# Anomaly & Outliers Detection

UNIVERSITÀ DI PISA

# What is an Outlier?

- Anomaly is a pattern in the data that does not conform to the expected behaviour (also referred ad outlier/exception)

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

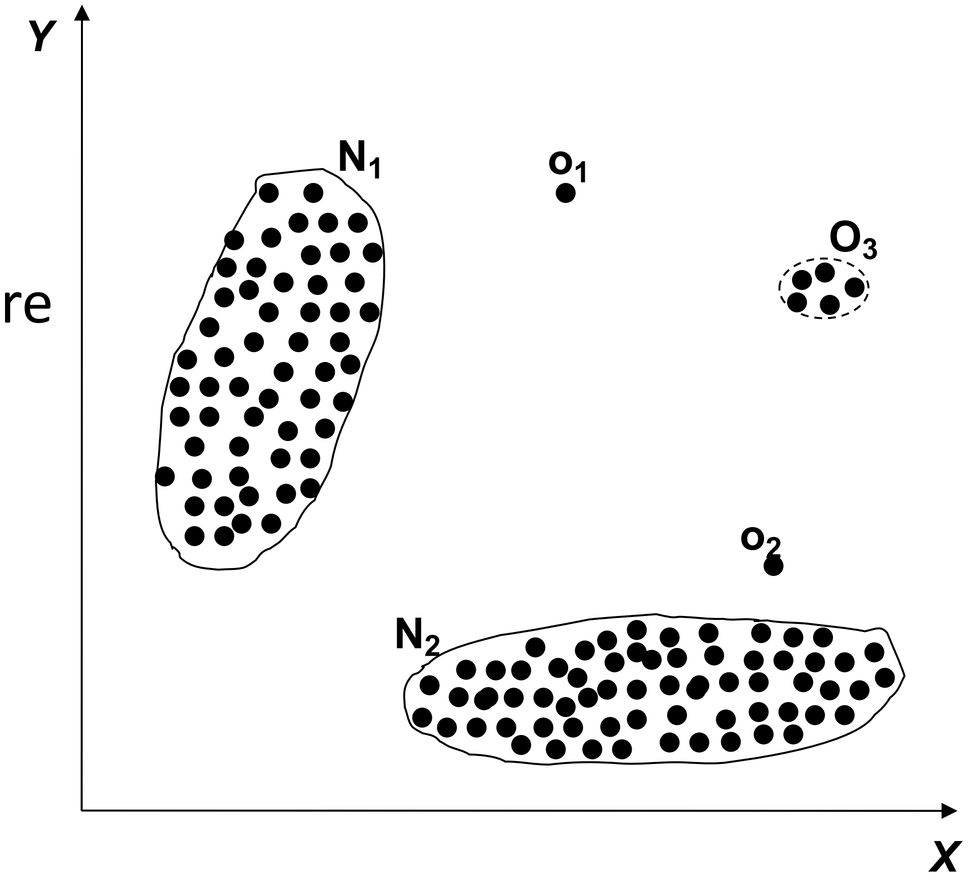
- Normal data objects follow a “generating mechanism”, e.g. some given statistical process
- **Abnormal objects** deviate from this generating mechanism

# 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

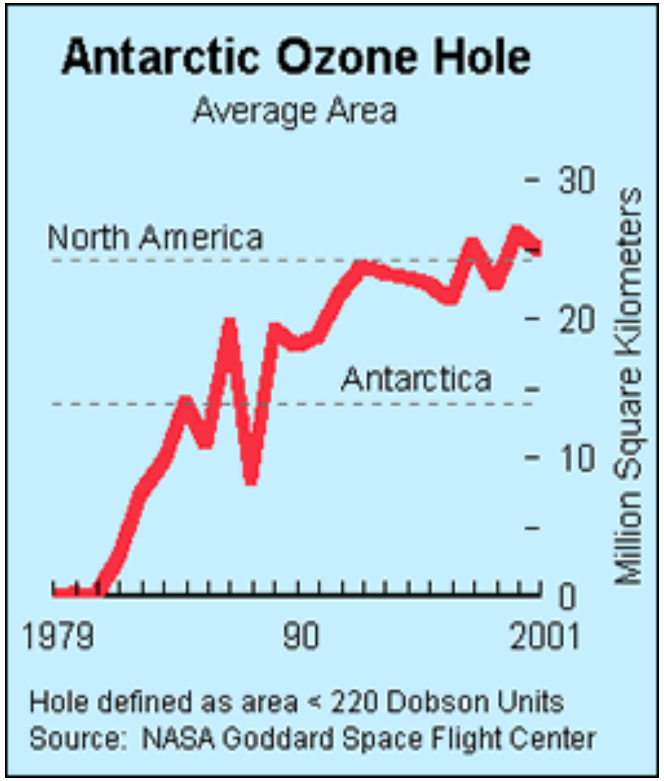
# Importance of Anomaly Detection

## 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/ Data Measurement and Collection 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**: normal objects are classified as outliers
  - **Masking**: the presence of several anomalies masks the presence of all

- **Evaluation**
  - How do you measure performance?
  - Supervised vs. unsupervised situations

- **Efficiency**
  - Classification models – expensive for learning the model and inexpensive to apply the mode
  - Proximity-based approaches – cost of the proximity matrix

- **Context**: global versus local perspective
  - A person is unusually tall w.r.t. the general population but not w.r.t. professional basketball team

# Variants of Anomaly Detection Problems

- Given a data set D, find all data points **x** $\in$ D with anomaly scores greater than some threshold *t*
- Given a data set D, find all data points **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
- Supervised
  - Anomalies are regarded as a rare class
  - Need to have training data

# Machine Learning for Outlier Detection

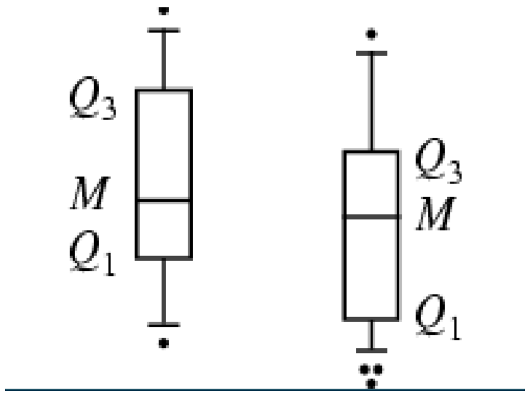
- If the ground truth of anomalies is available we can prepare a classification problem to unveil outliers.
- As classifiers we can use all the available machine learning approaches: Ensembles, SVM, DNN.
- The problem is that the dataset would be very unbalanced
- Thus, ad-hoc formulations/implementation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

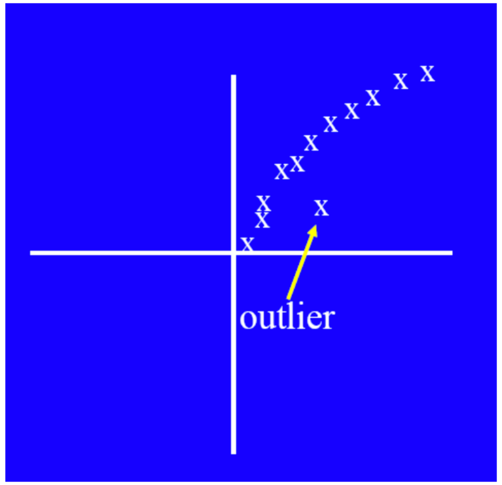
# Additional Anomaly Detection Techniques

- **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

# Graphical Approches

Boxplot (1-D), Scatter plot (2-D)




**Limitation**: It is Time Consuming

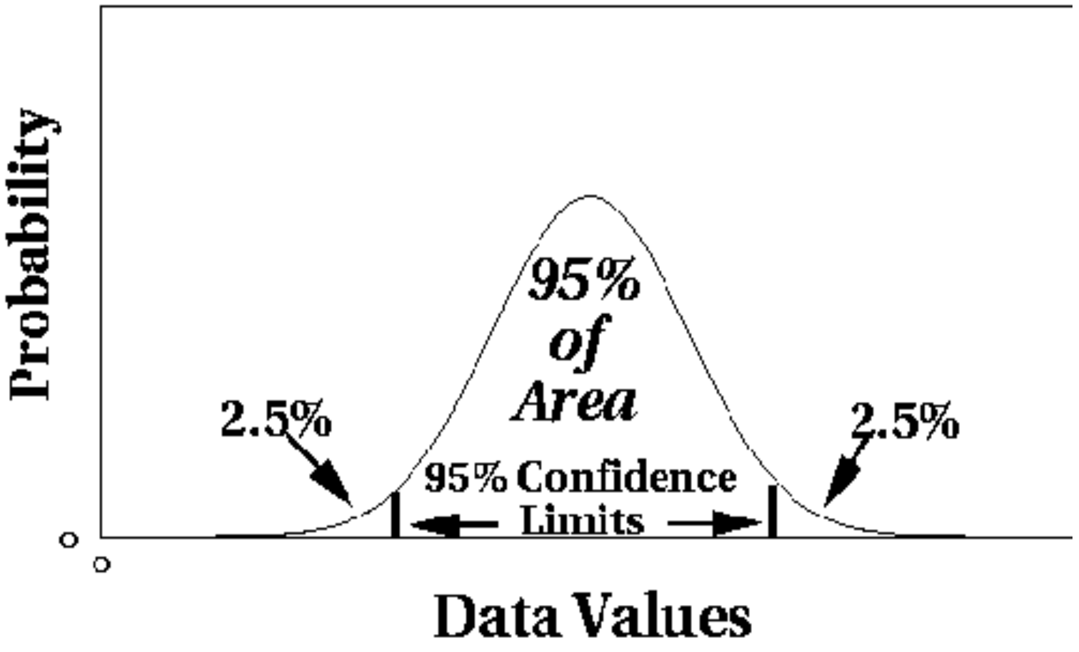
# Statistical Approaches

# 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: most of these approaches are applicable to single 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)=α (when c increas and α decreases)**
- We can apply this method on z-score values
- **α should be specified to use this method**

# Interquartile Range

- Divides data in quartiles
  - Q1: first quartile
  - Q3: third quartile

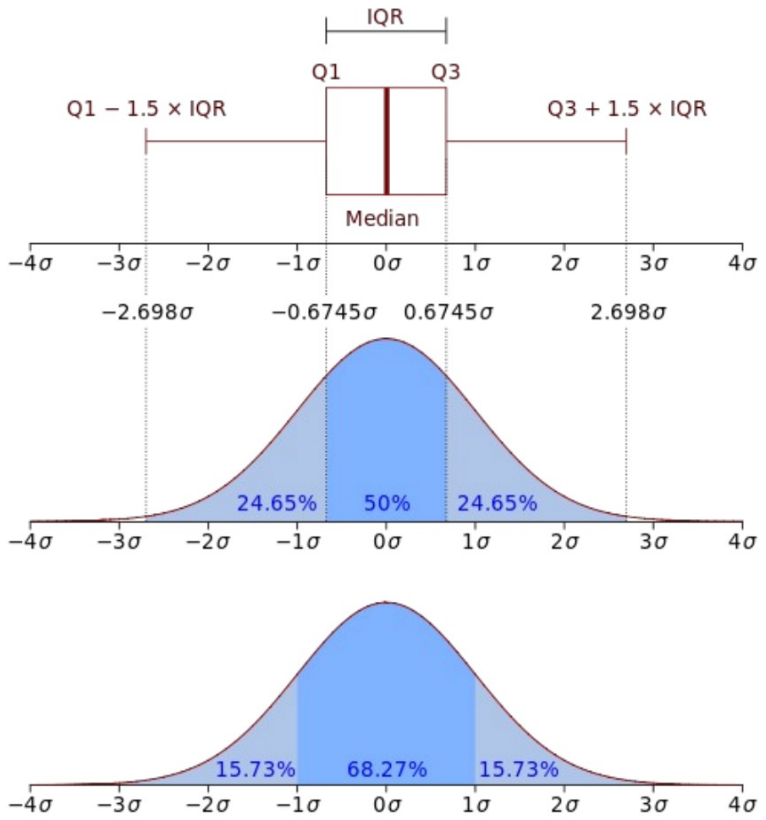
Definitions:

- IQR = Q3-Q1
- **Outlier detection:**
  - **All x values outside** [median-1.5*IQR ; median+1.5*IQR]

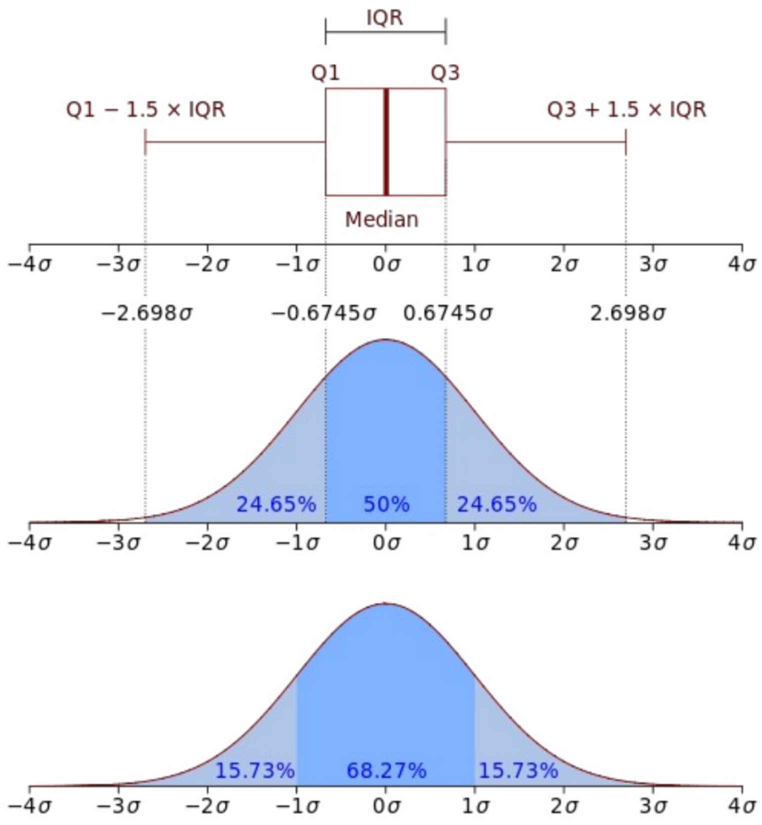
**Example**:

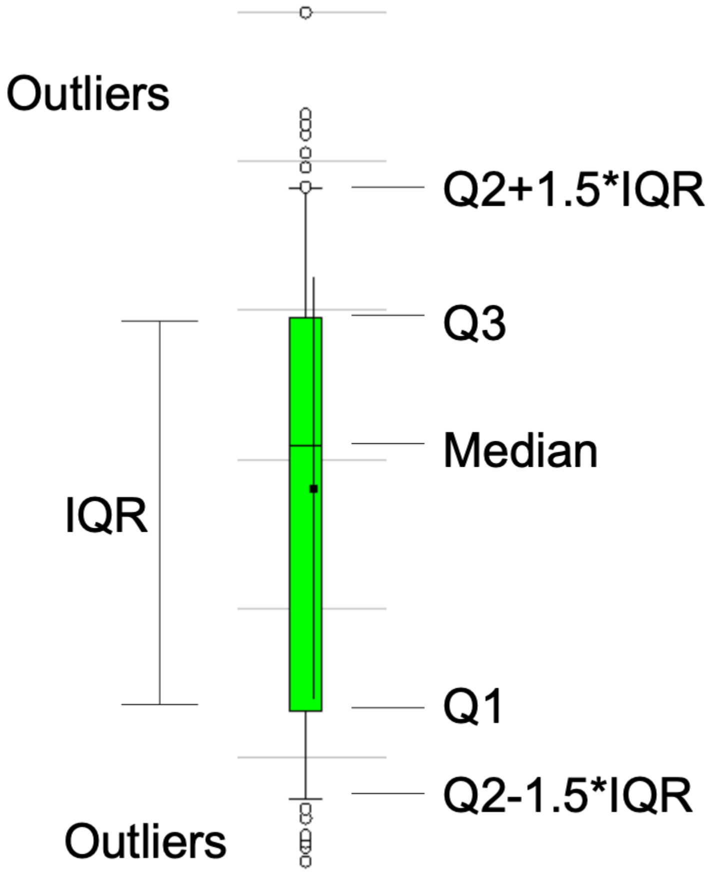
X = 0,1,1,3,3,5,7,42

- **Median= 3**, **Q1=1**, **Q3=7** → **IQR = 6**
- Allowed interval: [3 - 1.5*6 ; 3+1.5*6] = [-6 ; 12]
- Thus, 42 is an outlier



# IQR vs Box Plots



# Median Absolute Deviation (MAD)

- MAD is the median deviation from the median of a sample, i.e.

$$MAD := median_i(X_i - median_j(X_j))$$

- MAD can be used for outlier detection
- all values that are k*MAD away from the median are considered to be outliers
- e.g., k=3

**Example**

**X= 0,1,1,3,5,7,42**

- Median = 3, Deviations: 3,2,2,0,2,4,39 → MAD = 2
- allowed interval: [3-3*2 ; 3+3*2] = [-3;9]
- therefore, 42 is an outlier

# 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:

mean

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

std dev

the z-score of largest magnitude

- Reject H0 at **significance level** α if:

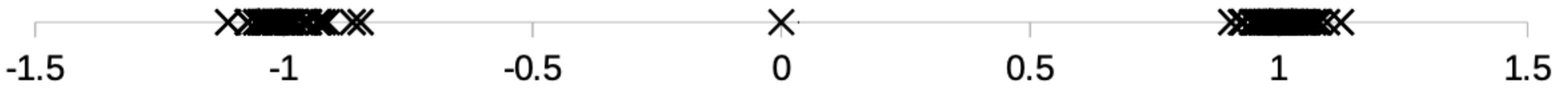
$$G > \frac{(N-1)}{\sqrt{N}} \sqrt{\frac{t^2_{(\alpha/N, N-2)}}{N - 2 + t^2_{(\alpha/N, N-2)}}}$$

**the upper critical value** of the **t-distribution** with N – 2 degrees of freedom and a significance level of α/(2N).

# Outliers vs. Extreme Values

So far, we have looked at extreme values only

- But outliers can occur as non-extremes
- Methods presented until now are able to detect 0 as an outlier?
    - In that case, methods like IQR fails



# 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

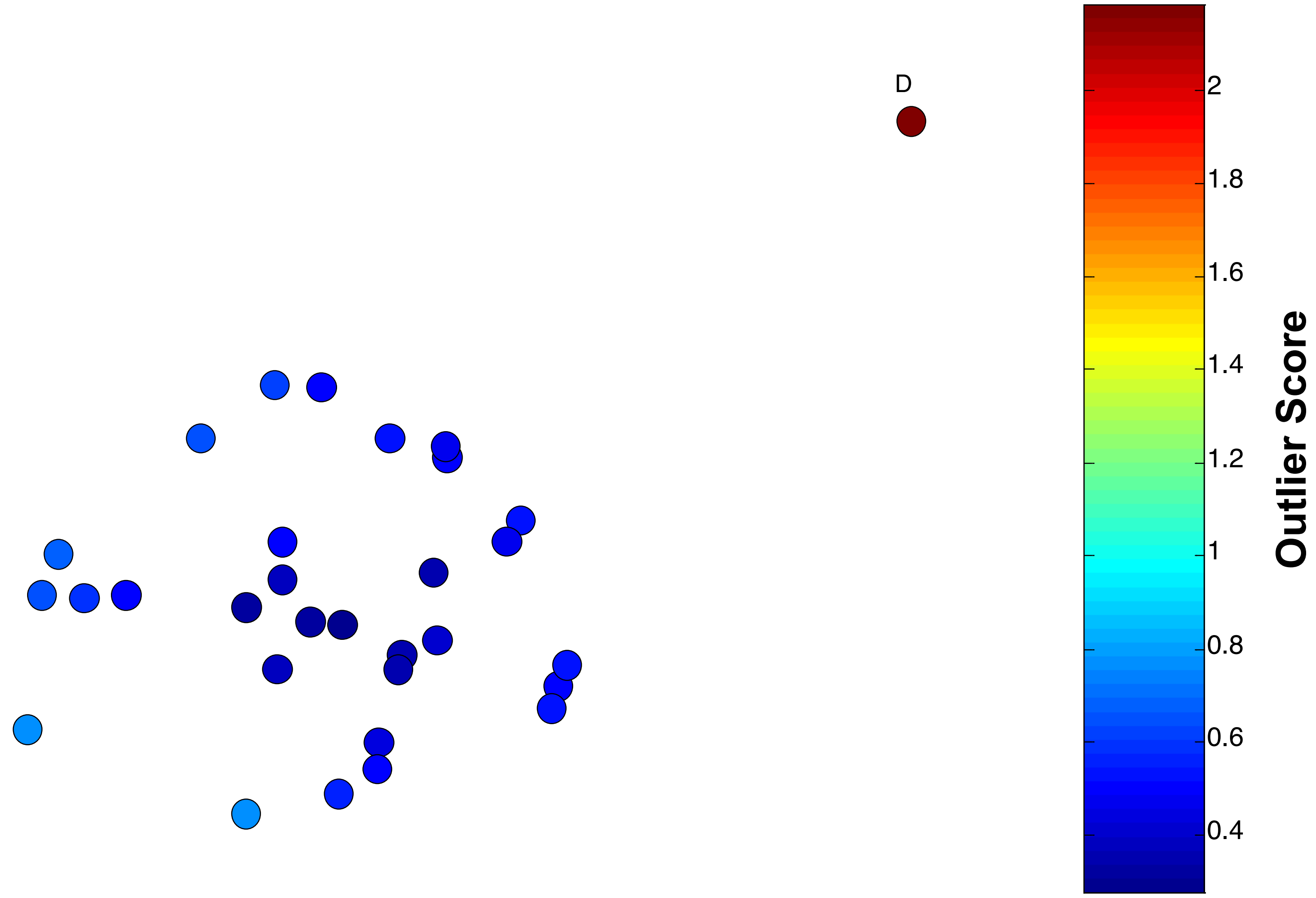
- f(x) = Distance between x and its k-nearest neighbor
- f(x) = Average distance between x and its k-nearest neighbors (less sensitive to k small or large)

**How does the approach work?** (in general):

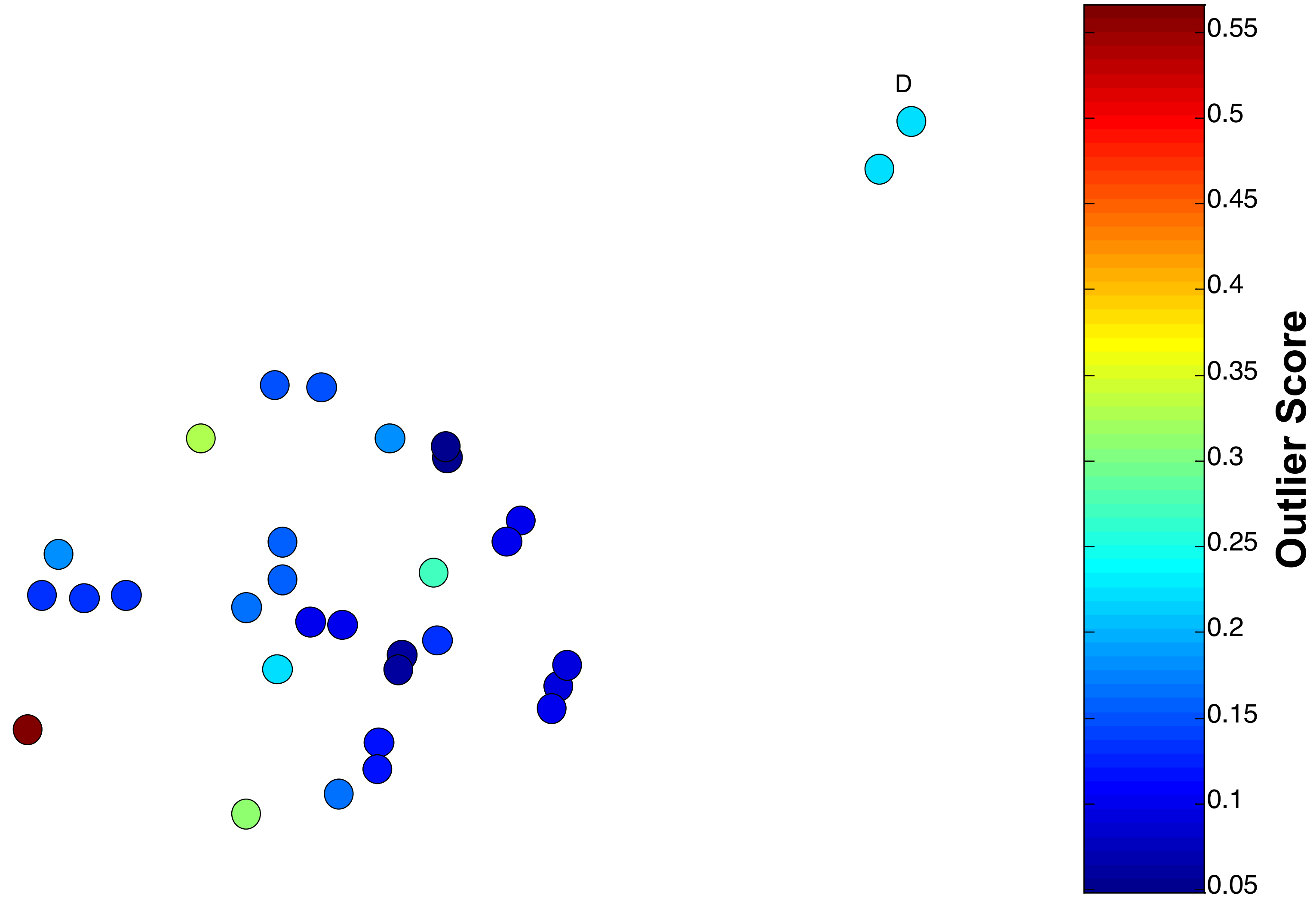
1. Calculate the anomaly score, f(x), for each data point in the dataset.
2. Use a threshold t on this score to determine outliers.

**x is an outlier iff f(x) > t**

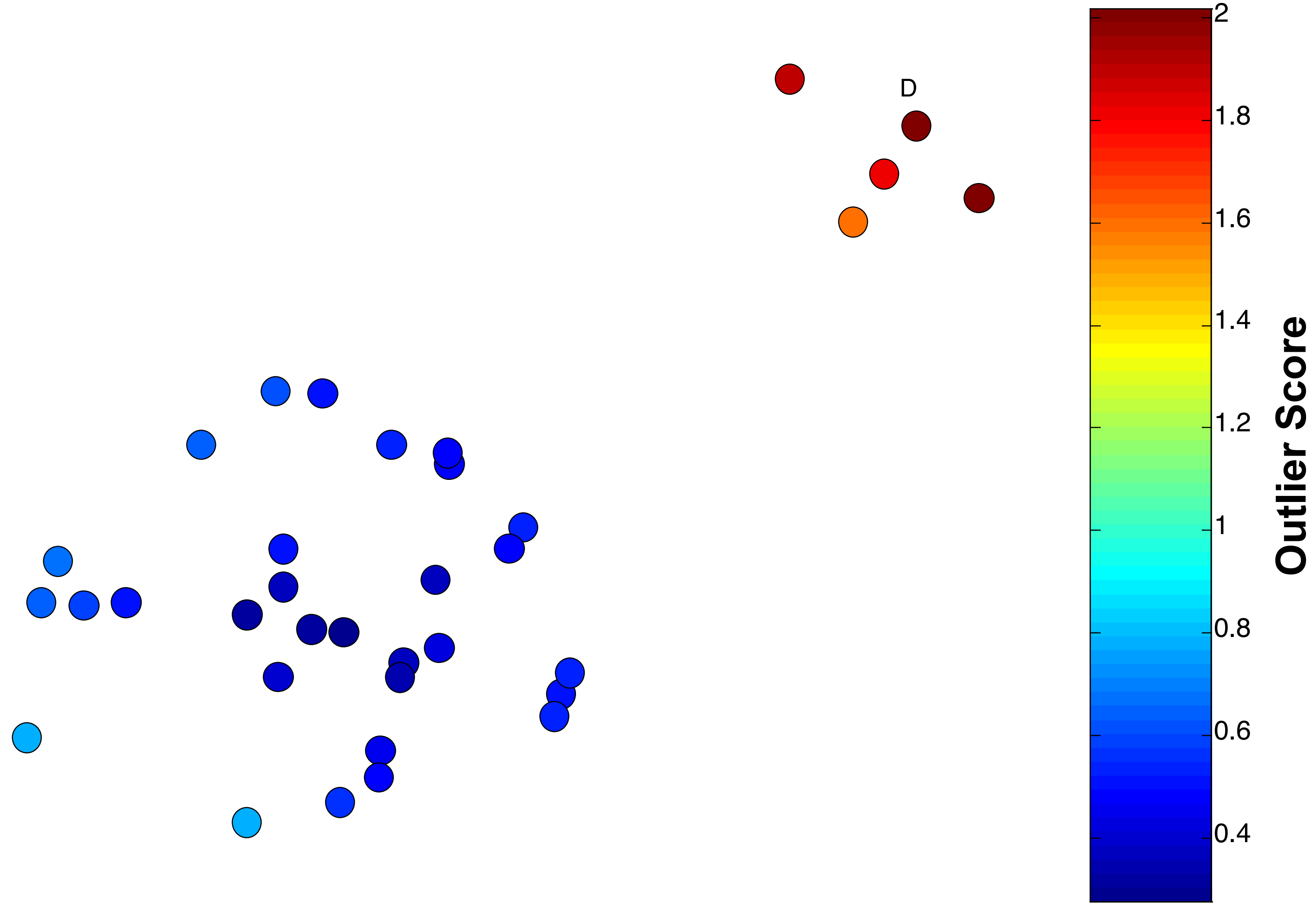
# 1 Nearest Neighbor - One Outlier



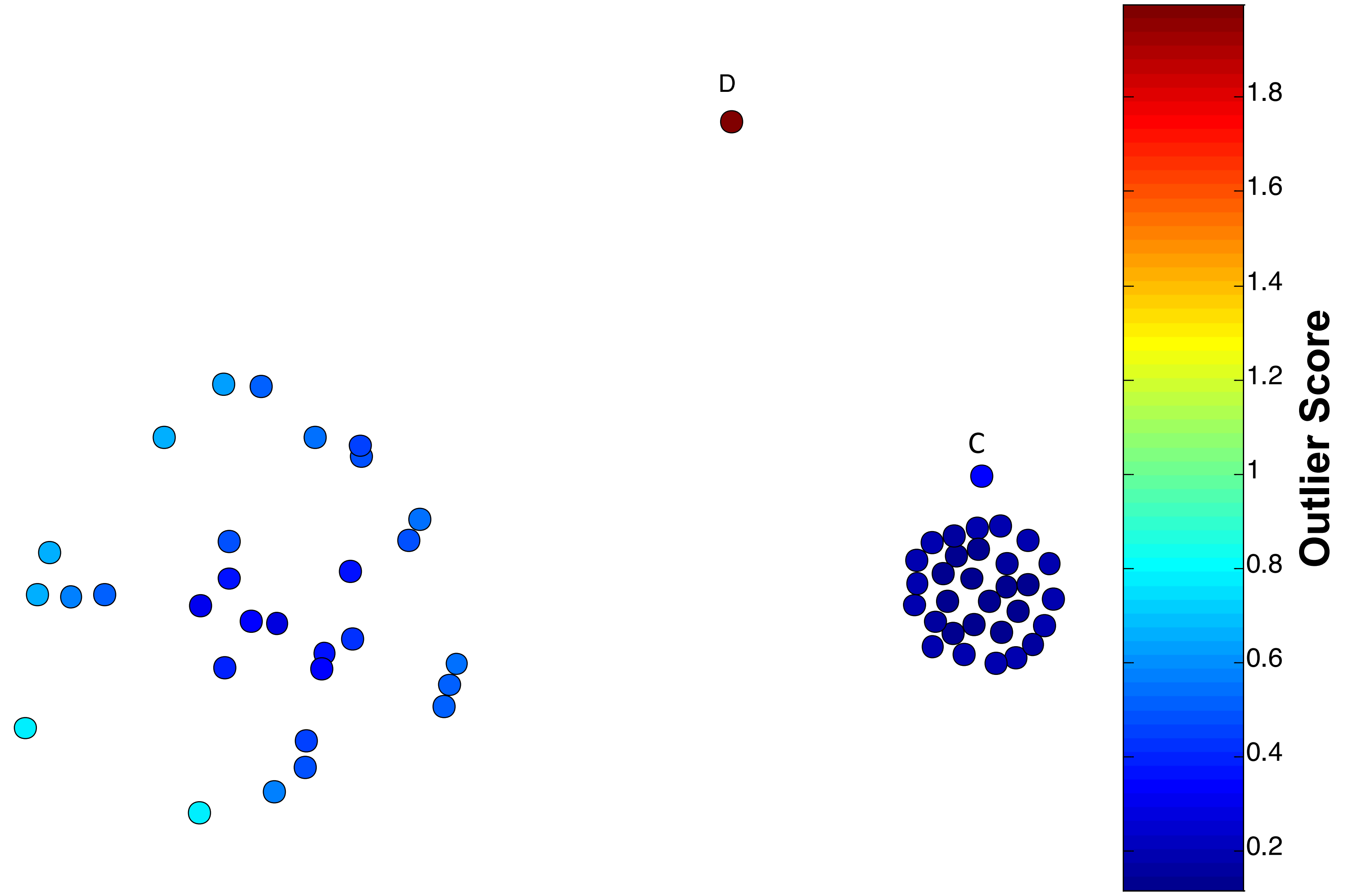
# 1 Nearest Neighbor - Two Outliers



# 5 Nearest Neighbors - Small Cluster



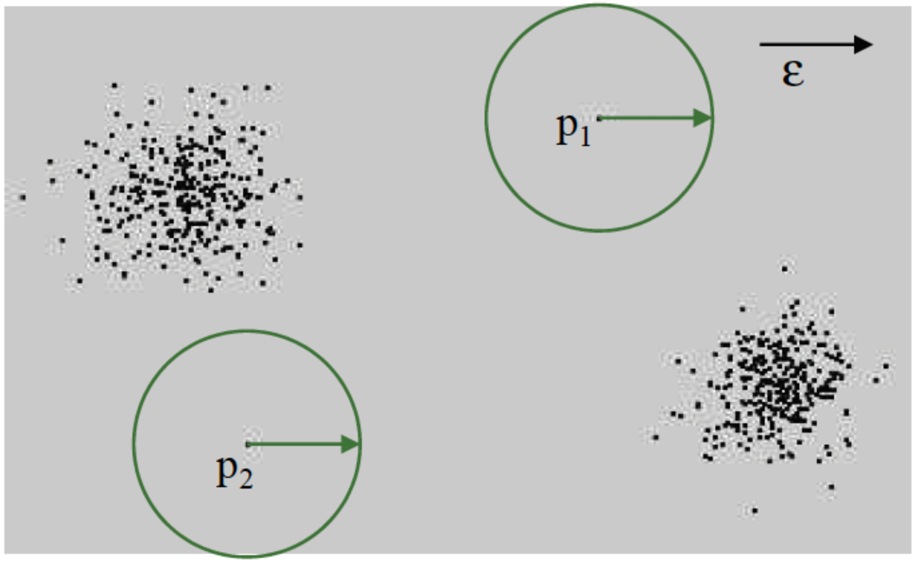
# 5 Nearest Neighbors - Differing Density



# 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*




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

range-query with radius ε

# General approach for computation

- **Efficient computation:** Nested loop algorithm
  - For any object p, calculate its distance from other objects
    - count the # of other objects in the ε-neighborhood.
    - If $\pi \cdot n$ other objects are within ε distance, terminate the inner loop
  - Otherwise, p 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]

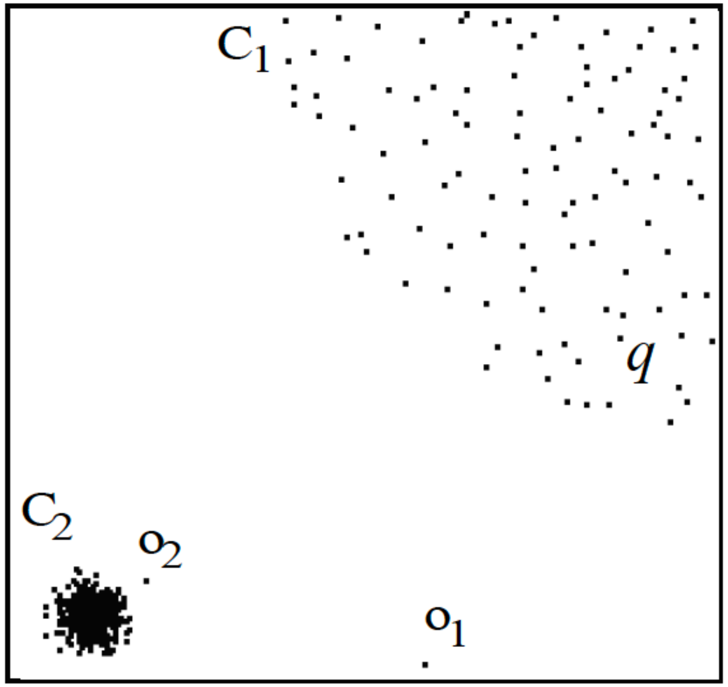
Motivation:

- 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 $\varepsilon$ and $\pi$ 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

$$density(\mathbf{x}, k) = \left( \frac{\sum_{\mathbf{y} \in N(\mathbf{x},k)} distance(\mathbf{x}, \mathbf{y})}{|N(\mathbf{x}, k)|} \right)^{-1}$$

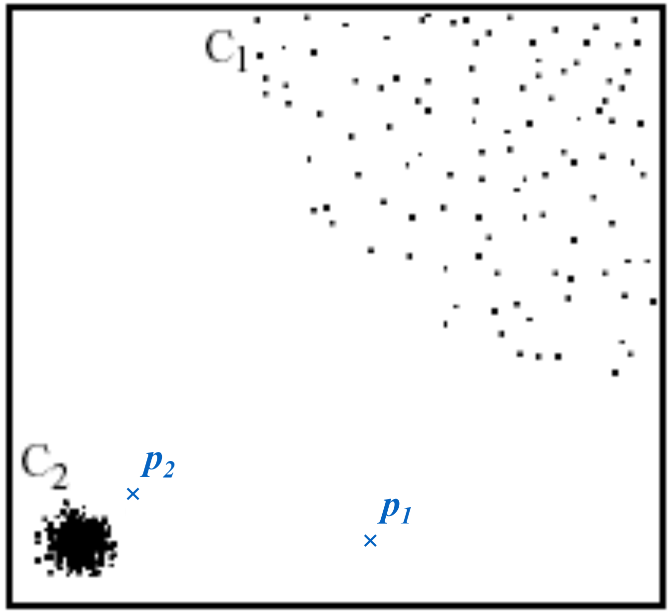
$$average\ relative\ density(\mathbf{x}, k) = \frac{density(\mathbf{x}, k)}{\sum_{\mathbf{y} \in N(\mathbf{x},k)} density(\mathbf{y}, k)/|N(\mathbf{x}, k)|}. \quad (10.7)$$

**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**

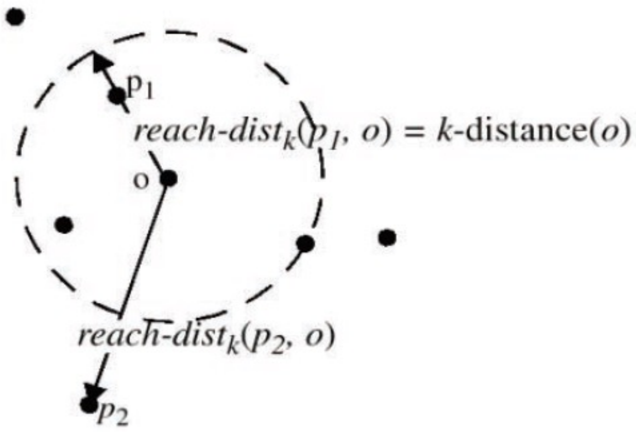
# Local Outlier Factor (LOF)

- 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

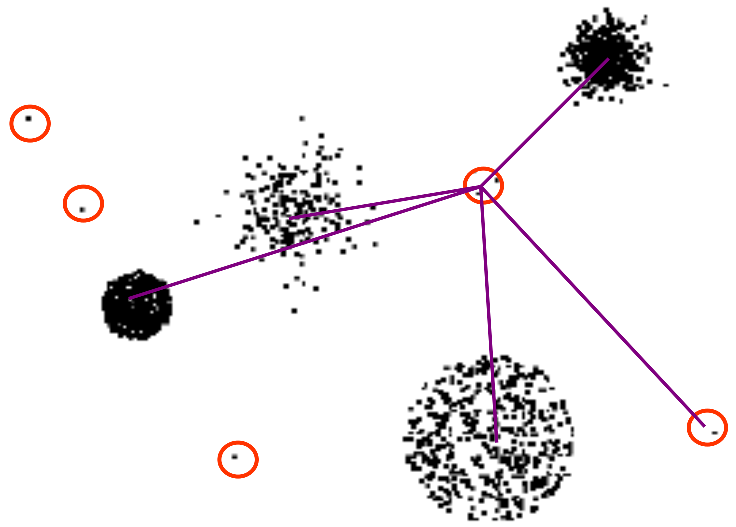
# Clustering-based Approaches

# Clustering and Anomaly Detection

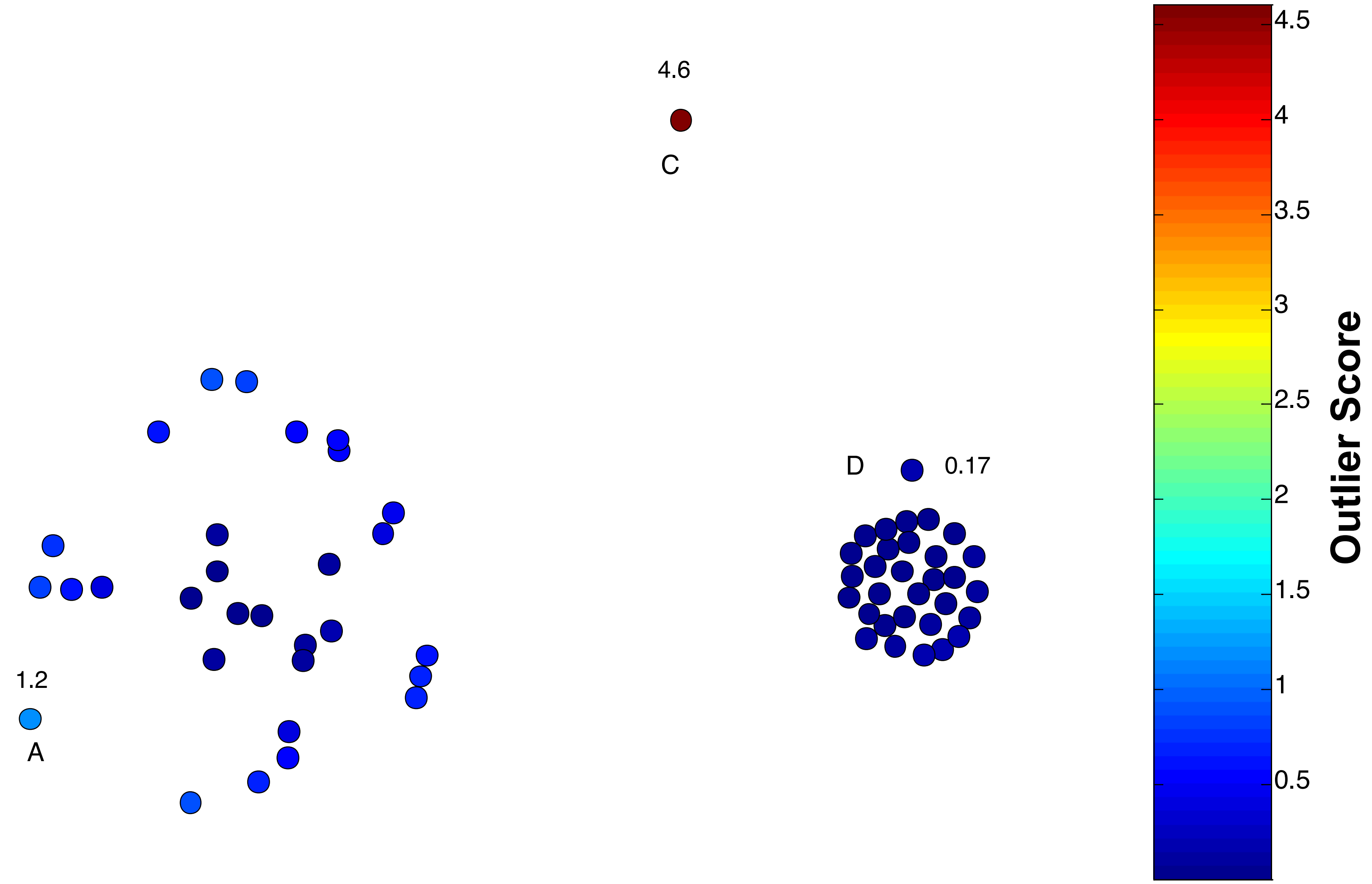
- Are outliers just a side product of some clustering algorithms?
  - Many clustering algorithms do not assign all points to clusters but account for noise objects (e.g. DBSCAN, OPTICS)
  - Look for outliers by applying one algorithm and retrieve the noise set
- Problem:
  - Clustering algorithms are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

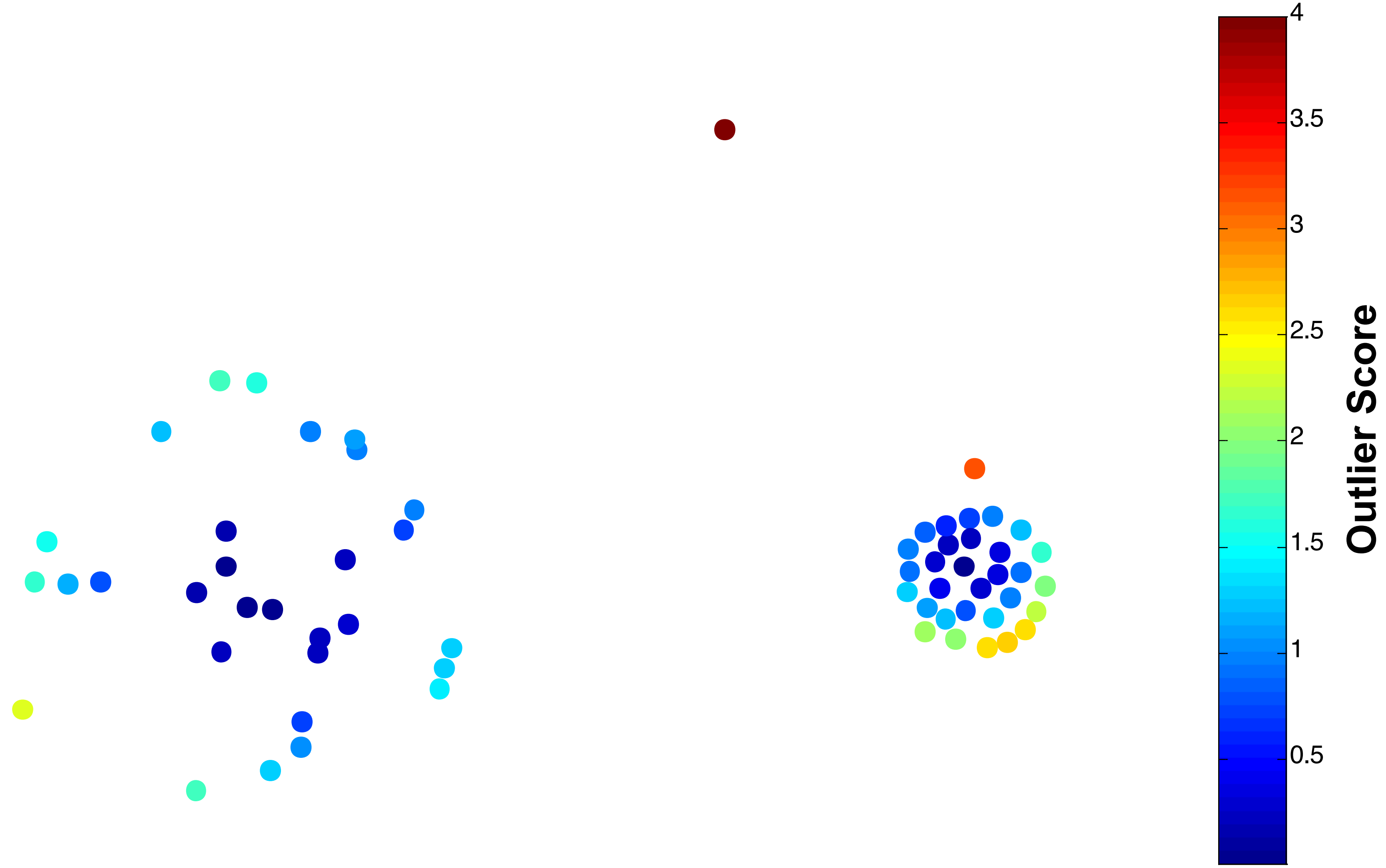
- **Clustering-based Outlier:** An object is a cluster-based outlier if it does not strongly belong to any cluster
  - For prototype-based clusters, an object is an outlier if it is not close enough to a cluster center
  - For density-based clusters, an object is an outlier if its density is too low
  - 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.