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Lecture 20: Anomaly Detection

COMP90049
Introduction to Machine Learning
Semester 1, 2023

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Acknowledgement: Lida Rashidi

Lecture Outline

- Anomaly Detection
  - Importance & Applications
  - Definition
  - Structure

- Anomaly Detection Algorithms
  - Statistical
  - Proximity-based
  - Density-based
  - Clustering-based

- Summary

Importance of Anomaly Detection I

Example use cases

- **Banking**. Unusually high purchases; withdrawal from an unusual location
- **Insurance**: high spend, fraudulent claim
- **Social media**: unusual postings; bots or hacked accounts
- **Surveillance**: Unusual behavior of groups or individuals in public spaces
- **Weather.** Abnormally hot summers? Seismic anomalies → earthquake
- **Companies**: sudden change in customer feedback or behavior
- **Health**: skin check for melanoma
- **Machine learning**: Removing outliers from the data set

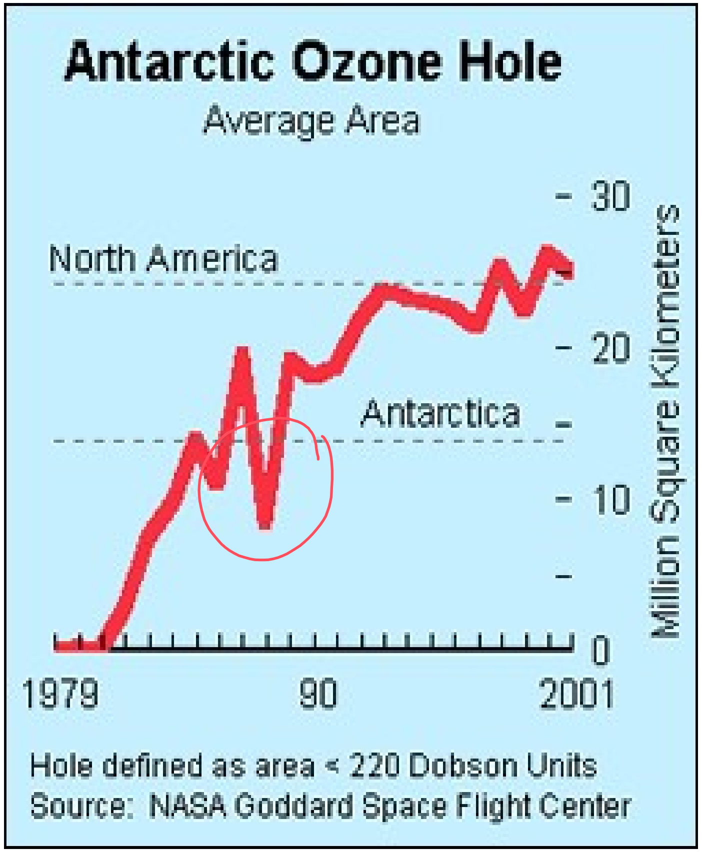
Importance of Anomaly Detection II

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 noise by a computer program and discarded!



What are Outliers/Anomalies?

- **Anomaly**: A data object that **deviates significantly** from the normal objects as if it were **generated by a different mechanism**
  - Ex.: Unusual credit card purchase, sports: Michael Jordan, …
- Anomalies are different from **noise**
  - Noise is random error or variance in a measured variable
  - Noise should be removed before anomaly detection
- Anomalies are **interesting**:
  - They violate the mechanism that generates the normal data
  - translate to significant (often critical) real life entities
    - Cyber intrusions
    - Credit card fraud

Variants of Anomaly Detection Problem

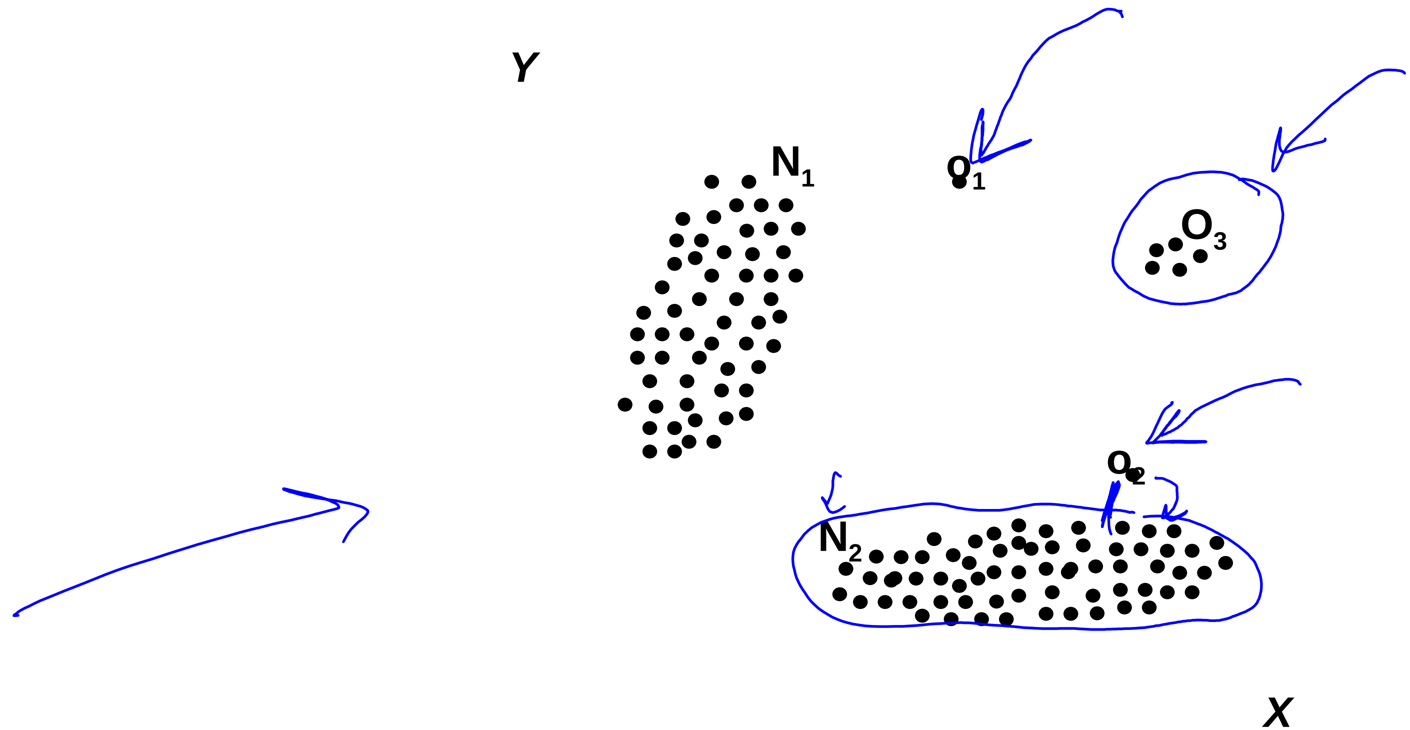
- Variants of Anomaly/Outlier Detection Problems
  - Given a database D, find all the data points **x** ∈ D with anomaly scores **greater than some threshold** t
  - Given a database D, find all the data points **x** ∈ D having the **top-n largest anomaly scores** f(**x**)
  - Given a database D, containing mostly normal (but unlabeled) data points, and a **test point** **x**, compute the **anomaly score** of **x** with respect to D

Structure of Anomalies

- Global/Point anomalies
- Contextual/Conditional anomalies
- Collective anomalies

Global/Point anomalies

- **Global Anomaly** (or point)
  - Object is O_g if it **significantly deviates from the rest of the data** set
  - Ex. Intrusion detection in computer networks
  - Issue: Find an appropriate measurement of deviation



Contextual anomalies

- **Contextual Anomaly** (or *conditional*)
  - Object is O_c if it **deviates significantly based on a selected context**

  - Attributes of data objects should be divided into two groups
    - **Contextual attributes**: defines the context, e.g., time & location
    - **Behavioral attributes**: characteristics of the object, used in anomaly evaluation, e.g., temperature

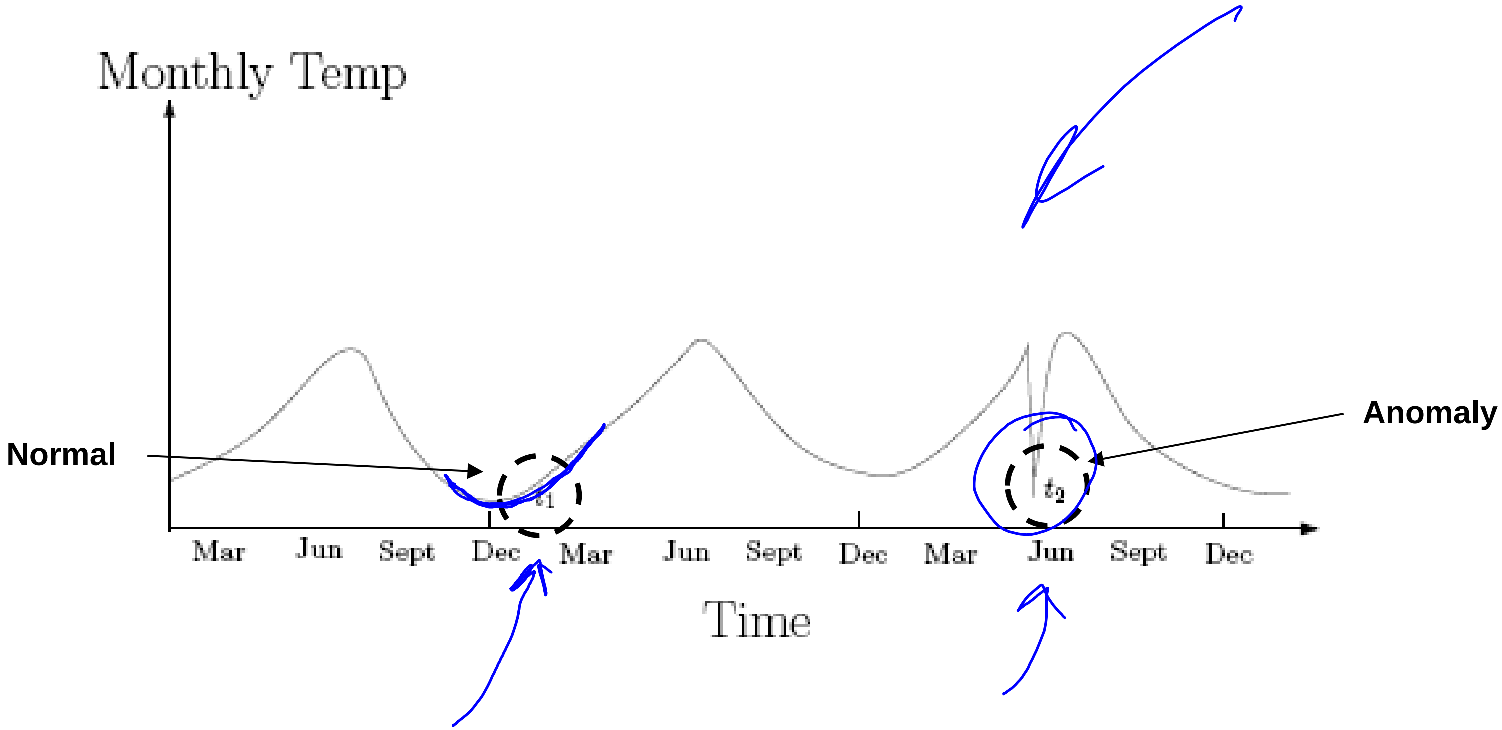
  - Can be viewed as a generalization of *local anomalies*—whose density significantly deviates from its local area

  - Issue: How to define or formulate meaningful context?

* Song, et al, “Conditional Anomaly Detection”, IEEE Transactions on Data and Knowledge Engineering, 2006.

Example of Contextual Anomalies

Ex. 10º C in Paris: Is this an anomaly?



Collective anomalies

Collective Anomalies

- A **subset** of data objects that ***collectively* deviate** significantly from the whole data set, even if the individual data objects may not be anomalies

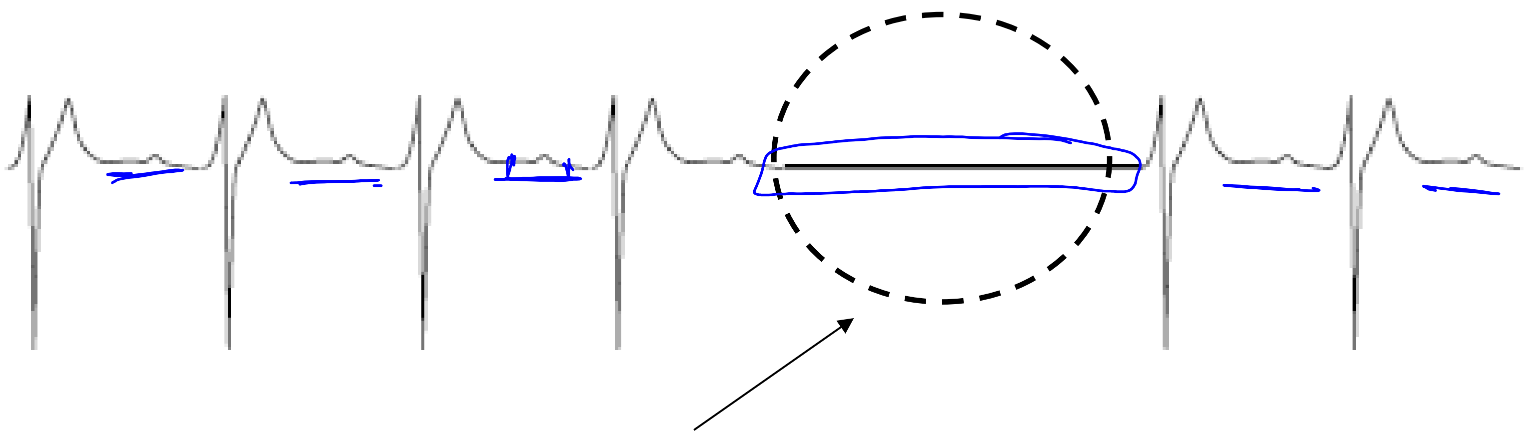
- E.g., *intrusion detection*:
  - When a number of computers keep sending denial-of-service packages to each other

- Detection of collective anomalies
  - Consider not only behavior of individual objects, but also that of **groups** of objects
  - Requires background **knowledge about the relationship** among data objects, such as a distance or similarity measure on objects.

Example of Collective anomalies

- Requires a relationship among data instances
  - Sequential data
  - Spatial data
  - Graph data

- The individual instances within a collective anomaly are not anomalous by themselves



Anomaly detection paradigms:

supervised, semi-supervised, and unsupervised

Supervised Anomaly Detection

Supervised anomaly detection

- Labels available for both **normal data and anomalies**
- Samples examined by domain experts used for training & testing
- Challenges
  - Require both **labels** from both normal and anomaly class
  - **Imbalanced** classes, i.e., anomalies are rare: Boost the anomaly class and make up some artificial anomalies
  - Cannot detect **unknown** and emerging anomalies
  - Catch as many outliers as possible, i.e., **recall** is more important than accuracy (i.e., not mislabeling normal objects as outliers)

Semi-supervised Anomaly Detection

Semi-Supervised anomaly detection

- Labels available only for **normal** data
- Model normal objects & report those not matching the model as outliers
- Challenges
  - Require **labels** from normal class
  - Possible high **false alarm** rate - previously unseen (yet legitimate) data records may be recognized as anomalies

Unsupervised Anomaly Detection I

Unsupervised anomaly detection

- Assume the **normal** objects are somewhat "clustered" into multiple **groups**, each having some **distinct features**
- An outlier is expected to be **far away from any groups** of normal objects
- **General steps**
  - Build a profile of “normal” behavior
    - summary statistics for overall population
    - model of multivariate data distribution
  - Use the “normal” profile to detect anomalies
    - anomalies are observations whose characteristics differ significantly from the normal profile

Unsupervised Anomaly Detection II

Unsupervised anomaly detection **Challenges**

- Normal objects may not share any strong patterns, but the collective outliers may share high similarity in a small area

- *Ex.* In some intrusion or virus detection, normal activities are diverse
  - Unsupervised methods may have a high false positive rate but still miss many real outliers.

Many clustering methods can be adapted for unsupervised methods

- Find clusters, then outliers: not belonging to any cluster

- *Problem 1*: Hard to distinguish noise from outliers

- *Problem 2*: Costly since first clustering: but far less outliers than normal objects

Unsupervised anomaly detection: Approaches

- Statistical (or: model-based)
  - Assume that normal data follow some statistical model
- Proximity-based
  - An object is an outlier if the nearest neighbors of the object are far away
- Density-based
  - Outliers are objects in regions of low density
- Clustering-based
  - Normal data belong to large and dense clusters

Statistical Anomaly detection

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Statistical anomaly detection

Anomalies are objects that are fit poorly by a statistical model.

- **Idea**: learn a model fitting the given data set, and then identify the objects in **low probability regions** of the model as anomalies

- **Assumption**: normal **data is generated by a parametric distribution** with parameter θ
  - The probability density function of the parametric distribution $f(x, \theta)$ gives the probability that object x is generated by the distribution
  - The smaller this value, the more likely x is an outlier

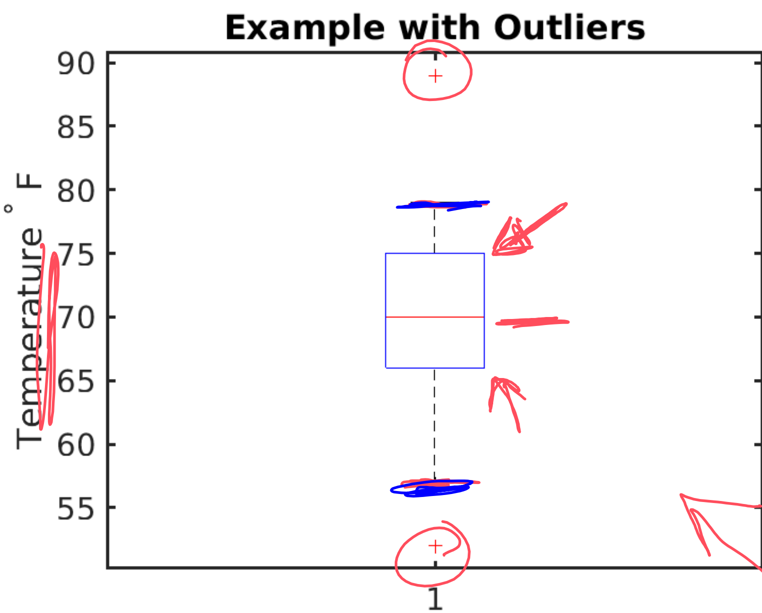
- **Challenges** of Statistical testing:
  - highly depends on whether the assumption of statistical model holds in the real data

Visualizing the data

Graphical Approaches

- Boxplot (1-D), Scatter plot (2-D), Spin plot (3-D)

- Limitations: Time consuming, Subjective



$f(\theta)$

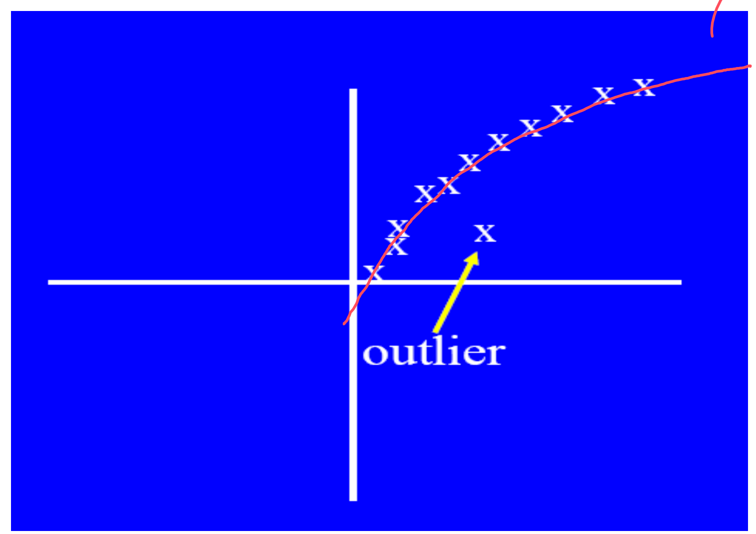


Image: https://en.wikipedia.org/wiki/Box_plot#/media/File:Boxplot_with_outlier.png

Univariate data -- General Approach

Avg. temp.: x={24.0, 28.9, 28.9, 29.0, 29.1, 29.1, 29.2, 29.2, 29.3, 29.4}

- Use the **maximum likelihood** method to estimate μ and σ

$$\hat{\mu} = \overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \overline{x})^2$$

- For the above data x with n = 10:

$$\hat{\mu} = 28.61 \qquad \hat{\sigma} = \sqrt{2.29} = 1.51$$

- Decide on a confidence limits, e.g.,

$$\mu \pm 3\sigma \text{ region contains } 99.7\% \text{ data}$$

- Then 24 is an outlier since:

$$(24 - 28.61) / 1.51 = -3.04 < -3$$

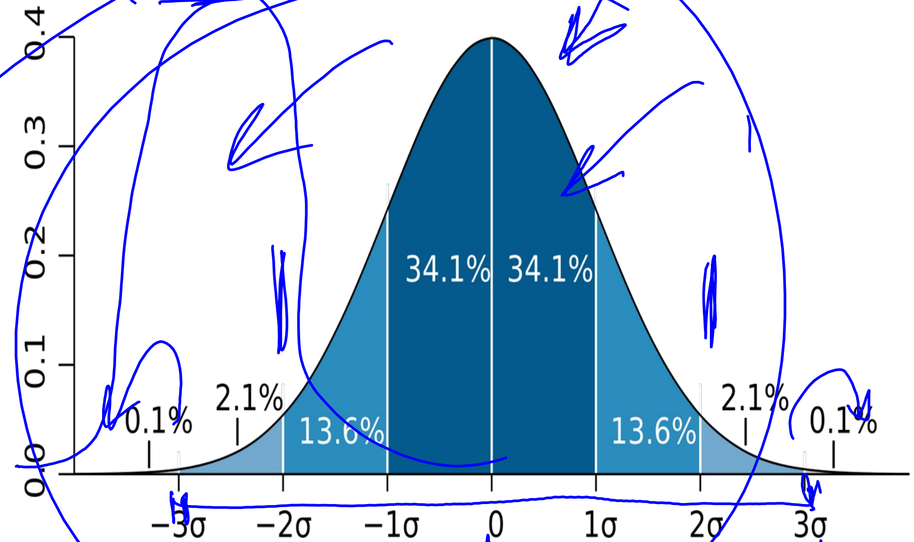


Image: https://en.wikipedia.org/wiki/Standard_deviation#/media/File:Standard_deviation_diagram.svg

Multivariate Data

- **Multivariate** Gaussian distribution
  - Outlier defined by **Mahalanobis distance**
  - Grubb's test on the distances

	Distance	
	~~Euclidean~~	Mahalanobis
A	5.7	35
B	7.1	24

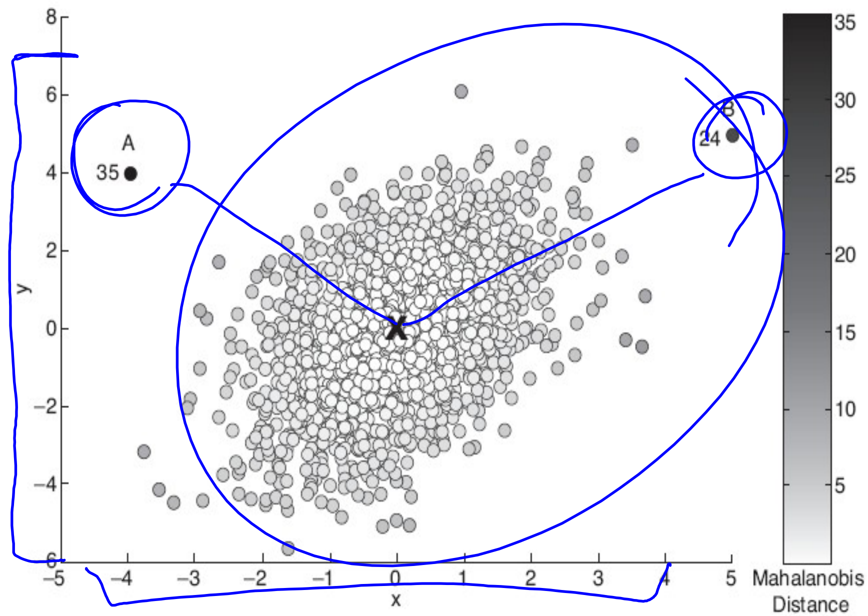
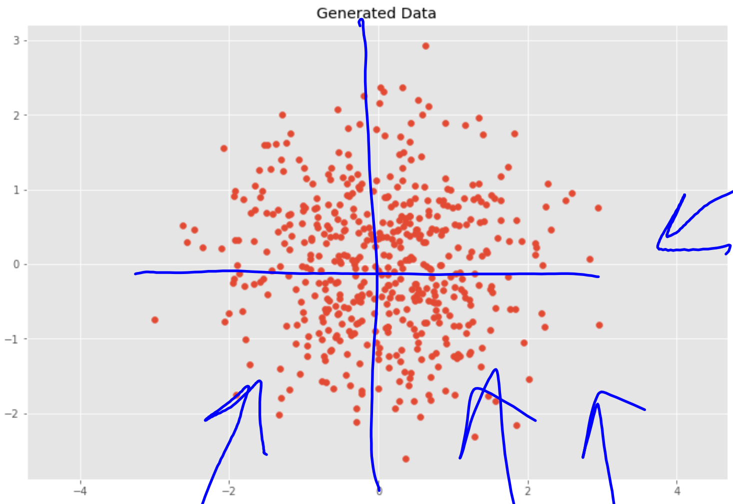
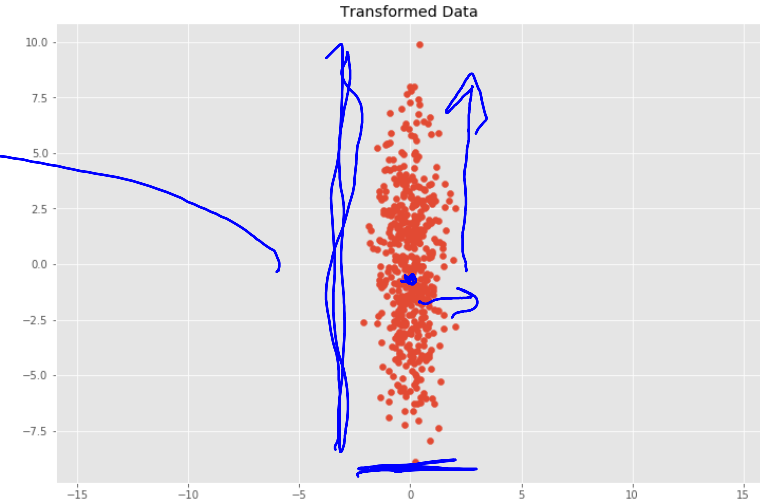
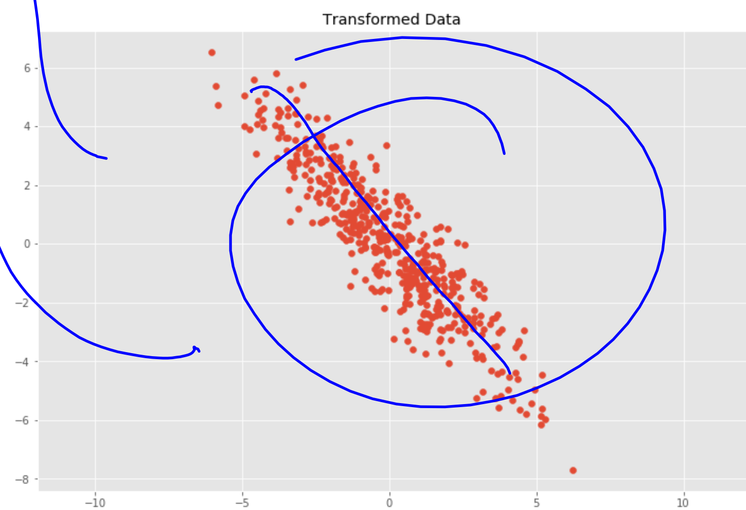


Figure 10.3. Mahalanobis distance of points from the center of a two-dimensional set of 2002 points.

Mahalanobis Distance







Mahalanobis Distance

- Mahalanobis Distance

$$y^2 = (\mathbf{x} - \bar{\mathbf{x}})' S^{-1} (\mathbf{x} - \bar{\mathbf{x}})$$

- S is the covariance matrix:

$$S = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \bar{X})(X_i - \bar{X})'$$

- For 2-dimensional data:

$$\begin{pmatrix} \sigma(x,x) & \sigma(x,y) \\ \sigma(y,x) & \sigma(y,y) \end{pmatrix}$$

Likelihood approach

- **Assume** the dataset 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

Likelihood approach

Data distribution, D = (1 – λ) M + λ A

- M is a probability distribution estimated from data
- A is initially assumed to be uniform distribution
- Likelihood at time t:

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

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

Statistical Anomaly detection

- **Pros**
  - Statistical tests are well-understood and well-validated.
  - Quantitative measure of degree to which object is an outlier.

- **Cons**
  - Data may be hard to model parametrically.
    - multiple modes
    - variable density
  - In high dimensions, data may be insufficient to estimate true distribution.

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Proximity-based Anomaly detection

Proximity-based Anomaly detection

Anomalies are objects far away from other objects.

- An object is an **anomaly** if the nearest neighbors of the object are **far** away, i.e., the **proximity** of the object significantly deviates from the proximity of most of the other objects in the same data set

- Common approach:
  - Outlier score is distance to k^{th} nearest neighbor.
  - Score sensitive to choice of k.

Proximity-based anomaly detection

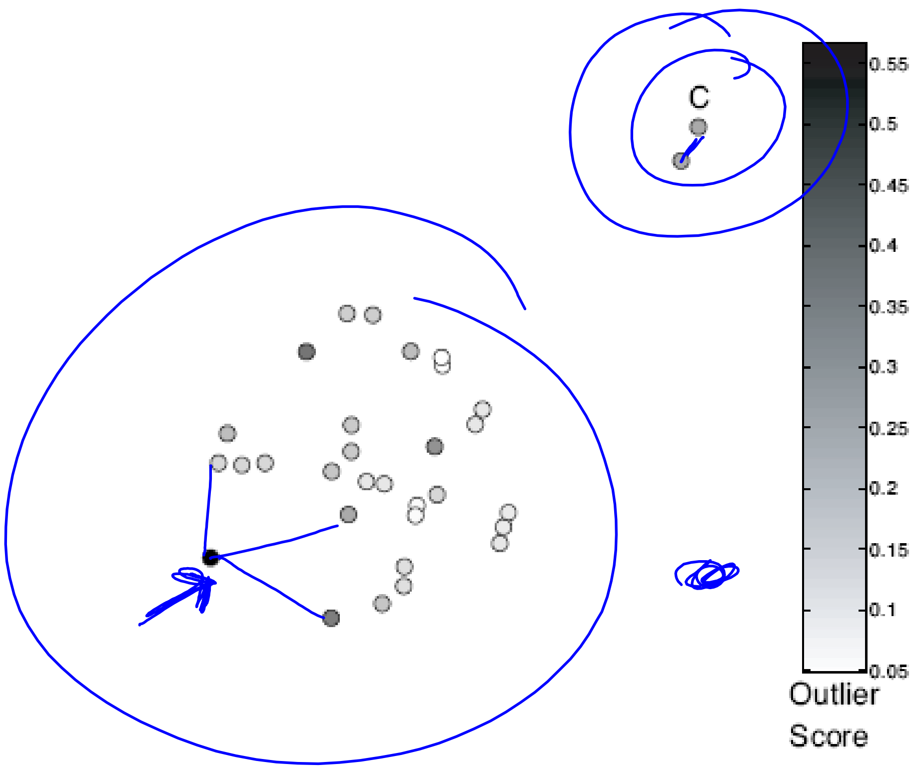


Figure 10.5. Outlier score based on the distance to the first nearest neighbor. Nearby outliers have low outlier scores.

Proximity-based anomaly detection

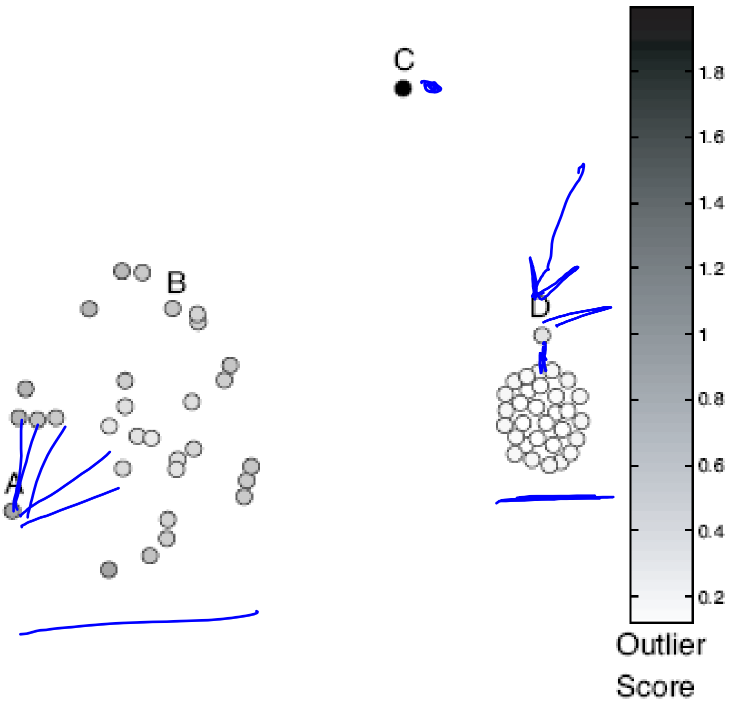


Figure 10.7. Outlier score based on the distance to the fifth nearest neighbor. Clusters of differing density.

Proximity-based outlier detection

Pros

- Easier to define a proximity measure for a dataset than determine its statistical distribution.
- Quantitative measure of degree to which object is an outlier.
- Deals naturally with multiple modes.

Cons

- $O(n^2)$ complexity.
- Score sensitive to choice of k.
- Does not work well if data has widely variable density.

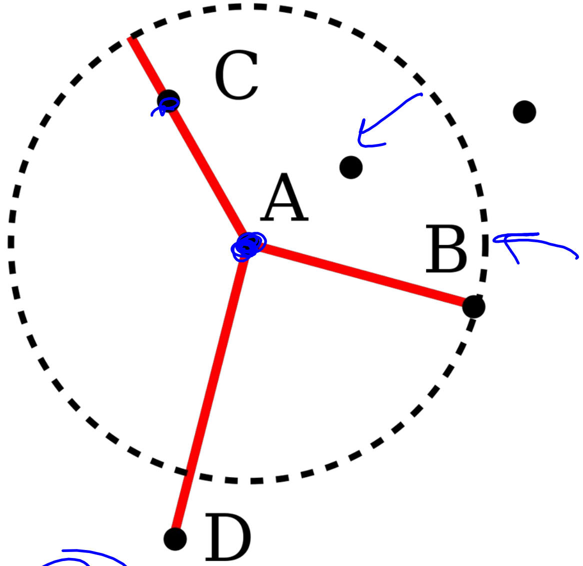
Density-based Anomaly detection

Density-based outlier detection

Outliers are objects in regions of low density.

- Outlier score is the **inverse of the density** around a point
- Scores usually based on **proximities**.
- Example scores:
  - # points within a fixed radius d
  - Reciprocal of average distance to *k* nearest neighbors:

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



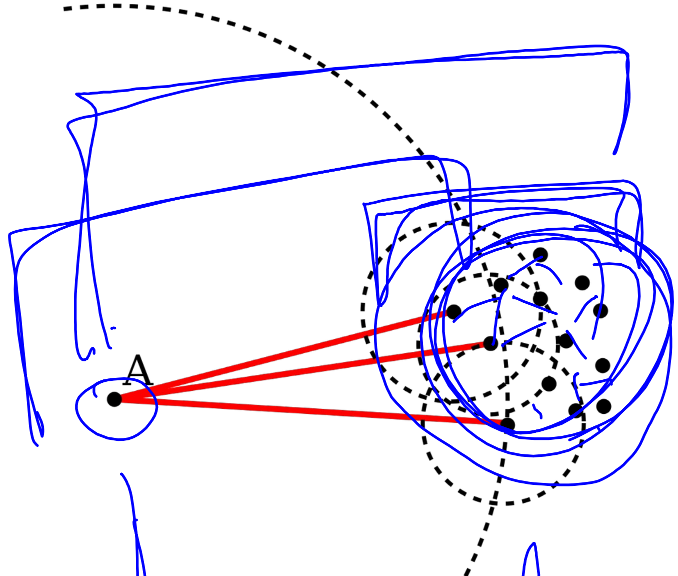
Tend to work **poorly** if data has **variable density**.

Image: https://en.wikipedia.org/wiki/Local_outlier_factor#/media/File:Reachability-distance.svg

Density-based outlier detection

Relative density outlier score

- Local Outlier Factor (LOF)
- **Reciprocal** of average distance to *k* nearest neighbors, relative to that of those *k* neighbors.

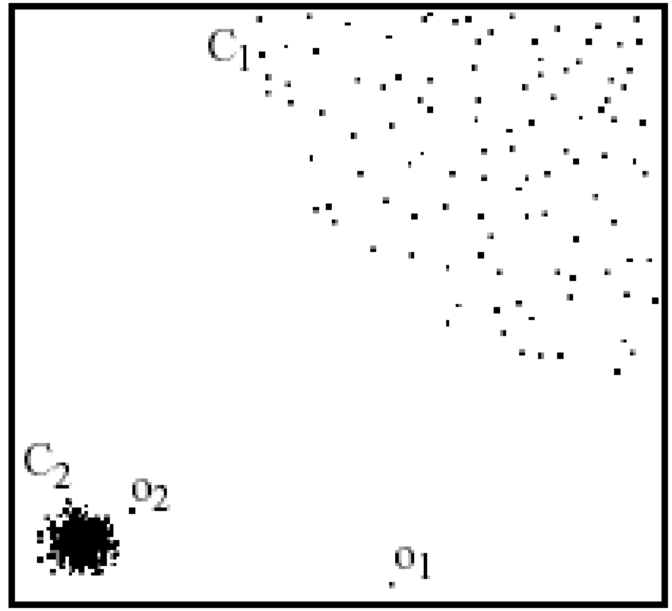


$$\text{relative density}(\mathbf{x}, k) = \frac{\text{density}(\mathbf{x}, k)}{\frac{1}{k}\sum_{\mathbf{y} \in N(\mathbf{x}, k)} \text{density}(\mathbf{y}, k)}$$

Image: https://en.wikipedia.org/wiki/File:LOF-idea.svg

Density-based outlier detection

In the NN approach, o_2 is not considered as outlier, while LOF approach find both o_1 and o_2 as outliers!



Density-based outlier detection

Pros

- Quantitative measure of degree to which object is an outlier.
- Can work well even if data has variable density.

Cons

- $O(n^2)$ complexity
- Must choose parameters
  - *k* for nearest neighbor
  - *d* for distance threshold

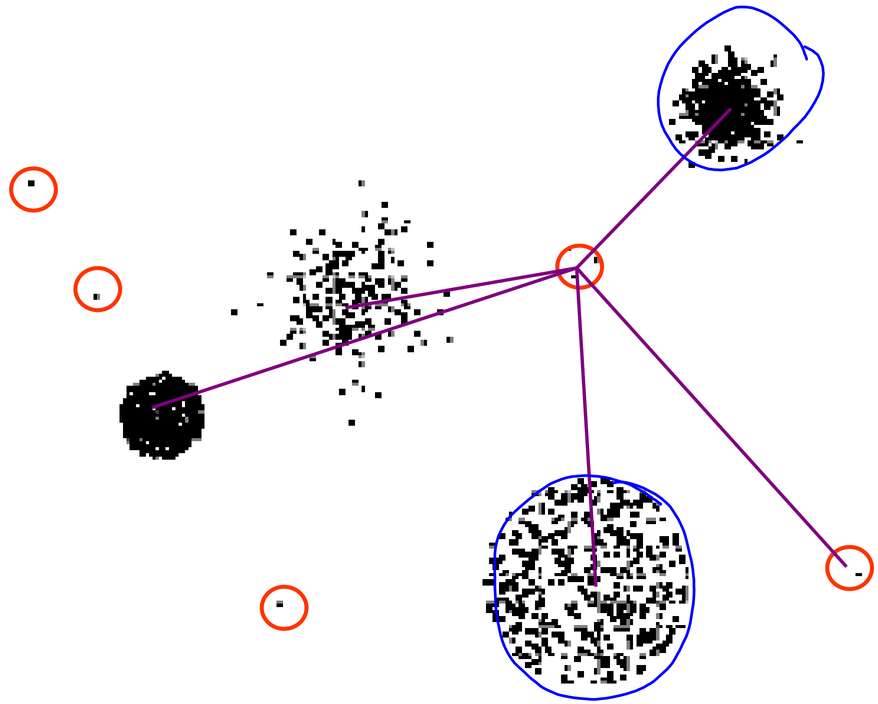
Cluster-based Anomaly Detection

Cluster-based outlier detection

Outliers are objects that do not belong strongly to any cluster.

Approaches:

- Assess degree to which object belongs to any cluster.
- Eliminate object(s) to improve objective function.
- Discard small clusters far from other clusters



Issue:

- Outliers may affect initial formation of clusters.

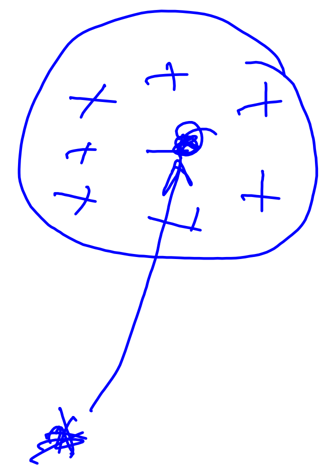
Cluster-based outlier detection

Assess degree to which object belongs to any cluster.

- For prototype-based clustering (e.g. k-means), use distance to cluster centers.

- To deal with variable density clusters, use relative distance:

$$\frac{\text{distance}(\mathbf{x}, centroid_C)}{\text{median}\left(\left\{\forall_{x'\in C}\ \text{distance}(\mathbf{x}', centroid_C)\right\}\right)}$$



- Similar concepts for density-based or connectivity-based clusters.

Cluster-based outlier detection

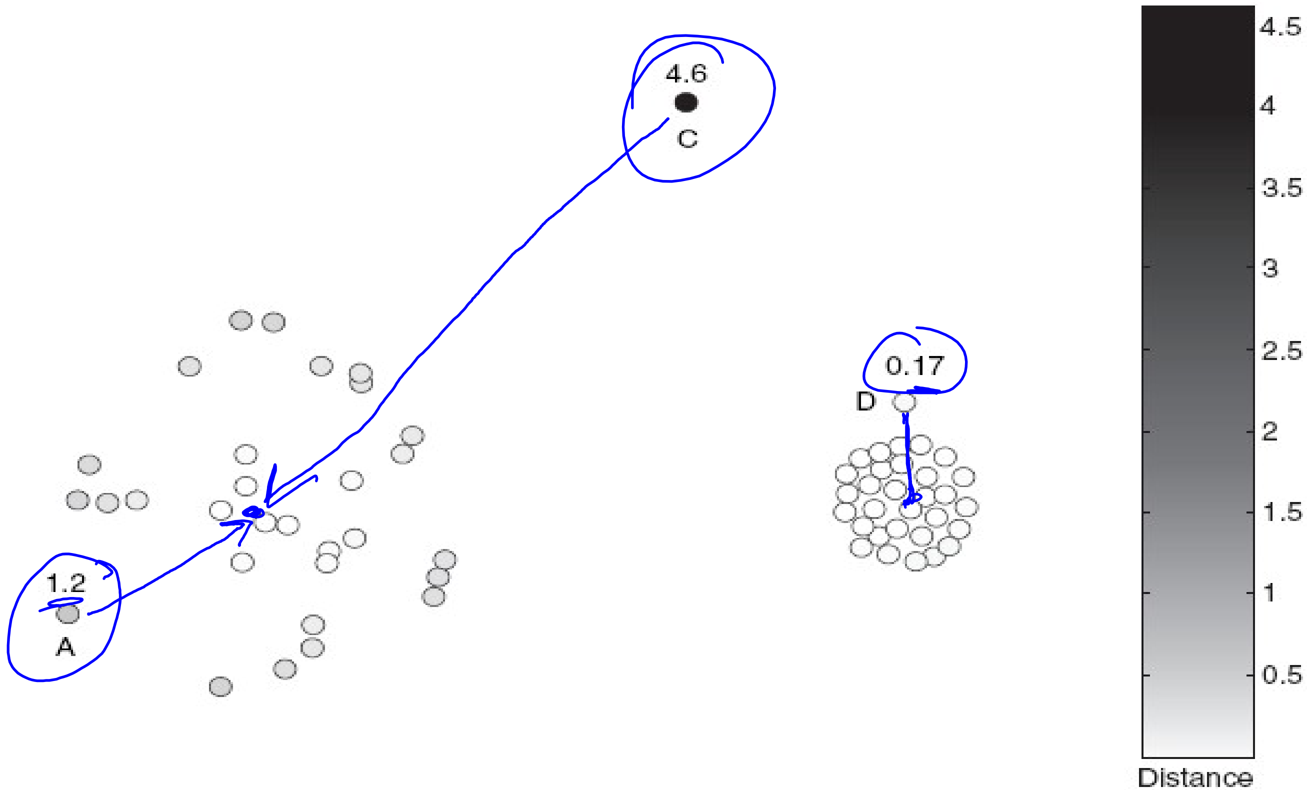


Figure 10.9. Distance of points from closest centroid.

distance of points from nearest centroid

Cluster-based outlier detection

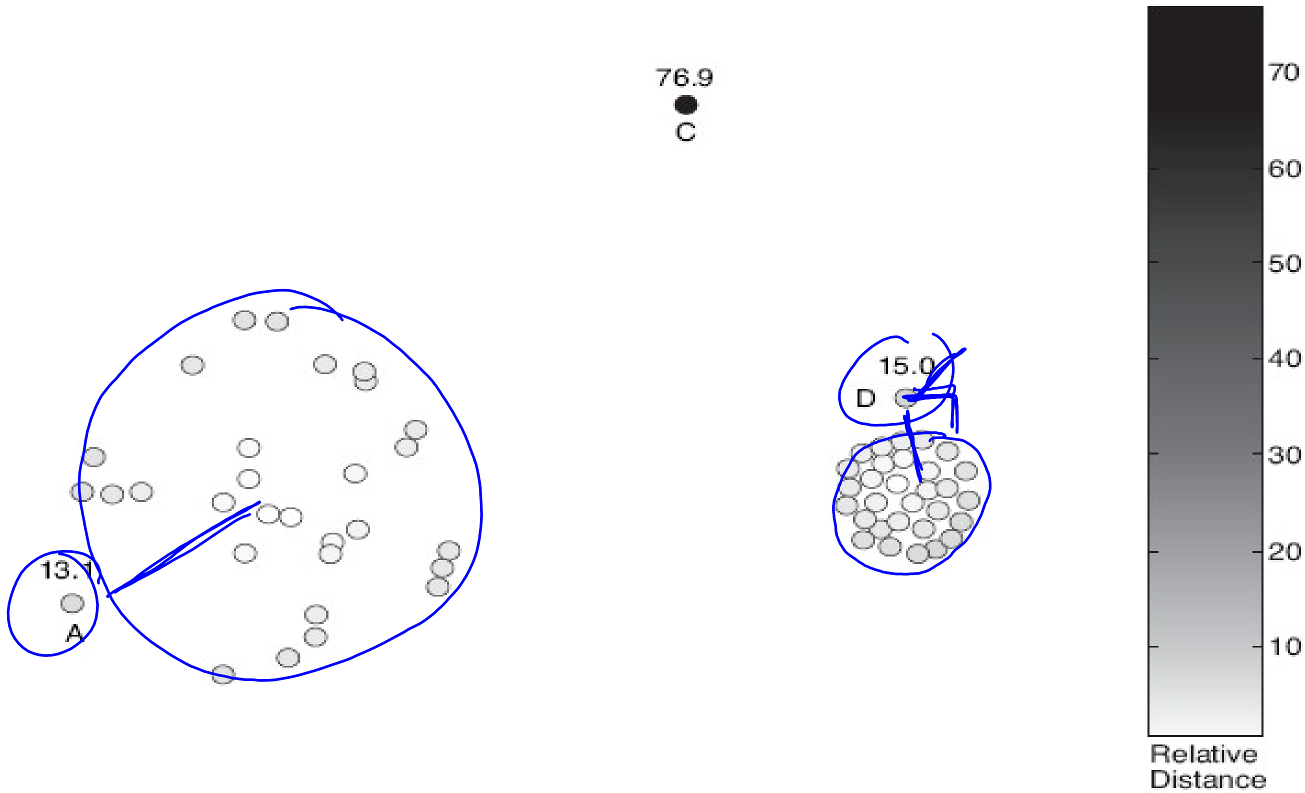


Figure 10.10. Relative distance of points from closest centroid.

relative distance of points from nearest centroid

Cluster-based outlier detection

Eliminate object(s) to improve objective function.

1) Form initial set of clusters.
2) Remove the object which most improves objective function.
3) Repeat step 2) until …

Discard small clusters far from other clusters.

- Need to define thresholds for “small” and “far”.

Cluster-based outlier detection

Pros:

- Some clustering techniques have *O*(*n*) complexity.
- Extends concept of outlier **from single objects to groups** of objects.

Cons:

- Requires thresholds for minimum size and distance.
- Sensitive to number of clusters chosen.
- Hard to associate outlier score with objects.
- Outliers may affect initial formation of clusters.

Summary

Today

- Anomalies – what are they and why are they important?
- Supervised, semi-supervised, or unsupervised anomaly detection
- Statistical, proximity-based, clustering-based anomaly detectoin

Next up

- Ethics in Machine Learning
- Friday: Recognizing and measuring (un)fairness in machine learning
- Next Tuesday: Responsible AI at seek.com (Guest lecture)

References

- *Tan et al (2006) Introduction to Data Mining. Section 4.3, pp 150-171. (Chapter 10)*
- V. Chandola, A. Banerjee, and V. Kumar, (2009). Anomaly detection: A survey. *ACM computing surveys (CSUR)*, *41*(3), 1-58.
- A. Banerjee, et al (2008). Tutorial session on anomaly detection. The SIAM Data Mining Conference (SDM08)