Anomaly & Outliers Detection

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What is an Outlier?

Definition of Hawkins [Hawkins 1980]:

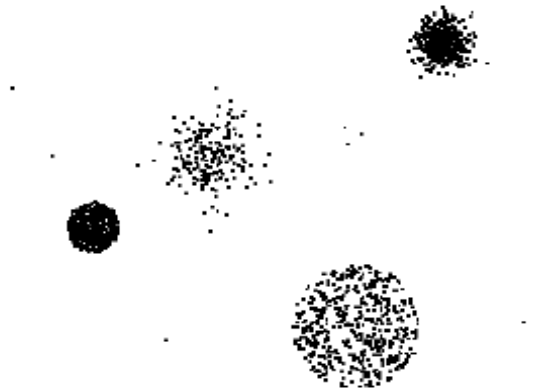
- “An outlier is an observation which deviates so much from the other observations as to arouse suspicions that it was generated by a different mechanism”

Statistics-based intuition

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

Anomaly/Outlier Detection

- What are anomalies/outliers?
  - The set of data points that are considerably different than the remainder of the data
- Natural implication is that anomalies are relatively rare
  - One in a thousand occurs often if you have lots of data
  - Context is important, e.g., freezing temps in July
- Can be important or a nuisance
  - 10 foot tall 2 years old
  - Unusually high blood pressure



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

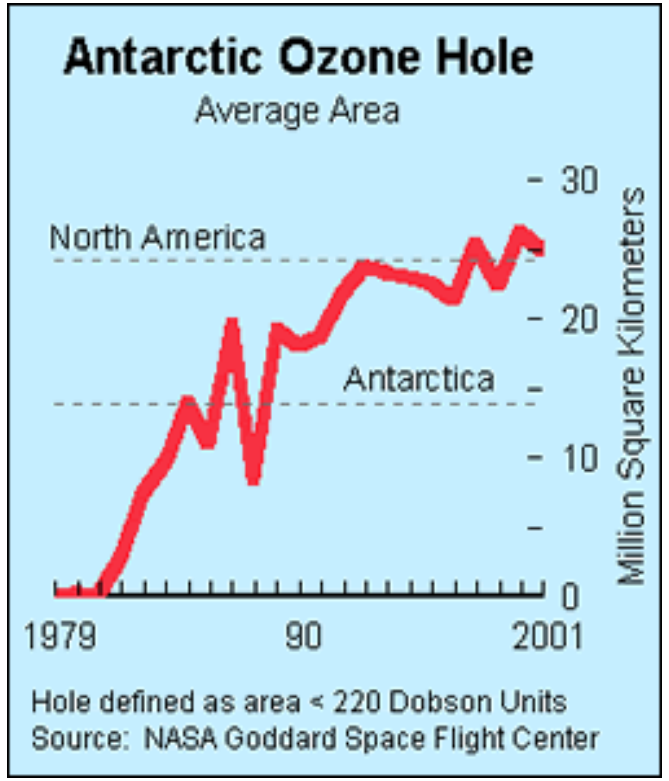
Importance of Anomaly Detection

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!



Causes of Anomalies

- Data from different classes
  - Measuring the weights of oranges, but a few grapefruit are mixed in
- Natural variation
  - Unusually tall people
- Data errors
  - 200 pound 2 year old

Distinction Between Noise and Anomalies

- Noise is erroneous, perhaps random, values or contaminating objects
  - Weight recorded incorrectly
  - Grapefruit mixed in with the oranges

- Noise doesn’t necessarily produce unusual values or objects
- Noise is not interesting
- Anomalies may be interesting if they are not a result of noise
- Noise and anomalies are related but distinct concepts

General Issues: Number of Attributes

- Many anomalies are defined in terms of a single attribute
  - Height
  - Shape
  - Color
- Can be hard to find an anomaly using all attributes
  - Noisy or irrelevant attributes
  - Object is only anomalous with respect to some attributes
- However, an object may not be anomalous in any one attribute

General Issues: Anomaly Scoring

- Many anomaly detection techniques provide only a binary categorization
  - An object is an anomaly, or it isn't
  - This is especially true of classification-based approaches
- Other approaches assign a score to all points
  - This score measures the degree to which an object is an anomaly
  - This allows objects to be ranked
- In the end, you often need a binary decision
  - Should this credit card transaction be flagged?
  - Still useful to have a score
- How many anomalies are there?

Other Issues for Anomaly Detection

- Find all anomalies at once or one at a time
  - Swamping
  - Masking
- Evaluation
  - How do you measure performance?
  - Supervised vs. unsupervised situations
- Efficiency
- Context
  - Professional basketball team

Variants of Anomaly Detection Problems

- Given a data set D, find all data points $\mathbf{x} \in$ D with anomaly scores greater than some threshold *t*
- Given a data set D, find all data points $\mathbf{x} \in$ D having the top-*n* largest anomaly scores
- Given a data set D, containing mostly normal (but unlabeled) data points, and a test point **x**, compute the anomaly score of **x** with respect to D

Model-Based Anomaly Detection

Build a model for the data and see

- Unsupervised
  - Anomalies are those points that don’t fit well
  - Anomalies are those points that distort the model
  - Examples:
    - Statistical distribution
    - Clusters
    - Regression
- Supervised
  - Anomalies are regarded as a rare class
  - Need to have training data

Machine Learning for Outlier Detection

- If the ground truth of anomalies is available we can prepare a classification problem to unveil outliers.
- As classifiers we can use all the available machine learning approaches: Ensembles, SVM, DNN.
- The problem is that the dataset would be very unbalanced
- Thus, ad-hoc formulations/implementation should be adopted.

Additional Anomaly Detection Techniques

- **Proximity-based**
  - Anomalies are points far away from other points
  - Can detect this graphically in some cases
- **Density-based**
  - Low density points are outliers
- **Pattern matching**
  - Create profiles or templates of atypical but important events or objects
  - Algorithms to detect these patterns are usually simple and efficient

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
- Notes
  - 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

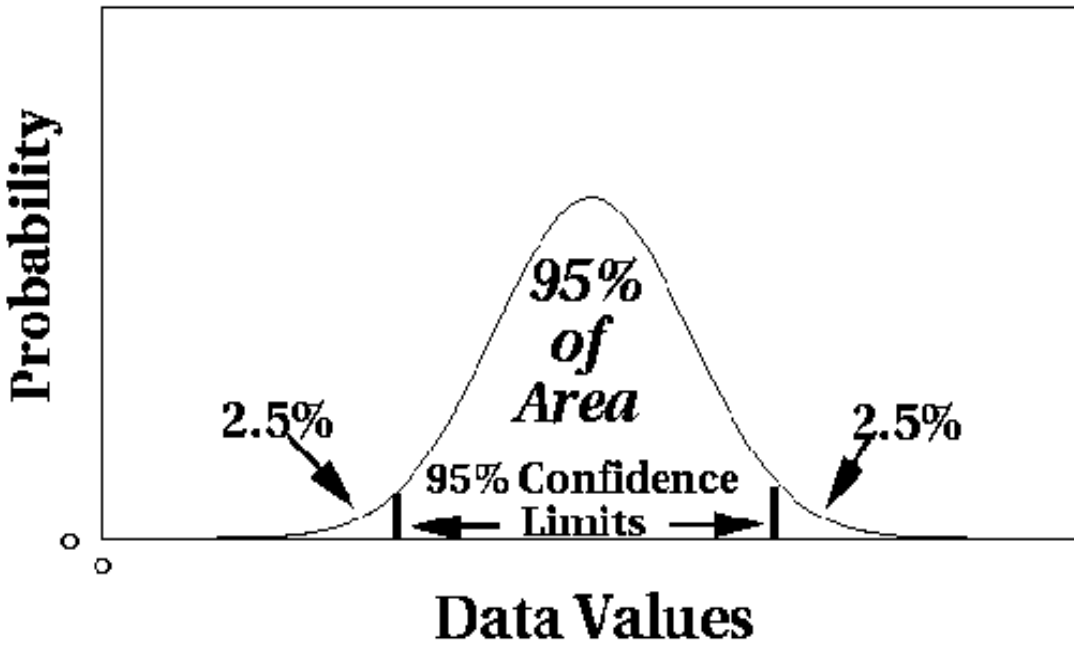
Statistical Approaches

Statistical Approaches

Probabilistic definition of an outlier: An outlier is an object that has a low probability with respect to a probability distribution model of the data.

- Usually assume a parametric model describing the distribution of the data (e.g., normal distribution)
- Apply a statistical test that depends on
  - Data distribution
  - Parameters of distribution (e.g., mean, variance)
  - Number of expected outliers (confidence limit)
- Issues
  - Identifying the distribution of a data set
    - Heavy tailed distribution
  - Number of attributes
  - Is the data a mixture of distributions?

Normal Distributions



One-dimensional Gaussian

The distance of a value x from the center of a N(0,1) distribution is directly related to the prob(x)

- Low probability for values in the tails
- **A data point x is an Outlier if $|x| > c$ and $prob(|x|>c)=\alpha$**

Statistical-based – 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:

$$G = \frac{\max\left|X - \overline{X}\right|}{s}$$

mean

std dev

- Reject H_0 if:

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

alpha significance

t – Student's distribution

Statistical-based – Likelihood Approach

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

Statistical-based – Likelihood Approach

- 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:

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

$$LL_t(D) = |M_t| \log(1-\lambda) + \sum_{x_i \in M_t} \log P_{M_t}(x_i) + |A_t| \log \lambda + \sum_{x_i \in A_t} \log P_{A_t}(x_i)$$

Strengths/Weaknesses of Statistical Approaches

Pros

- Firm mathematical foundation
- Can be very efficient
- Good results if distribution is known

Cons

- In many cases, data distribution may not be known
- For high dimensional data, it may be difficult to estimate the true distribution
- Anomalies can distort the parameters of the distribution
  - Mean and standard deviation are very sensitive to outliers

Distance-based Approaches

Distance-based Approaches

- 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

Distance-based Approaches

- Several different techniques
- **Approach 1:** The outlier score of an object is the distance to its *k*-th nearest neighbor
- **Approach 2:** An object is an outlier if a specified fraction of the objects is more than a specified distance away (Knorr, Ng 1998)

Distance-based Approaches

Definition of Outlier:

Proximity-based definition of outlier using distance to k-nearest neighbor

Anomaly score function:

Given a data instance x from a dataset D and a value k

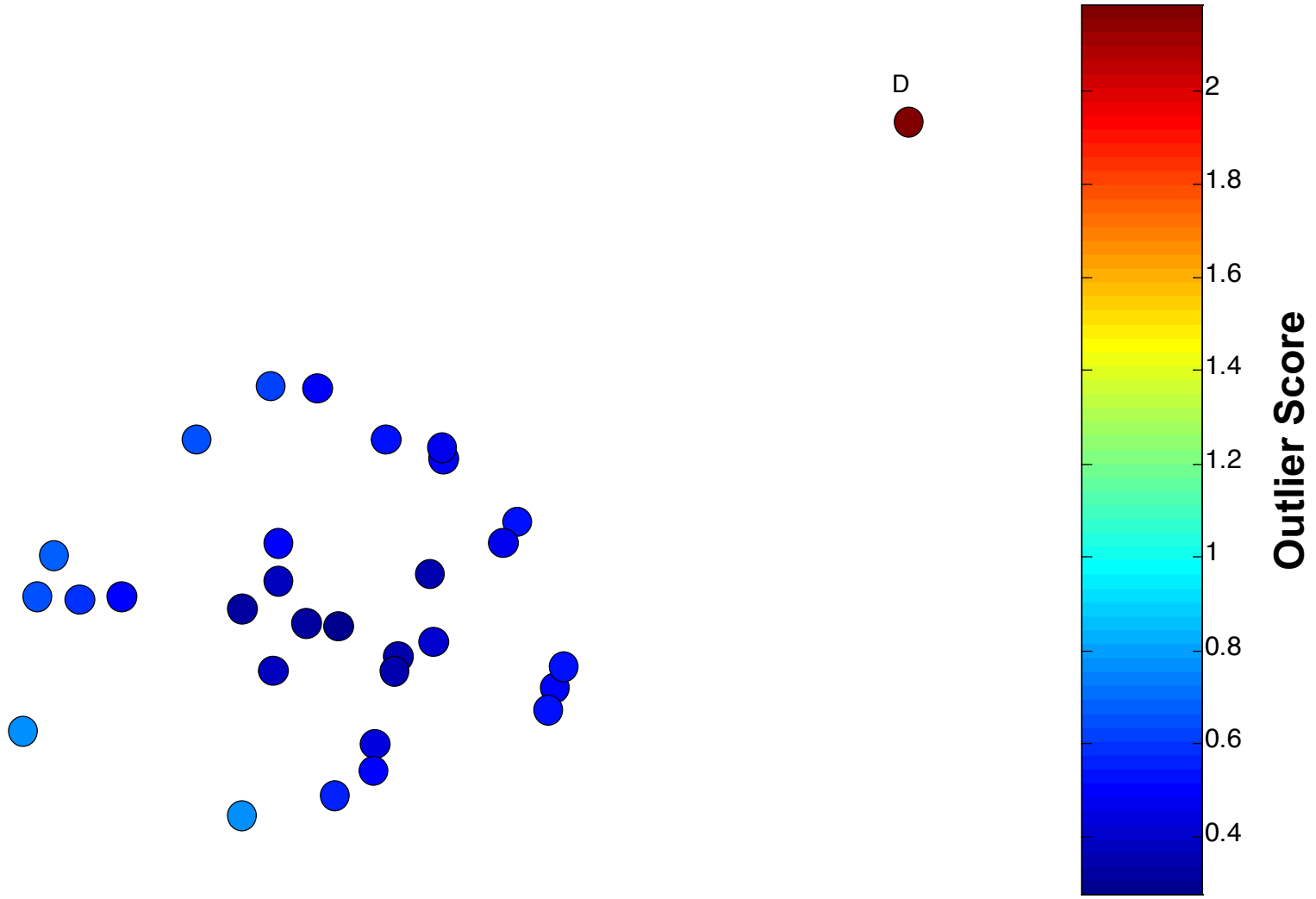
- f(x) = Distance between x and its k-nearest neighbor
- f(x) = Average distance between x and its k-nearest neighbors

How does the approach work? (in general):

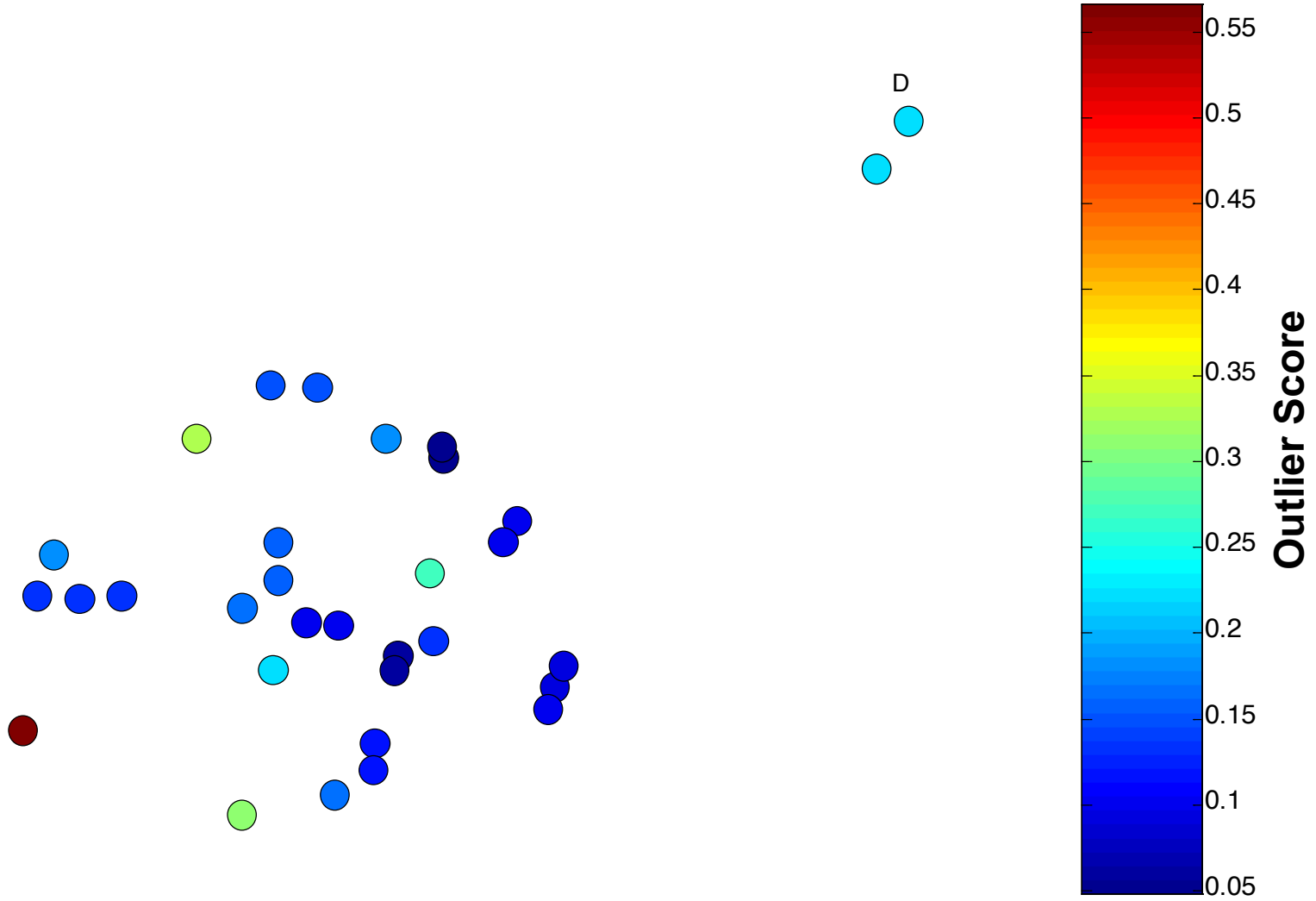
1. Calculate the anomaly score, f(x), for each data point in the dataset.
2. Use a threshold t on this score to determine outliers.

x is an outlier iff f(x) > t

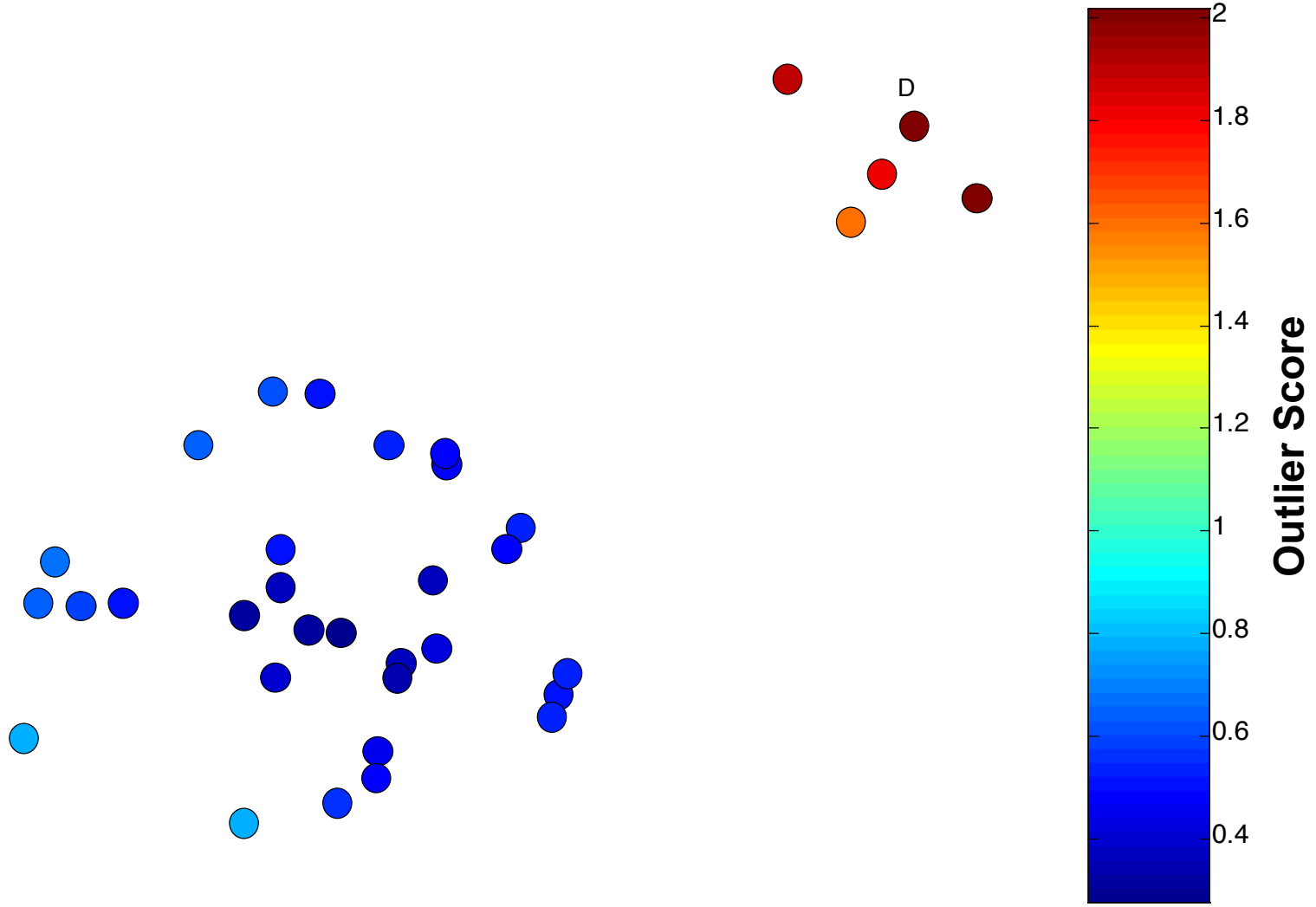
One Nearest Neighbor - One Outlier



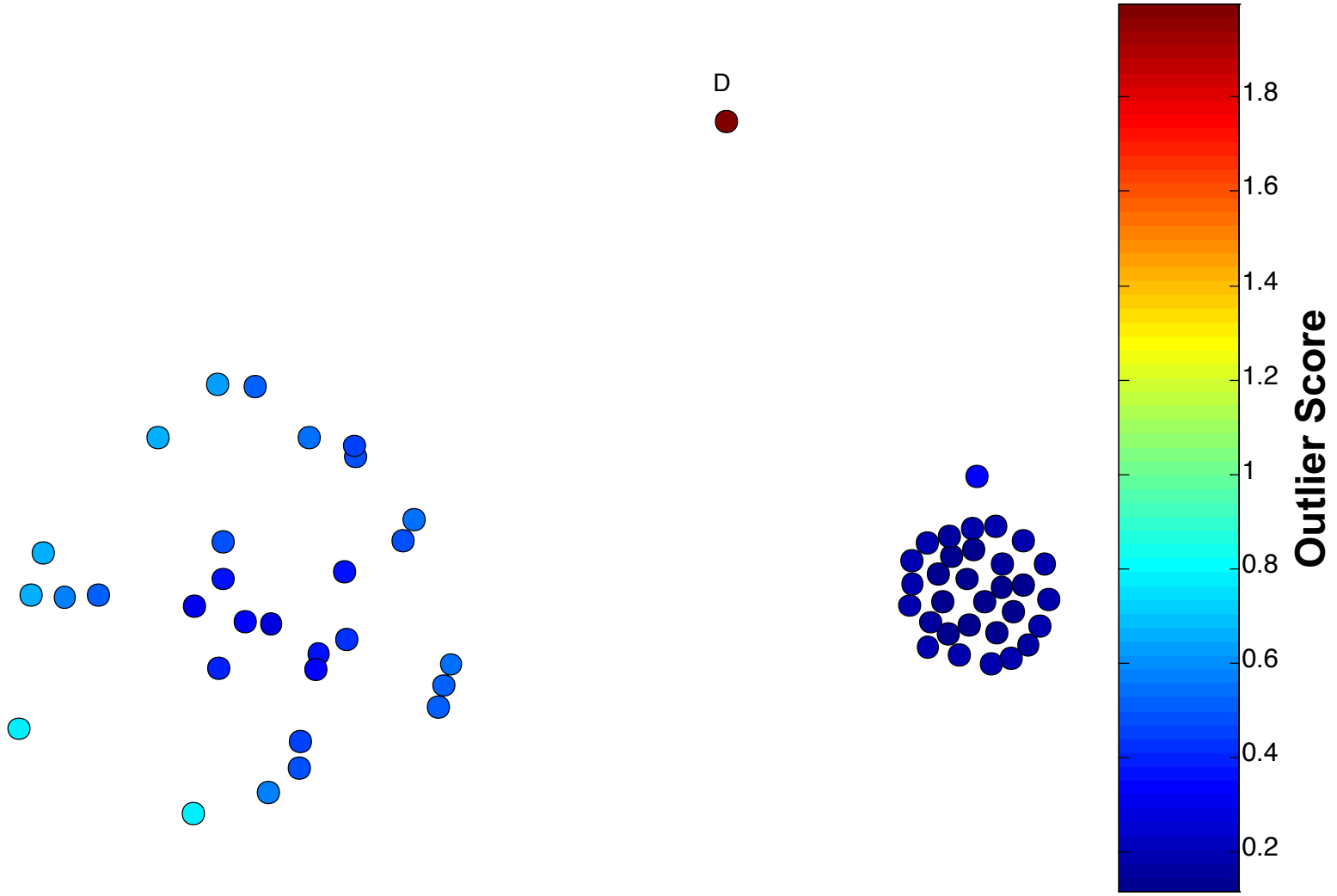
One Nearest Neighbor - Two Outliers



Five Nearest Neighbors - Small Cluster



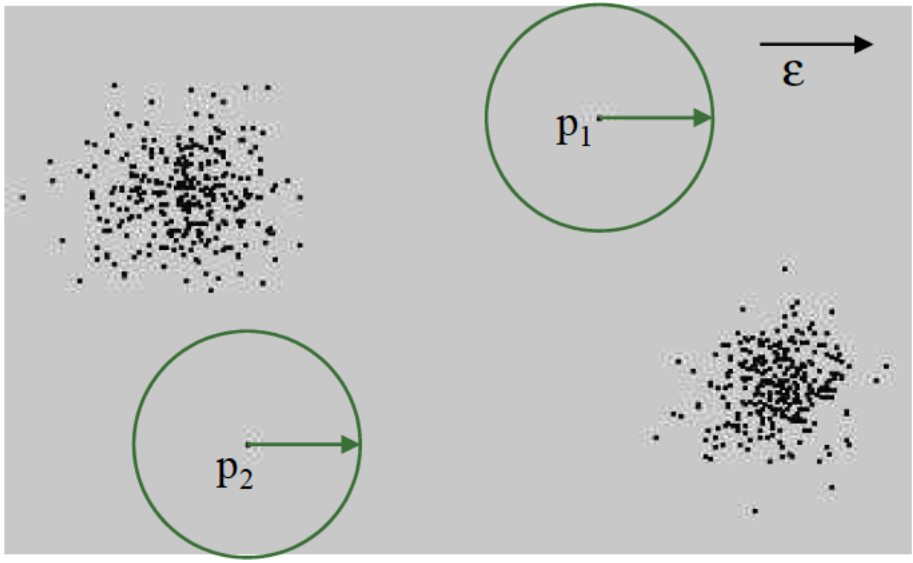
Five Nearest Neighbors - Differing Density



Distance-based Approaches

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, i.e., it is close to few points*



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

range-query with radius ε

General approach for computation

- **Efficient computation:** Nested loop algorithm
  - For any object o, calculate its distance from other objects, and count the # of other objects in the ε-neighborhood.
  - If $\pi \cdot n$ other objects are within ε distance, terminate the inner loop
  - Otherwise, o is a DB(ε, π) outlier
- **Efficiency**: Actually, CPU time is not $O(n^2)$ but linear to the data set size since for most non-outlier objects, the inner loop terminates early

Strengths/Weaknesses of Distance-Based Approaches

Pros

- Simple

Cons

- Expensive – $O(n^2)$
- Sensitive to parameters
- Sensitive to variations in density
- Distance becomes less meaningful in high-dimensional space

Density-based Approaches

Density-based Approaches

- 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 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

Density-based Approaches

- **Density-based Outlier:** The outlier score of an object is the inverse of the density around the object.
  - Can be defined in terms of the *k* nearest neighbors
  - One definition: Inverse of distance to *k*th neighbor
  - Another definition: Inverse of the average distance to *k* neighbors
  - DBSCAN definition

- If there are regions of different density, this approach can have problems

Local Outlier Factor (LOF) [Breunig et al. 1999], [Breunig et al. 2000]

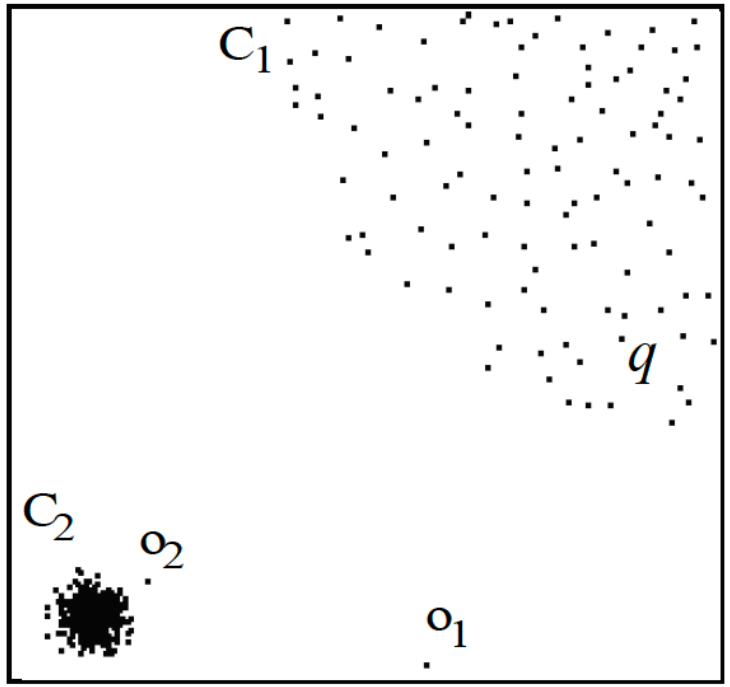
Motivation:

- 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 C_1 (e.g. q) are larger than the kNN-distance of o_2

Solution: consider relative density



Relative Density

- Consider the density of a point relative to that of its k nearest neighbors

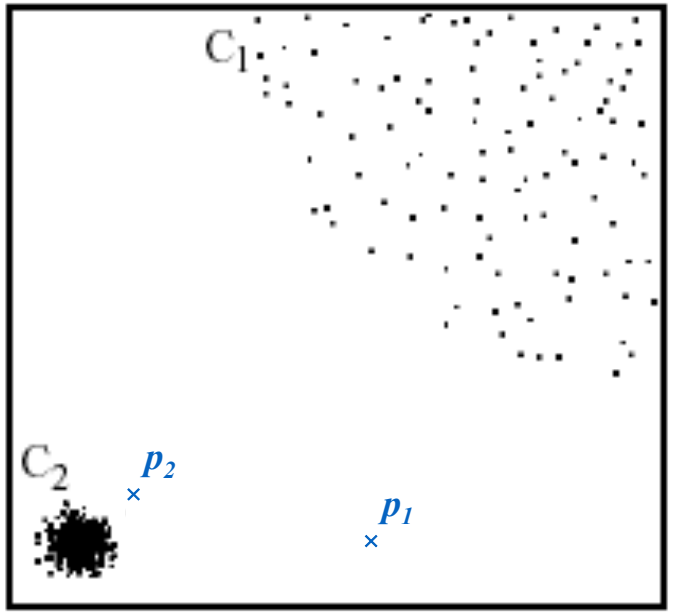
$$average\ relative\ density(\mathbf{x}, k) = \frac{density(\mathbf{x}, k)}{\sum_{\mathbf{y} \in N(\mathbf{x},k)} density(\mathbf{y}, k)/|N(\mathbf{x}, k)|}. \quad (10.7)$$

Algorithm 10.2 Relative density outlier score algorithm.

1: {k is the number of nearest neighbors}
2: **for all** objects $\mathbf{x}$ **do**
3: Determine $N(\mathbf{x}, k)$, the k-nearest neighbors of $\mathbf{x}$.
4: Determine $density(\mathbf{x}, k)$, the density of $\mathbf{x}$, using its nearest neighbors, i.e., the objects in $N(\mathbf{x}, k)$.
5: **end for**
6: **for all** objects $\mathbf{x}$ **do**
7: Set the $outlier\ score(\mathbf{x}, k) = average\ relative\ density(\mathbf{x}, k)$ from Equation 10.7.
8: **end for**

Local Outlier Factor (LOF)

- For each point, compute the density of its local neighborhood
- Compute local outlier factor (LOF) of a sample *p* as the average of the ratios of the density of sample *p* and the density of its nearest neighbors
- Outliers are points with largest LOF value

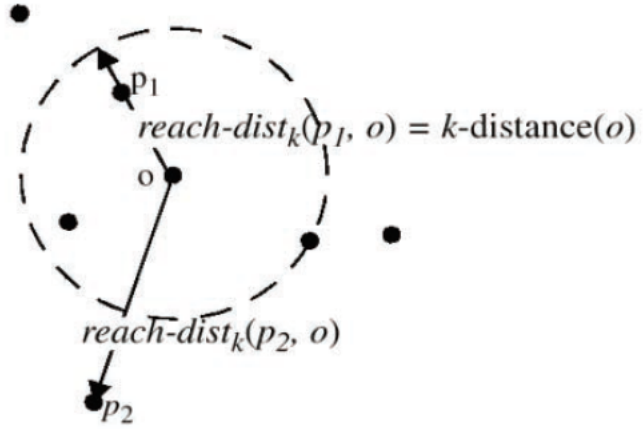


In the NN approach, p_2 is not considered as outlier, while LOF approach find both p_1 and p_2 as outliers

Local Outlier Factor (LOF)

- Reachability distance
  - Introduces a smoothing factor

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



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

$$lrd_k(p) = 1 \Big/ \left(\frac{\sum_{o \in kNN(p)} reach-dist_k(p,o)}{Card(kNN(p))} \right)$$

- Local outlier factor (LOF) of point *p*
  - Average ratio of *lrds* of neighbors of *p* and *lrd* of *p*

$$LOF_k(p) = \frac{\sum_{o \in kNN(p)} \frac{lrd_k(o)}{lrd_k(p)}}{Card(kNN(p))}$$

Strengths/Weaknesses of Density-Based Approaches

Pros

- Simple

Cons

- Expensive – $O(n^2)$
- Sensitive to parameters
- Density becomes less meaningful in high-dimensional space

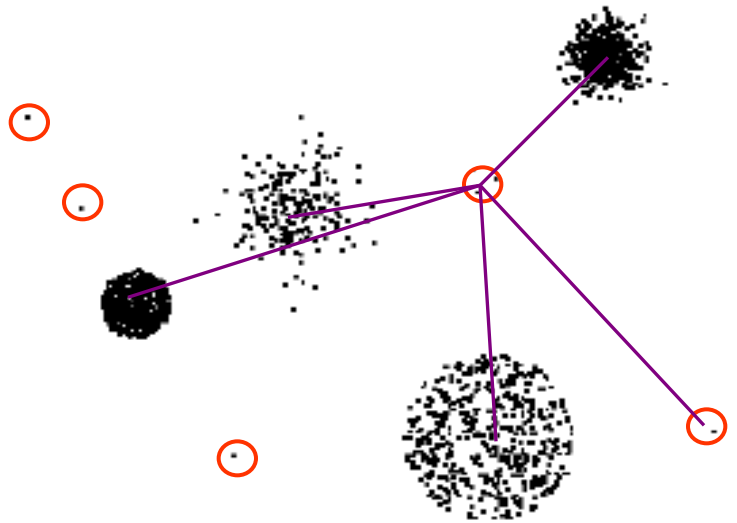
Clustering-based Approaches

Clustering and Anomaly Detection

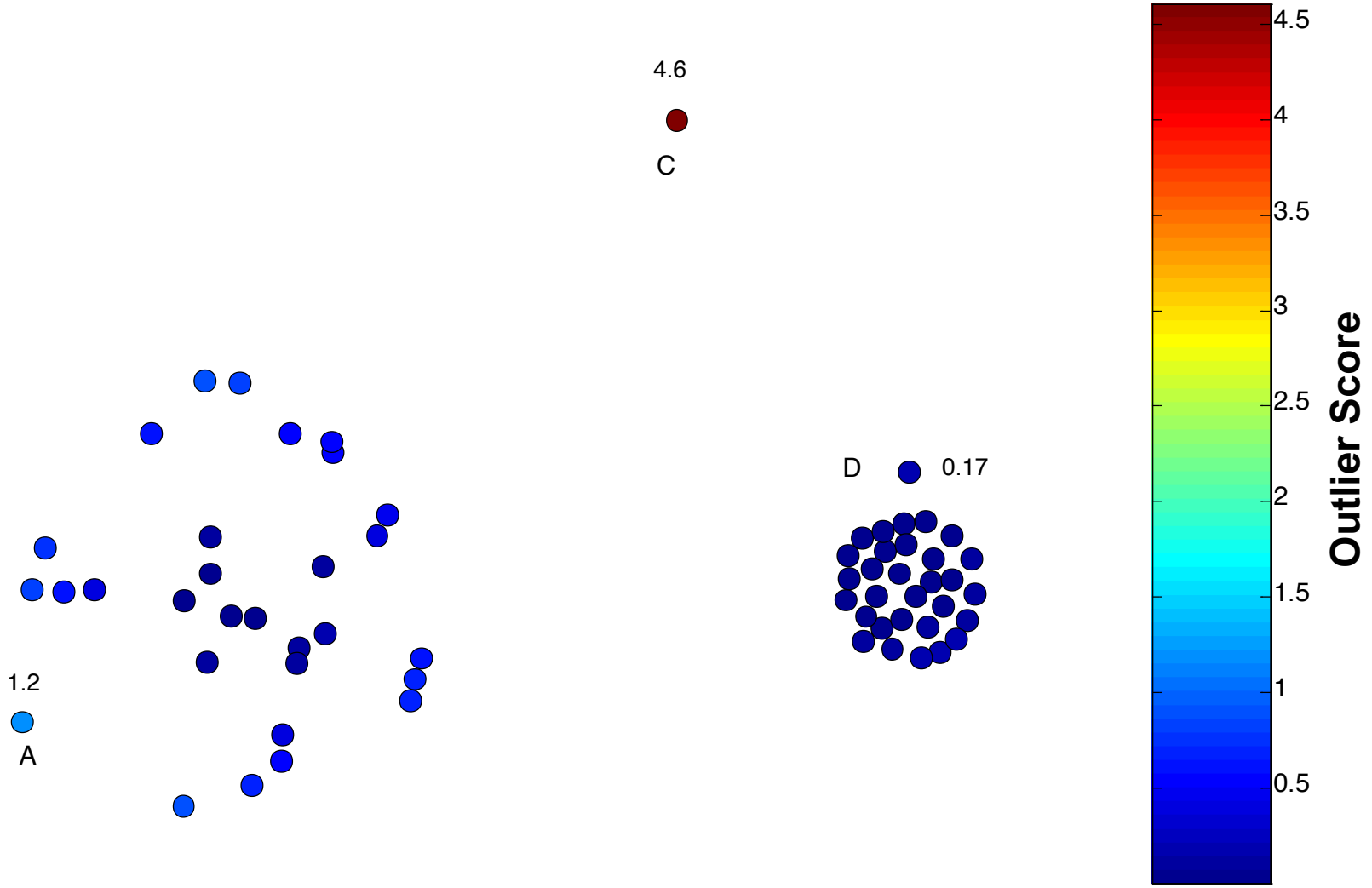
- Are outliers just a side product of some clustering algorithms?
  - Many clustering algorithms do not assign all points to clusters but account for noise objects (e.g. DBSCAN, OPTICS)
  - Look for outliers by applying one algorithm and retrieve the noise set
- Problem:
  - Clustering algorithms are 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

Clustering-Based Approaches

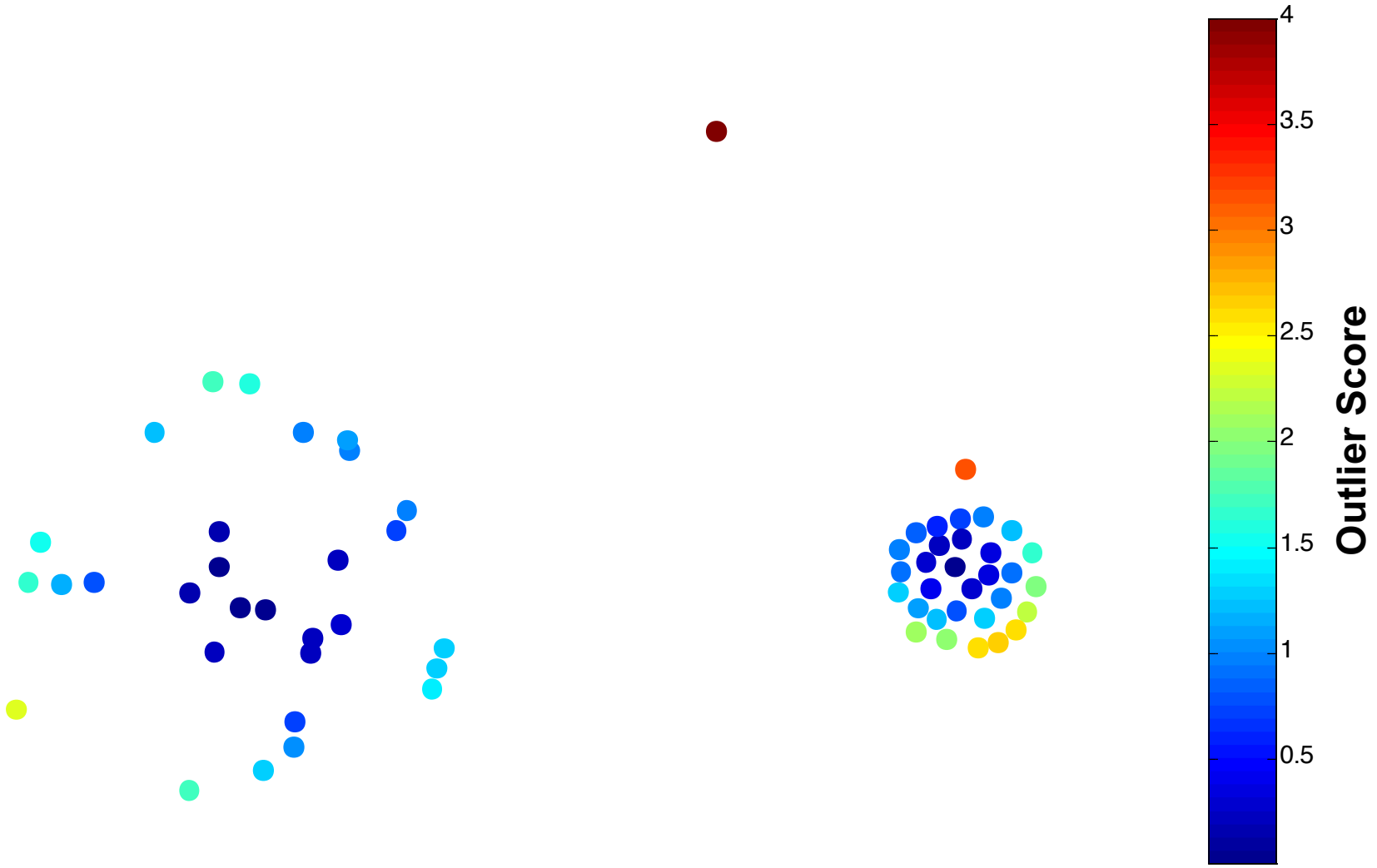
- **Clustering-based Outlier:** An object is a cluster-based outlier if it does not strongly belong to any cluster
  - For prototype-based clusters, an object is an outlier if it is not close enough to a cluster center
  - For density-based clusters, an object is an outlier if its density is too low
  - For graph-based clusters, an object is an outlier if it is not well connected
- Other issues include the impact of outliers on the clusters and the number of clusters



Distance of Points from Closest Centroids



Relative Distance of Points from Closest Centroid



Strengths/Weaknesses of Clustering-Based Approaches

Pros

- Simple
- Many clustering techniques can be used

Cons

- Can be difficult to decide on a clustering technique
- Can be difficult to decide on number of clusters
- Outliers can distort the clusters

Summary

- Different models are based on different assumptions
- 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

References

- Anomaly Detection. Chapter 10. Introduction to Data Mining.