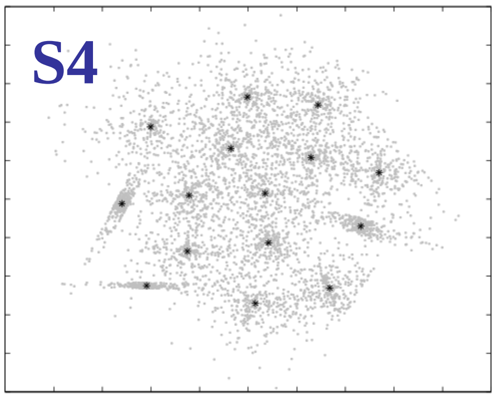
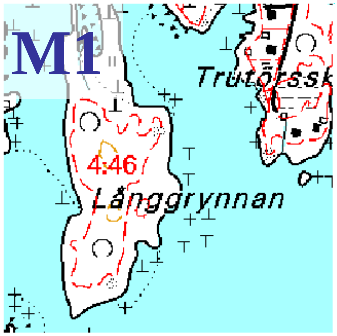
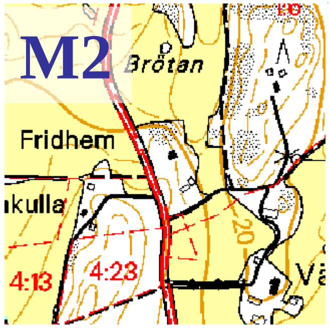
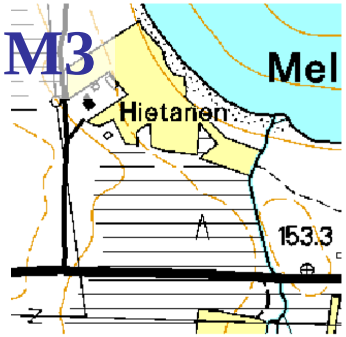


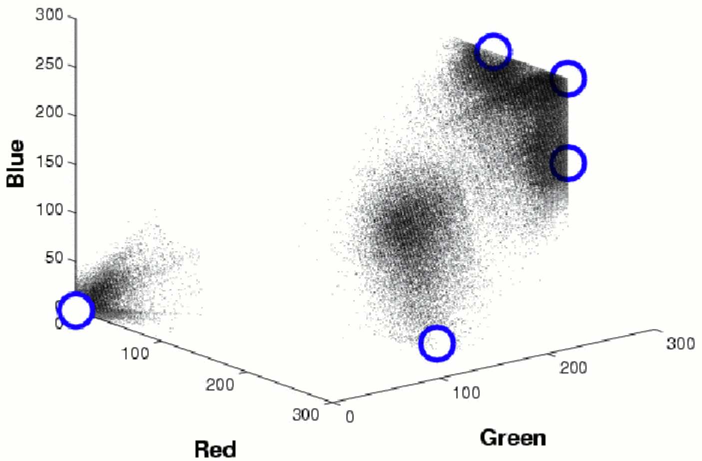
Image data sets







Plot of M2



Comparison

Algorithm	A1	S3	S4	M1	M2	M3
K-means	60	5719	7100	47	32	26
EM	525	3586	3507	46	49	35
CERES	56	3329	2813	45	13	23

Literature

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6. V. Hautamäki, S. Cherednichenko, I. Kärkkäinen, T. Kinnunen and P. Fränti, Improving K-Means by Outlier Removal, In *Proc. 14th Scand. Conf. on Image Analysis* (SCIA'2005), 978-987, Joensuu, Finland, June, 2005.
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