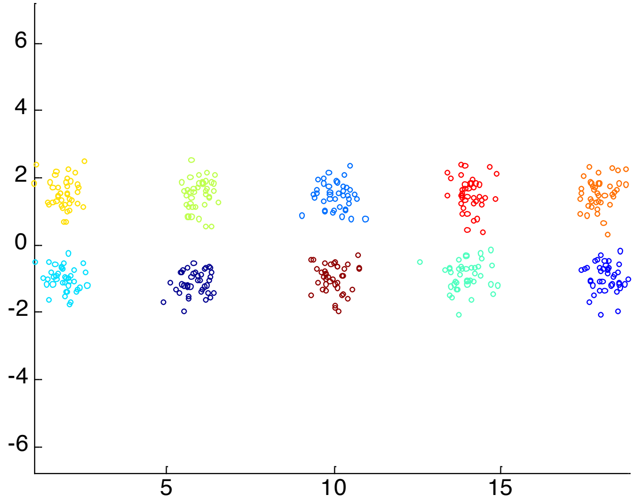
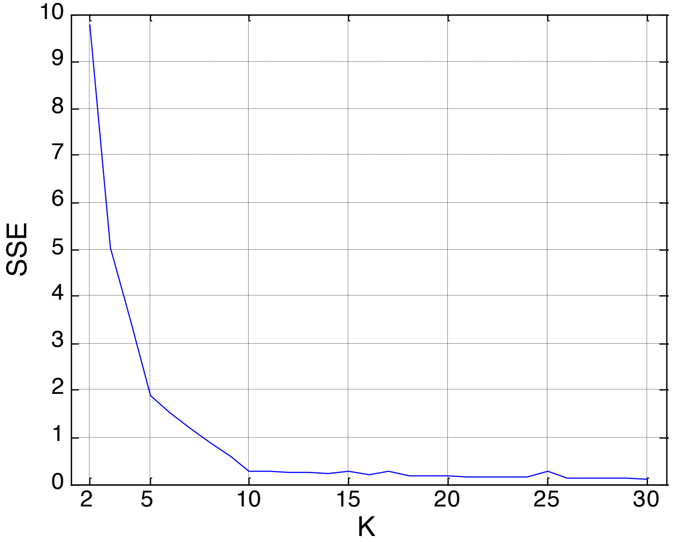
Internal Measures: SSE

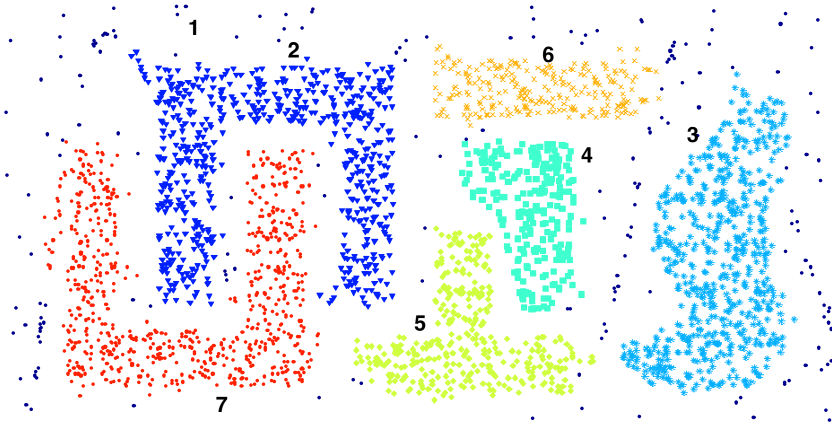
- Clusters in more complicated figures aren’t well separated
- Internal Index: Used to measure the goodness of a clustering structure without respect to external information
  - SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of clusters

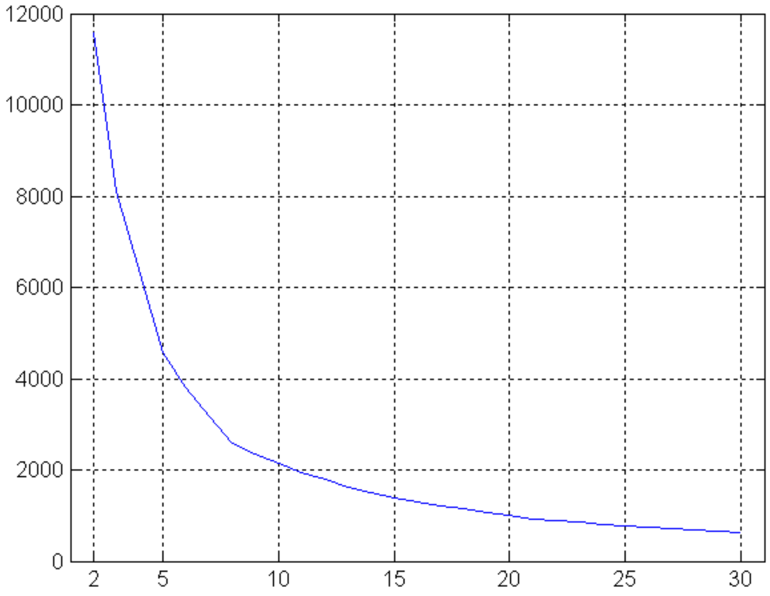




Internal Measures: SSE

- SSE curve for a more complicated data set





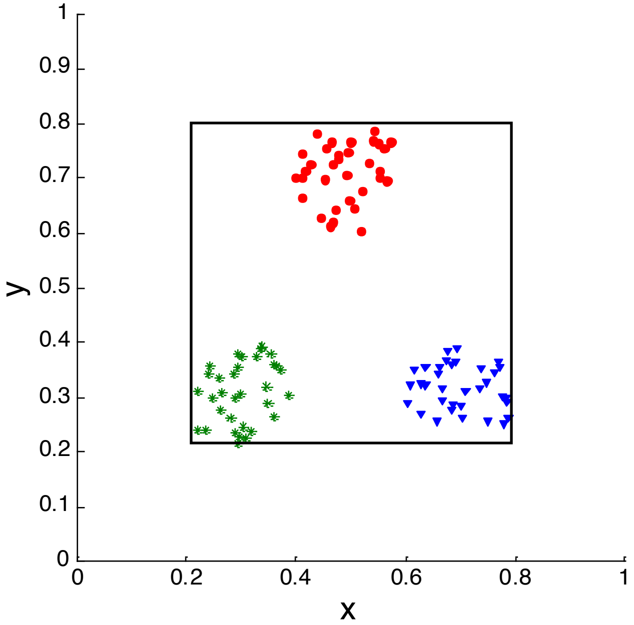
SSE of clusters found using K-means

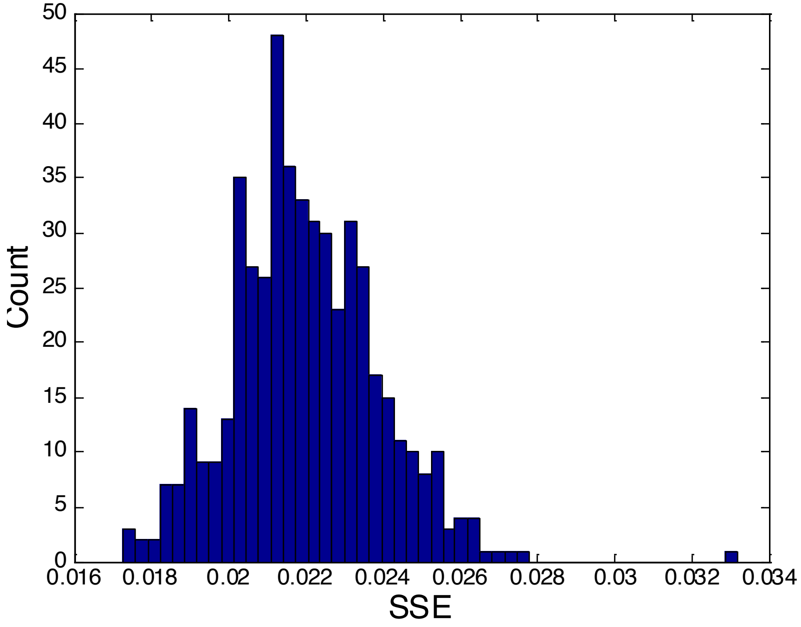
Framework for Cluster Validity

- Need a framework to interpret any measure.
  - For example, if our measure of evaluation has the value, 10, is that good, fair, or poor?
- Statistics provide a framework for cluster validity
  - The more "atypical" a clustering result is, the more likely it represents valid structure in the data
  - Can compare the values of an index that result from random data or clusterings to those of a clustering result.
    - If the value of the index is unlikely, then the cluster results are valid
  - These approaches are more complicated and harder to understand.
- For comparing the results of two different sets of cluster analyses, a framework is less necessary.
  - However, there is the question of whether the difference between two index values is significant

Statistical Framework for SSE

- Example
  - Compare SSE of 0.005 against three clusters in random data
  - Histogram shows SSE of three clusters in 500 sets of random data points of size 100 distributed over the range 0.2 – 0.8 for x and y values





Internal Measures: Cohesion and Separation

- Cluster Cohesion: Measures how closely related are objects in a cluster
  - Example: SSE
- Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters
- Example: Squared Error
  - Cohesion is measured by the within cluster sum of squares (SSE)

$$\boldsymbol{WSS} = \sum_{\boldsymbol{i}} \sum_{\boldsymbol{x} \in \boldsymbol{C}_i} (\boldsymbol{x} - \boldsymbol{m_i})^2$$

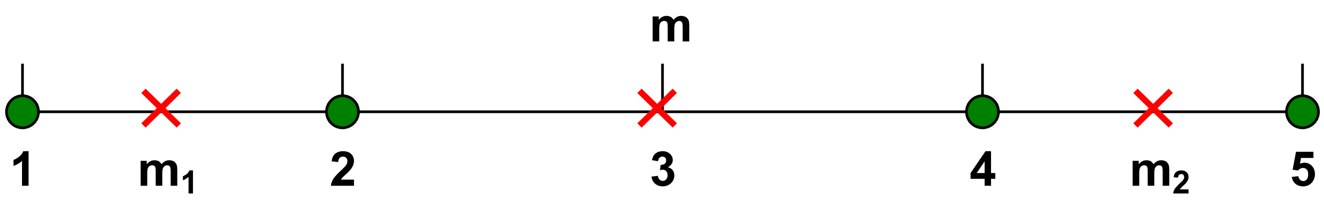
  - Separation is measured by the between cluster sum of squares

$$BSS = \sum_i |C_i| (m - m_i)^2$$

  - Where $|C_i|$ is the size of cluster i

Internal Measures: Cohesion and Separation

- Example: SSE
  - BSS + WSS = constant



K=1 cluster:

$$WSS = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$

$$BSS = 4 \times (3-3)^2 = 0$$

$$Total = 10 + 0 = 10$$

K=2 clusters:

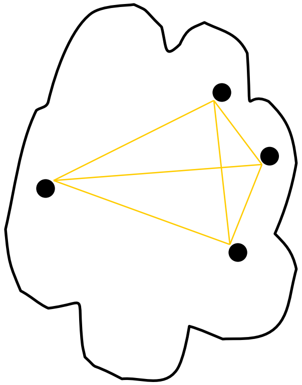
$$WSS = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

$$BSS = 2 \times (3-1.5)^2 + 2 \times (4.5-3)^2 = 9$$

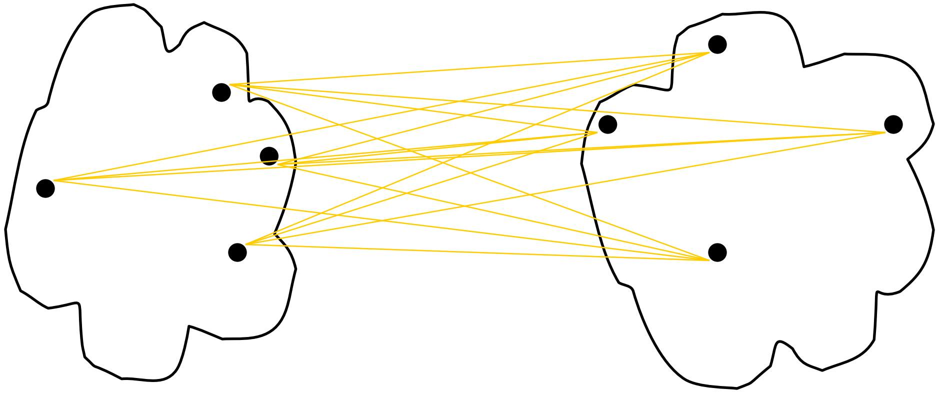
$$Total = 1 + 9 = 10$$

Internal Measures: Cohesion and Separation

- A proximity graph based approach can also be used for cohesion and separation.
  - Cluster cohesion is the sum of the weight of all links within a cluster.
  - Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.



cohesion



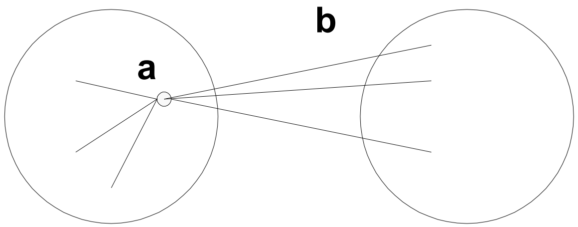
separation

Internal Measures: Silhouette Coefficient

- Silhouette Coefficient combine ideas of both cohesion and separation, but for individual points, as well as clusters and clusterings
- For an individual point, *i*
  - Calculate ***a*** = average distance of *i* to the points in its cluster
  - Calculate ***b*** = min (average distance of *i* to points in another cluster)
  - The silhouette coefficient for a point is then given by

    $s = 1 – a/b$ if $a < b$, (or $s = b/a - 1$ if $a \geq b$, not the usual case)

  - Typically between 0 and 1.
  - The closer to 1 the better.



- Can calculate the Average Silhouette width for a cluster or a clustering

External Measures of Cluster Validity: Entropy and Purity

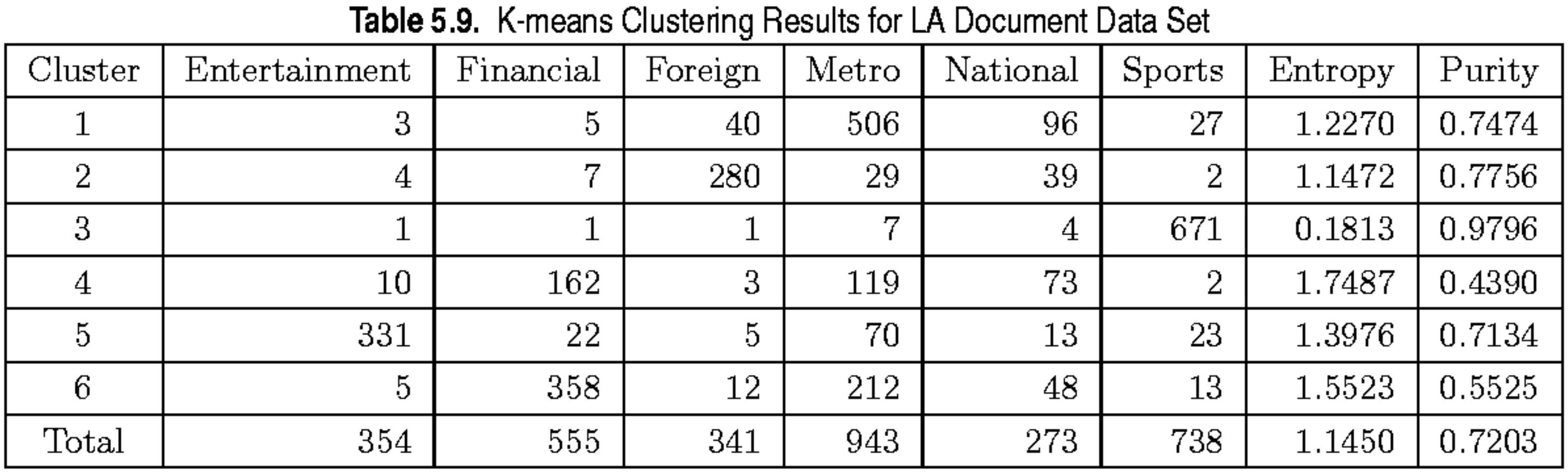
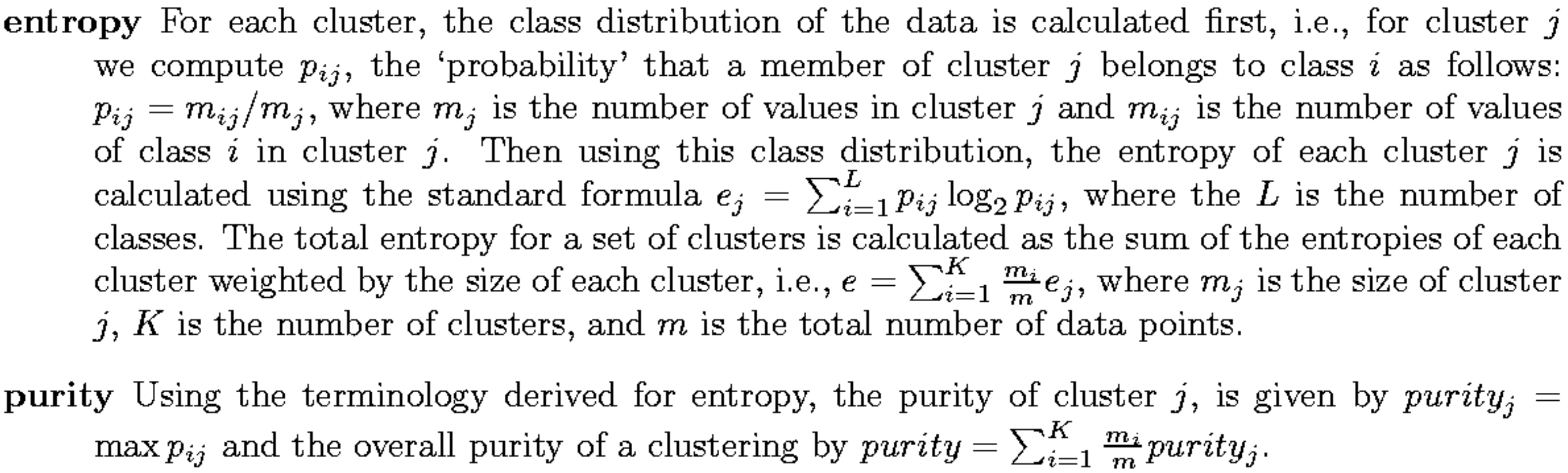


Table 5.9. K-means Clustering Results for LA Document Data Set

Cluster	Entertainment	Financial	Foreign	Metro	National	Sports	Entropy	Purity
1	3	5	40	506	96	27	1.2270	0.7474
2	4	7	280	29	39	2	1.1472	0.7756
3	1	1	1	7	4	671	0.1813	0.9796
4	10	162	3	119	73	2	1.7487	0.4390
5	331	22	5	70	13	23	1.3976	0.7134
6	5	358	12	212	48	13	1.5523	0.5525
Total	354	555	341	943	273	738	1.1450	0.7203



entropy For each cluster, the class distribution of the data is calculated first, i.e., for cluster j we compute p_{ij}, the 'probability' that a member of cluster j belongs to class i as follows: $p_{ij} = m_{ij}/m_j$, where m_j is the number of values in cluster j and m_{ij} is the number of values of class i in cluster j. Then using this class distribution, the entropy of each cluster j is calculated using the standard formula $e_j = \sum_{i=1}^{L} p_{ij} \log_2 p_{ij}$, where the L is the number of classes. The total entropy for a set of clusters is calculated as the sum of the entropies of each cluster weighted by the size of each cluster, i.e., $e = \sum_{i=1}^{K} \frac{m_i}{m} e_j$, where m_j is the size of cluster j, K is the number of clusters, and m is the total number of data points.

purity Using the terminology derived for entropy, the purity of cluster j, is given by $purity_j = \max p_{ij}$ and the overall purity of a clustering by $purity = \sum_{i=1}^{K} \frac{m_i}{m} purity_j$.

Final Comment on Cluster Validity

"The validation of clustering structures is the most difficult and frustrating part of cluster analysis.

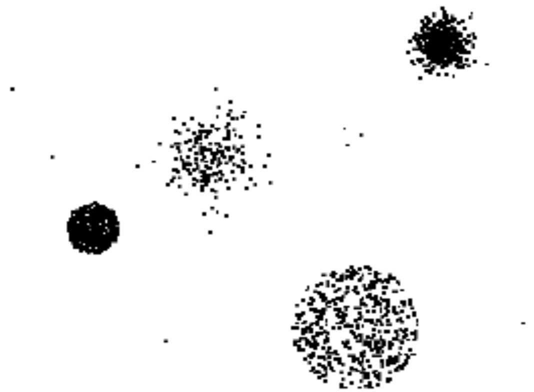
Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage."

Algorithms for Clustering Data, Jain and Dubes

Cluster Analysis: Anomaly/Outlier Detection

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 year old
  - Unusually high blood pressure

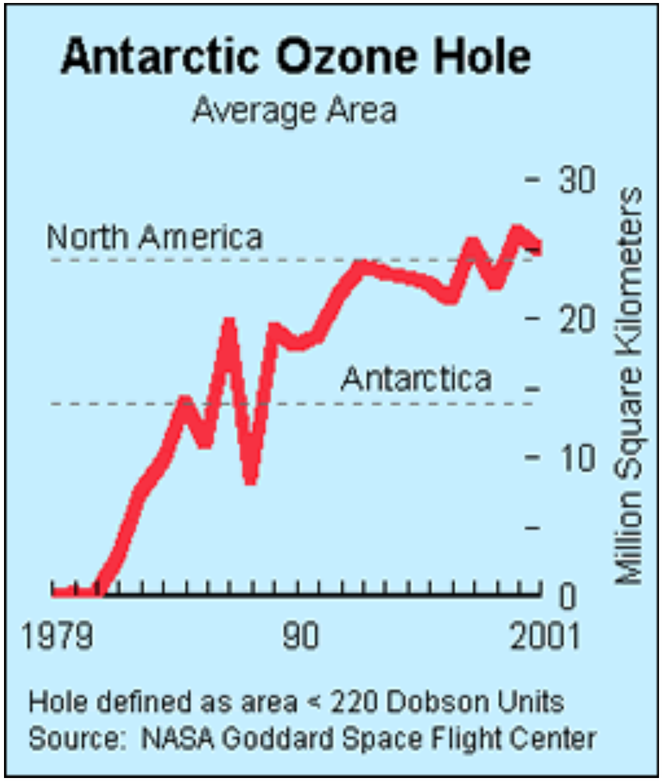
Importance of Anomaly Detection

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!



Hole defined as area < 220 Dobson Units
Source: NASA Goddard Space Flight Center

Sources:
http://exploringdata.cqu.edu.au/ozone.html
http://www.epa.gov/ozone/science/hole/size.html

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 **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

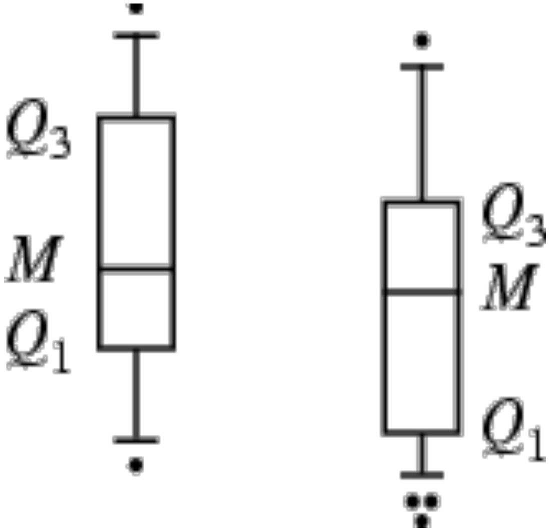
- Build a model for the data and see
  - Unsupervised
    - Anomalies are those points that don't fit well
    - Anomalies are those points that distort the model
    - Examples:
      - Statistical distribution
      - Clusters
      - Regression
      - Geometric
      - Graph
  - Supervised
    - Anomalies are regarded as a rare class
    - Need to have training data

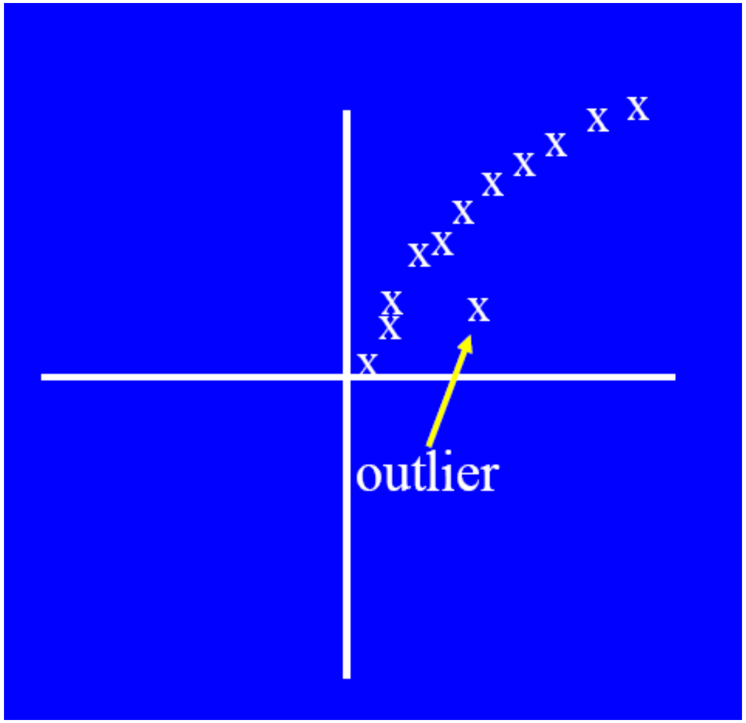
Additional Anomaly Detection Techniques

- 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

Visual Approaches

- Boxplots or scatter plots
- Limitations
  - Not automatic
  - Subjective



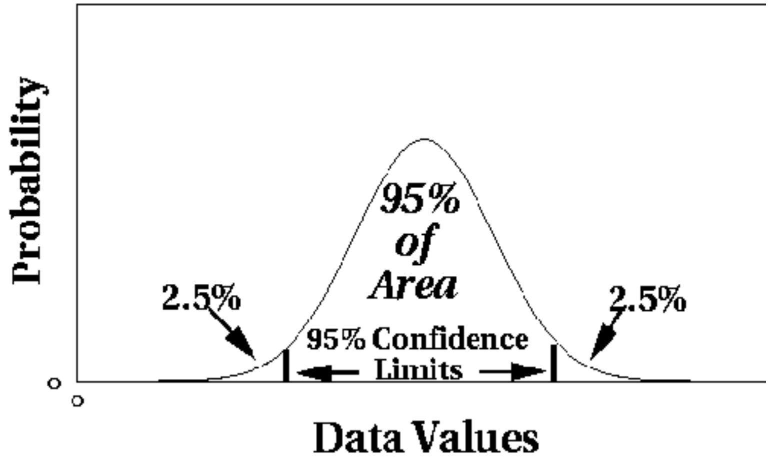


Statistical Approaches

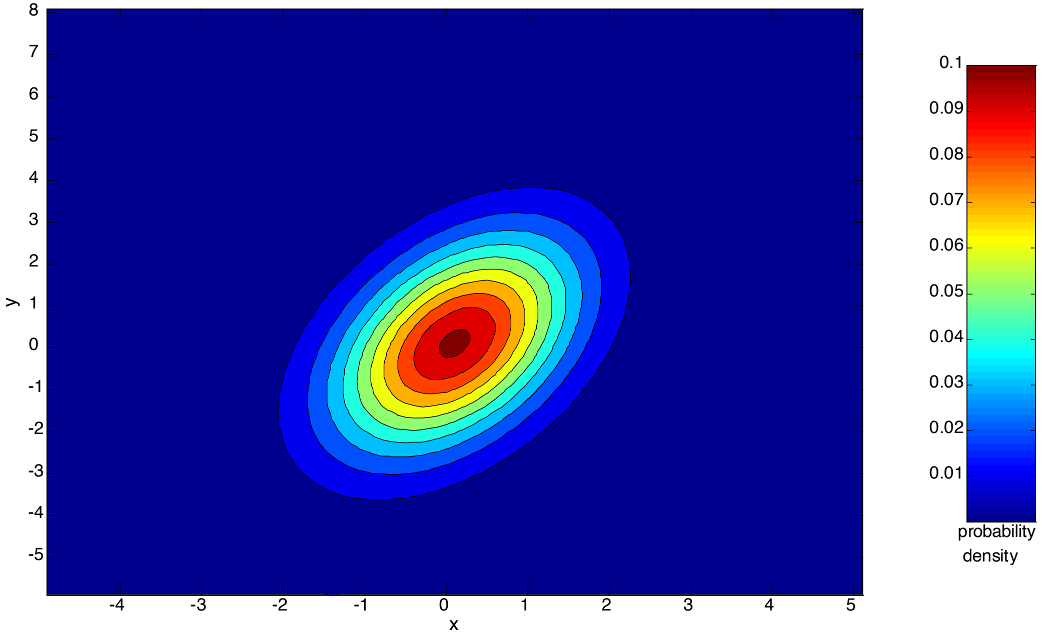
Probabilistic definition of an outlier: An outlier is an object that has a low probability with respect to a probability distribution model of the data.

- 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



Two-dimensional Gaussian

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:

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

- Reject H_0 if:

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

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 – λ) M + λ 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:

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

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

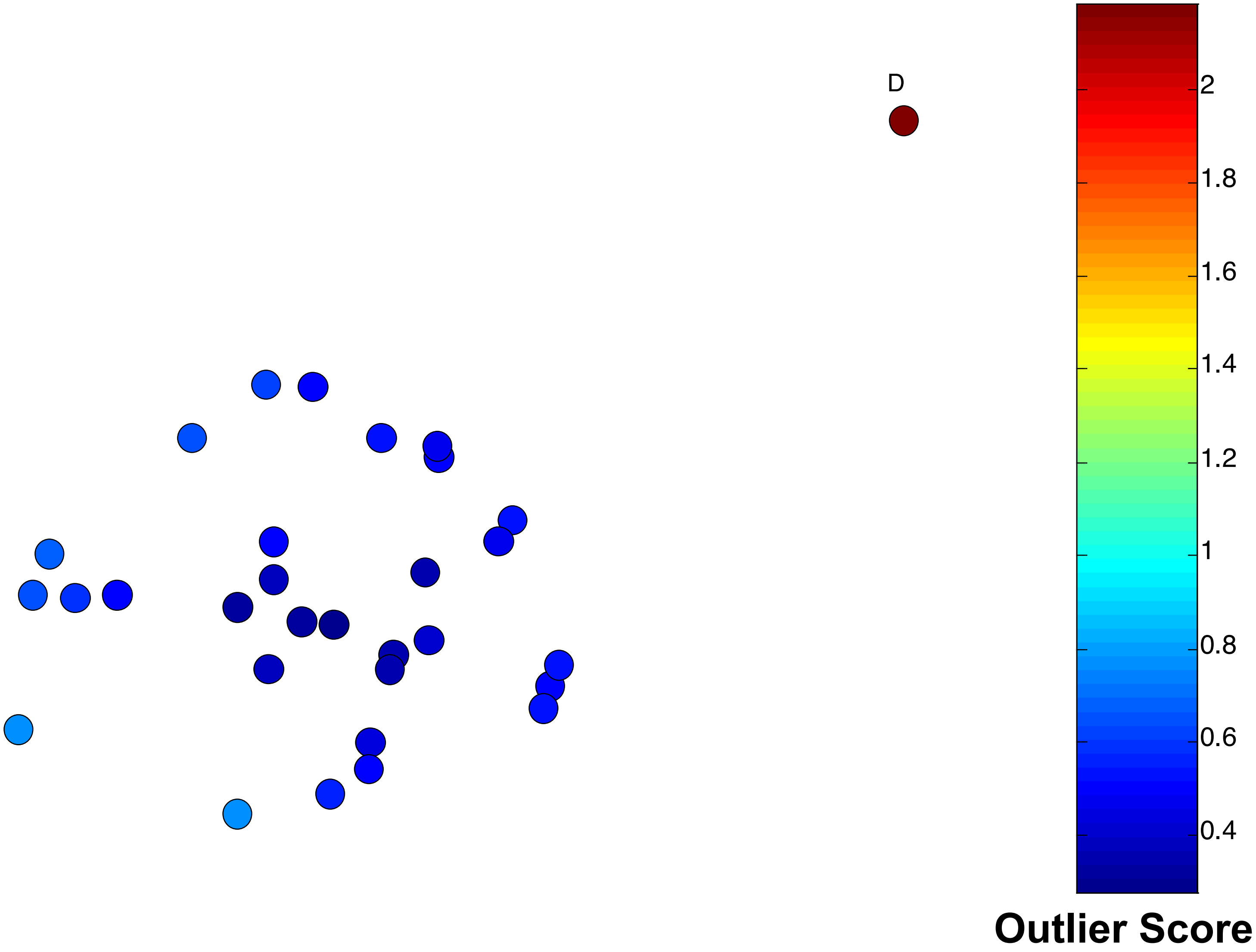
Strengths/Weaknesses of Statistical Approaches

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

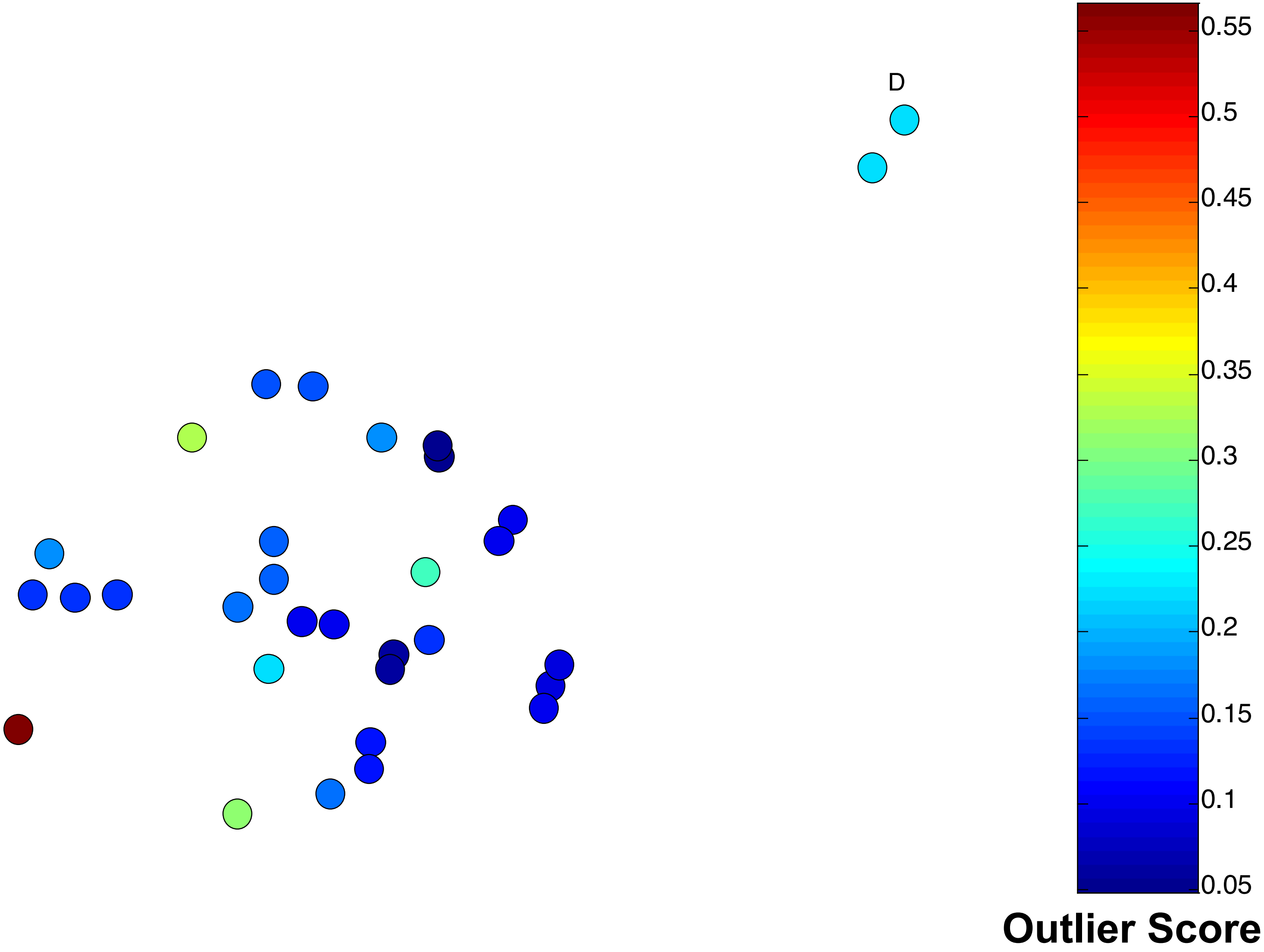
Distance-Based Approaches

- Several different techniques
- An object is an outlier if a specified fraction of the objects is more than a specified distance away (Knorr, Ng 1998)
  - Some statistical definitions are special cases of this
- The outlier score of an object is the distance to its kth nearest neighbor

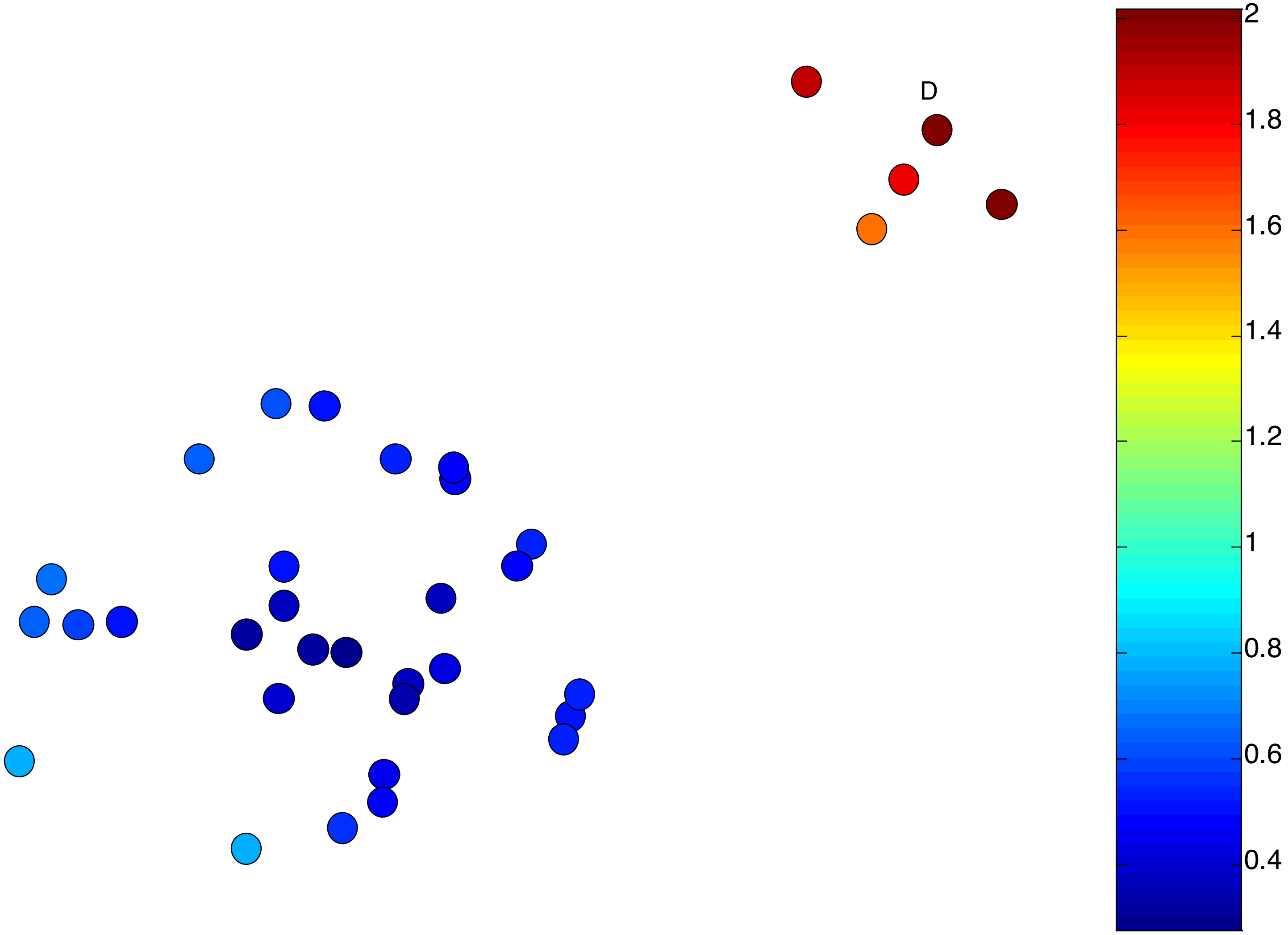
One Nearest Neighbor - One Outlier



One Nearest Neighbor - Two Outliers

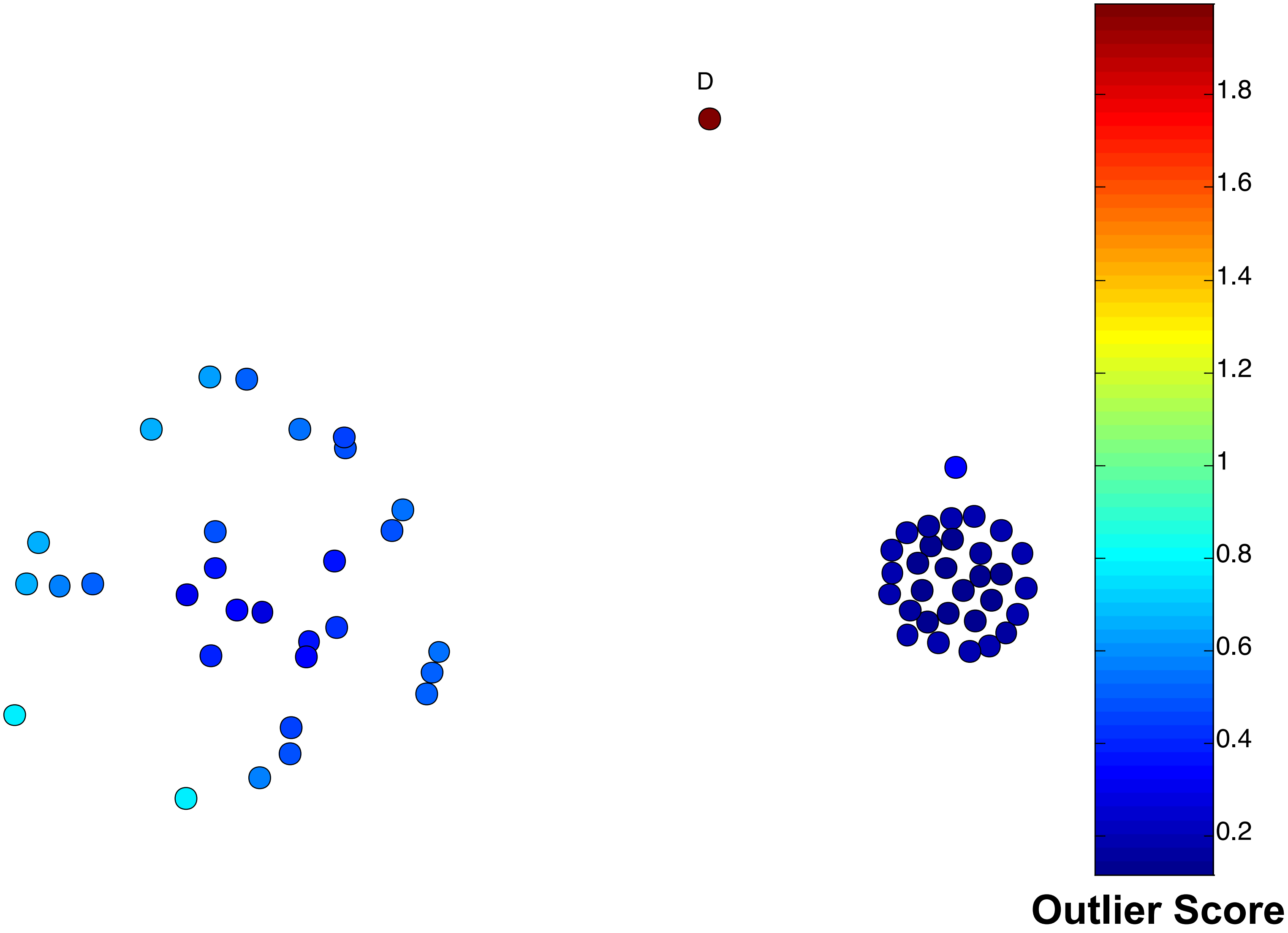


Five Nearest Neighbors - Small Cluster



Outlier Score

Five Nearest Neighbors - Differing Density



Strengths/Weaknesses of Distance-Based Approaches

- Simple
- 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 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 kth 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

Relative Density

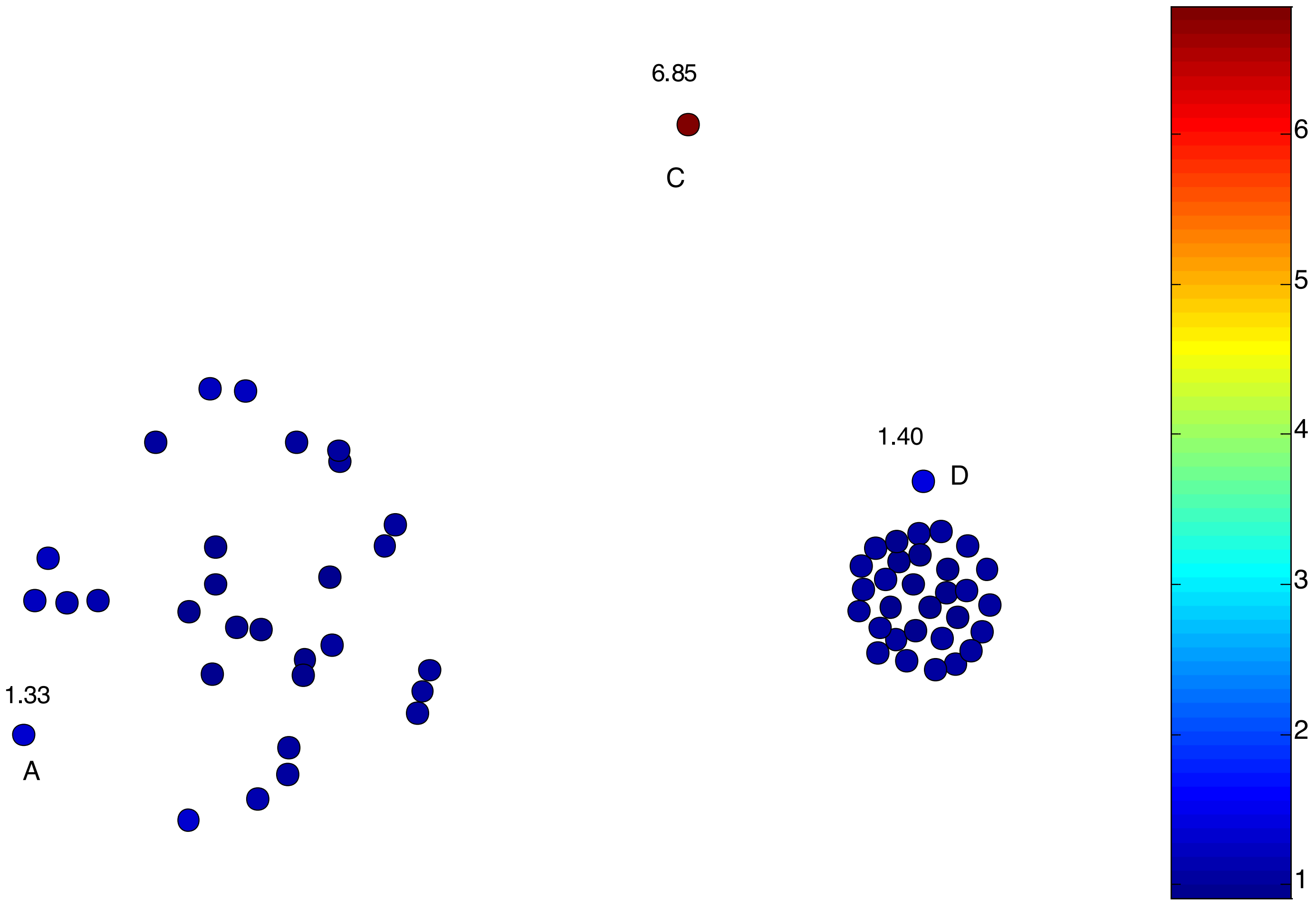
- Consider the density of a point relative to that of its k nearest neighbors

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

Algorithm 10.2 Relative density outlier score algorithm.

```
{$k$ is the number of nearest neighbors}
for all objects $\mathbf{x}$ do
    Determine $N(\mathbf{x}, k)$, the $k$-nearest neighbors of $\mathbf{x}$.
    Determine $density(\mathbf{x}, k)$, the density of $\mathbf{x}$, using its nearest neighbors, i.e., the
    objects in $N(\mathbf{x}, k)$.
end for
for all objects $\mathbf{x}$ do
    Set the $outlier\ score(\mathbf{x}, k) = average\ relative\ density(\mathbf{x}, k)$ from Equation
    10.7.
end for
```

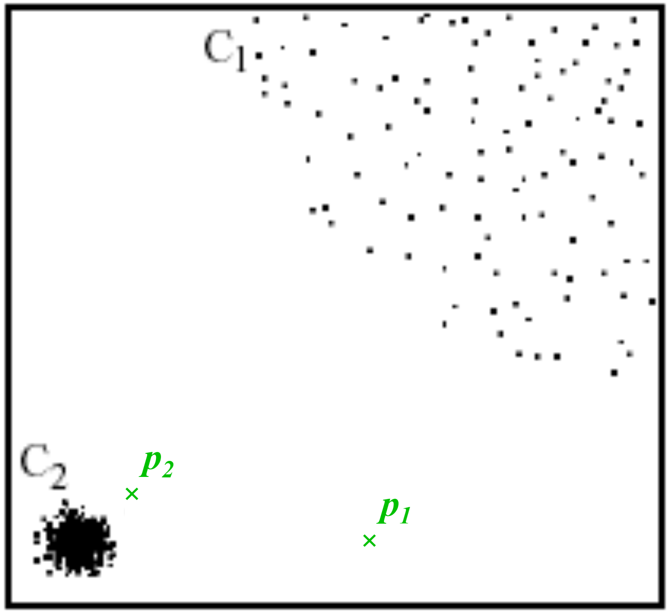
Relative Density Outlier Scores



Outlier Score

Density-based: LOF approach

- 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



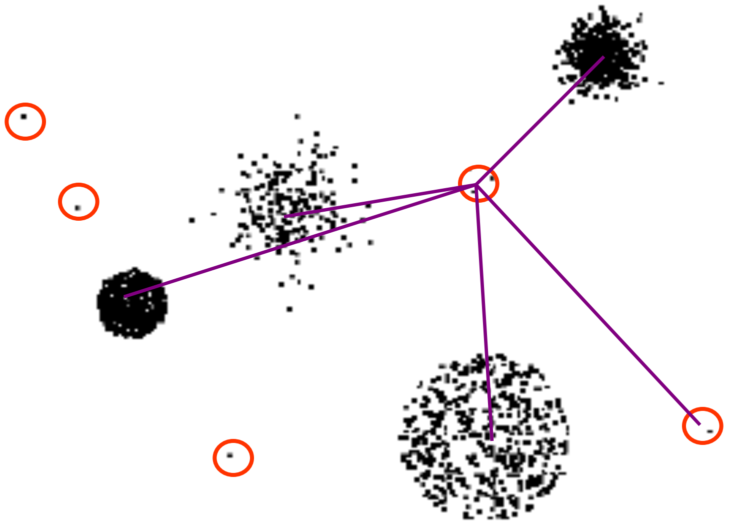
In the NN approach, p_2 is not considered as outlier, while LOF approach find both p_1 and p_2 as outliers

Strengths/Weaknesses of Density-Based Approaches

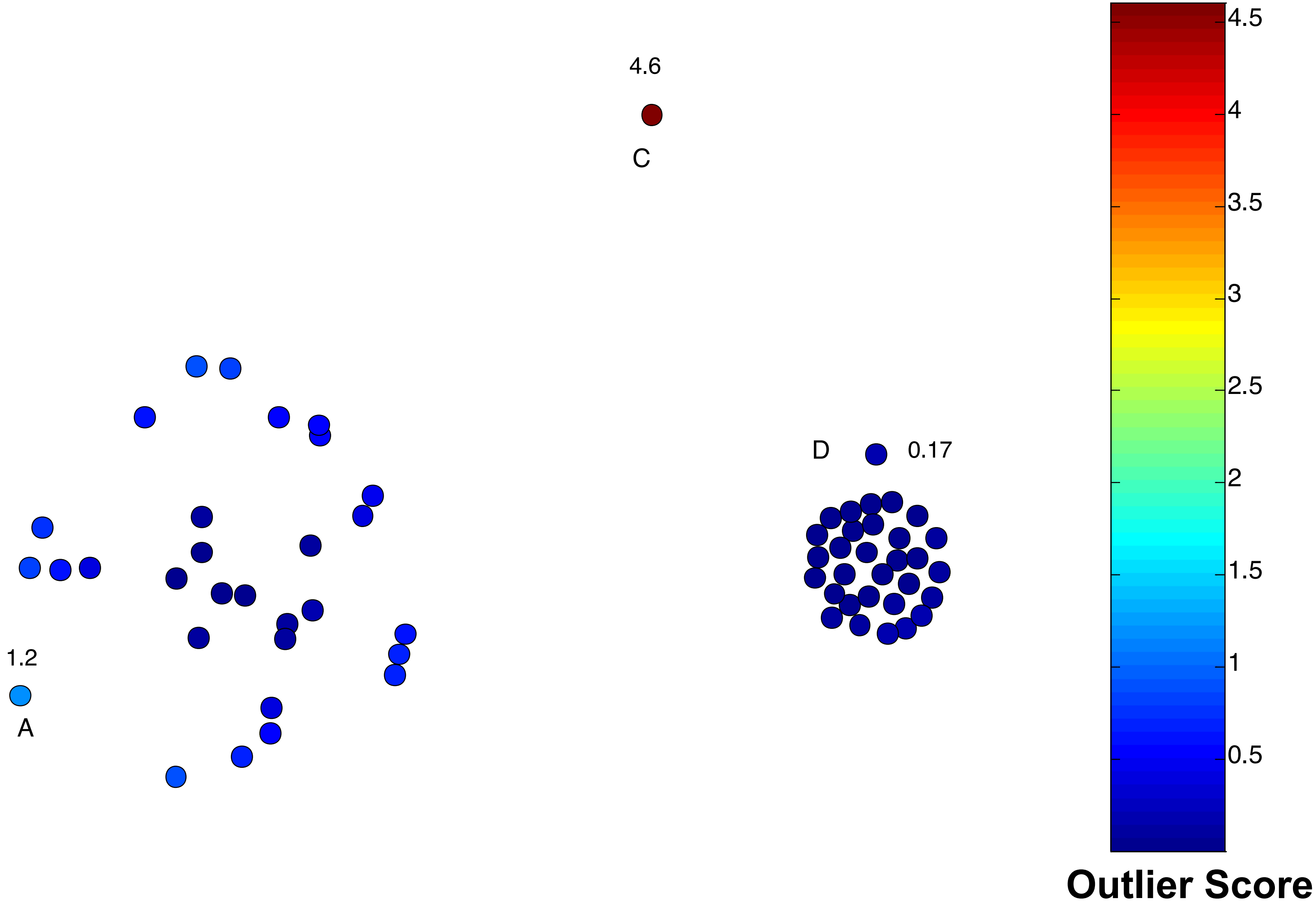
- Simple
- Expensive – O(n^2)
- Sensitive to parameters
- Density becomes less meaningful in high-dimensional space

Clustering-Based Approaches

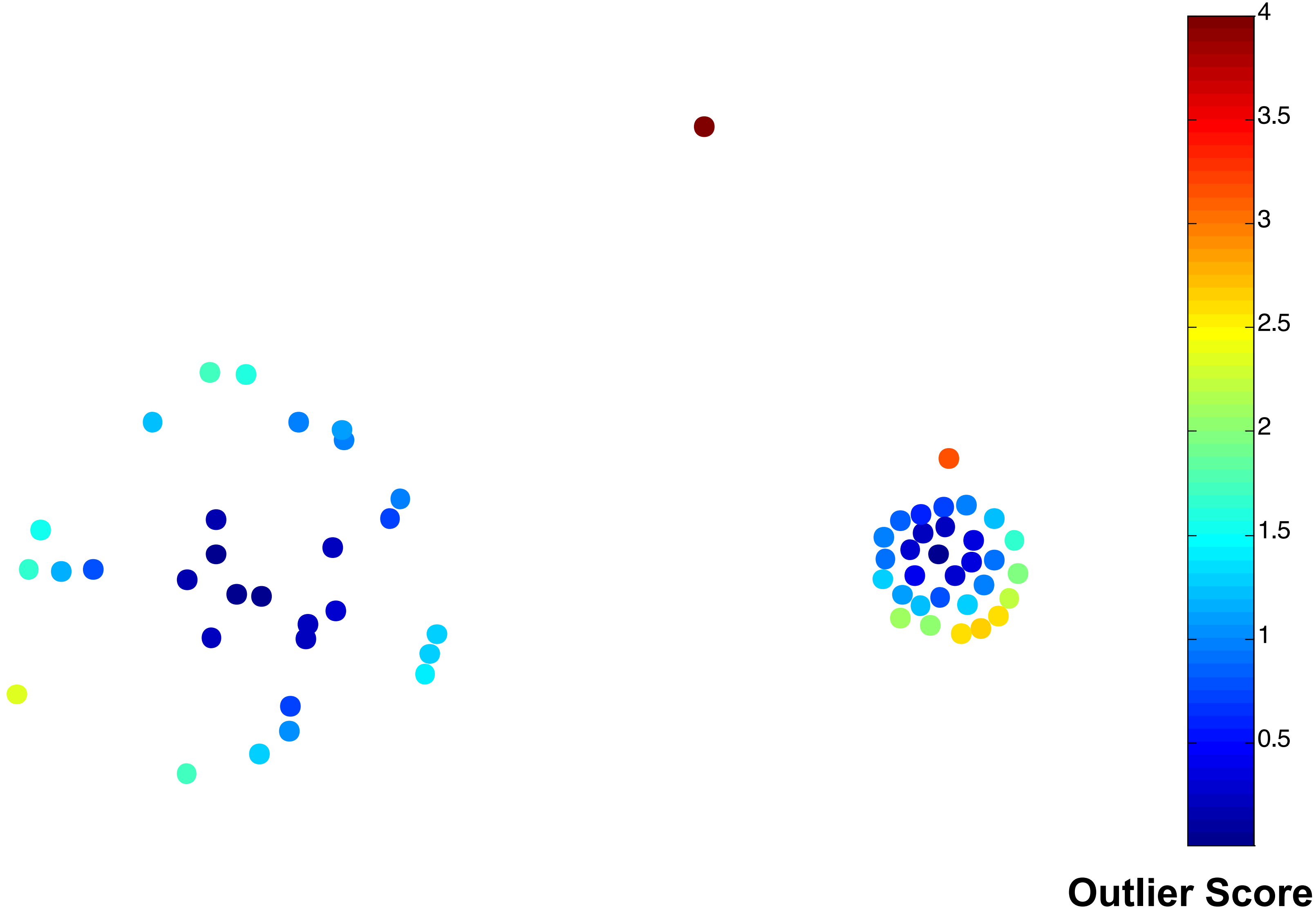
- **Clustering-based Outlier:** An object is a cluster-based outlier if it does not strongly belong to any cluster
  - For prototype-based clusters, an object is an outlier if it is not close enough to a cluster center
  - For density-based clusters, an object is an outlier if its density is too low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

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