Anomaly Detection

Lecture Notes for Chapter 9

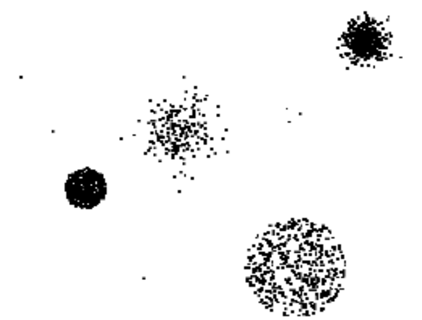
Introduction to Data Mining, 2nd Edition

by

Tan, Steinbach, Karpatne, Kumar

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
  - Unusually high blood pressure
  - 200 pound, 2 year old

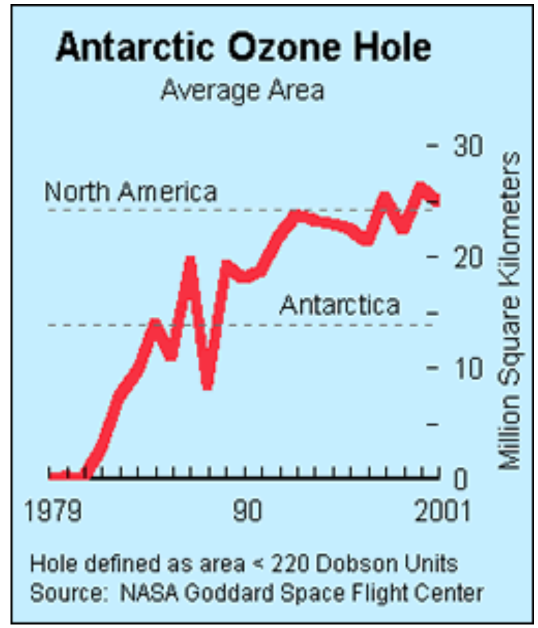
Importance of Anomaly Detection

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!



Source:
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

https://umn.zoom.us/my/kumar001

  – Unusually tall people

- Data errors
  – 200 pound 2 year old

Distinction Between Noise and Anomalies

- Noise doesn’t necessarily produce unusual values or objects

- Noise is not interesting

- Noise and anomalies are related but distinct concepts

Model-based vs Model-free

- Model-based Approaches
  - Model can be parametric or non-parametric
  - Anomalies are those points that don't fit well
  - Anomalies are those points that distort the model
- Model-free Approaches
  - Anomalies are identified directly from the data without building a model
- Often the underlying assumption is that the most of the points in the data are normal

General Issues: Label vs Score

- Some anomaly detection techniques provide only a binary categorization

- Other approaches measure the degree to which an object is an anomaly
  - This allows objects to be ranked
  - Scores can also have associated meaning (e.g., statistical significance)

Anomaly Detection Techniques

- Statistical Approaches

- Proximity-based
  - Anomalies are points far away from other points

- Clustering-based
  - Points far away from cluster centers are outliers
  - Small clusters are outliers

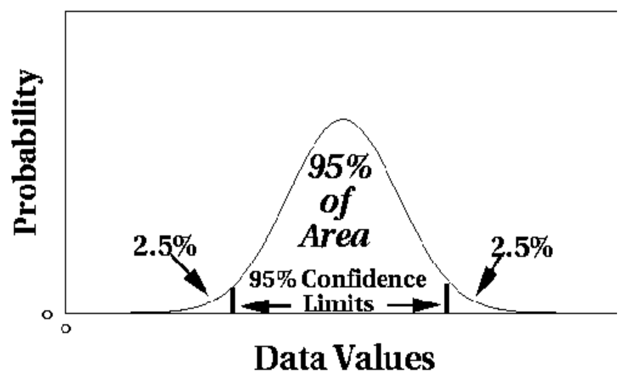
- Reconstruction Based

Statistical Approaches

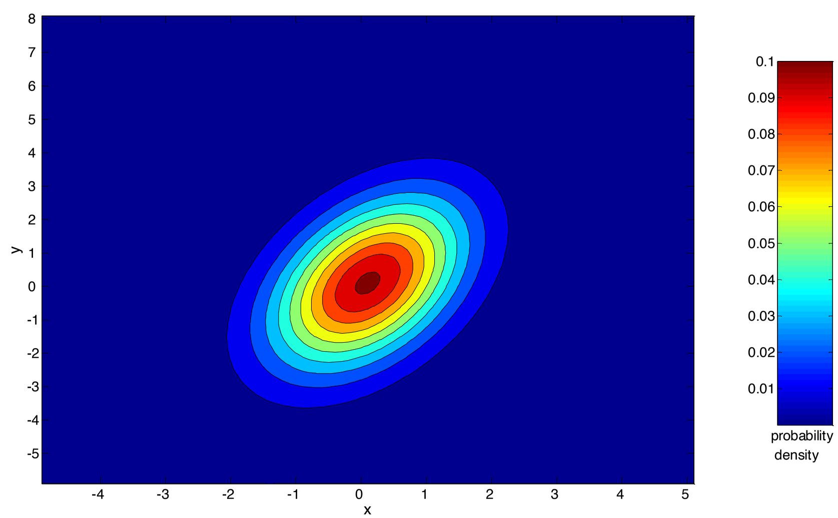
Probabilistic definition of an outlier: An outlier is an object that has a low probability with respect to a probability distribution model of the data.

- 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:

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

Statistically-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

Statistically-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:

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

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

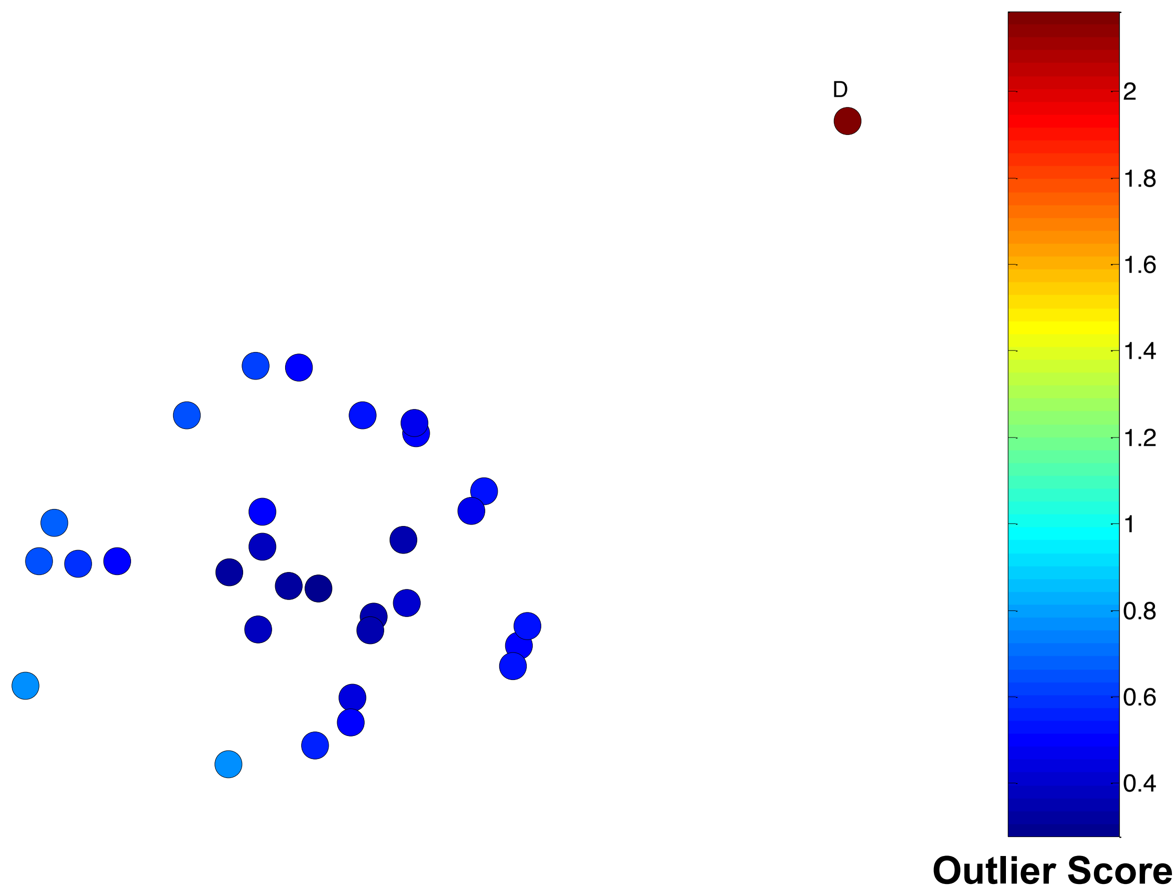
Strengths/Weaknesses of Statistical Approaches

- 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

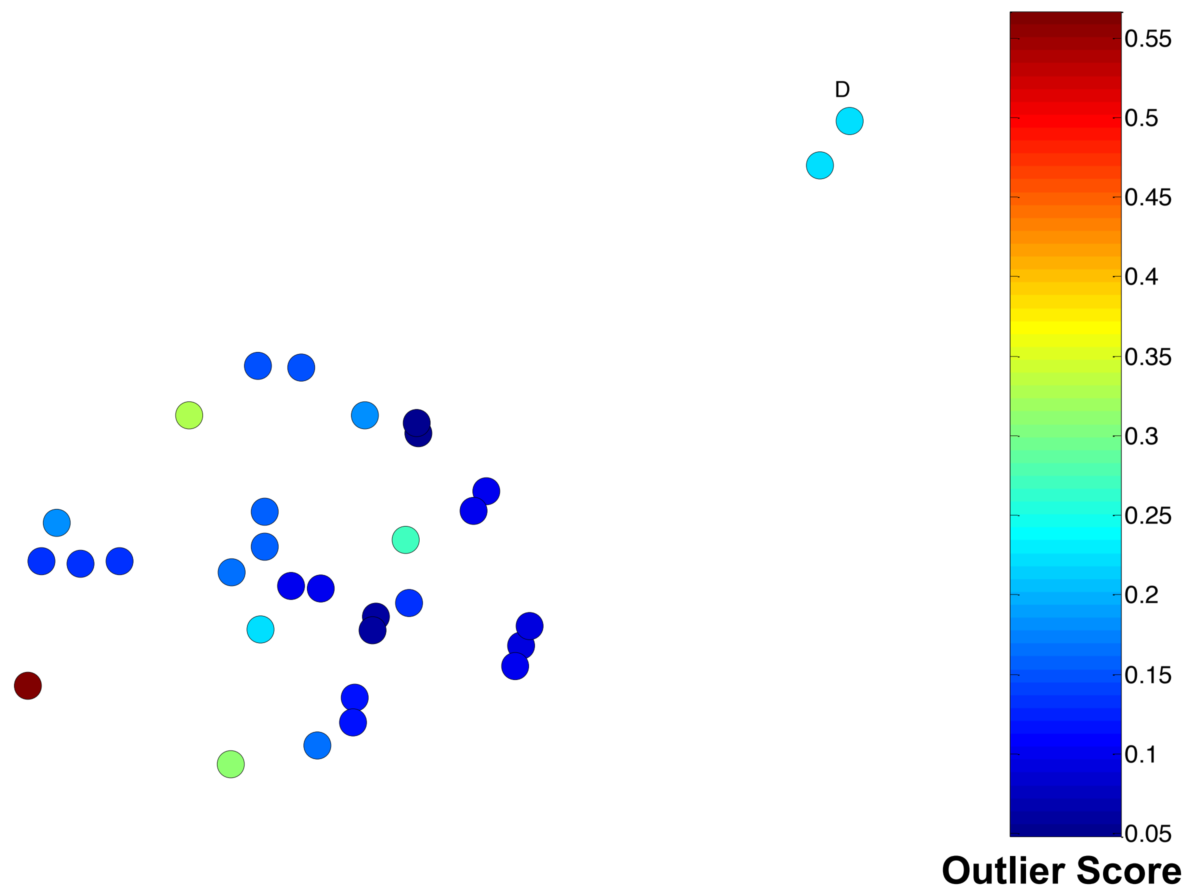
Distance-Based Approaches

- The outlier score of an object is the distance to its kth nearest neighbor

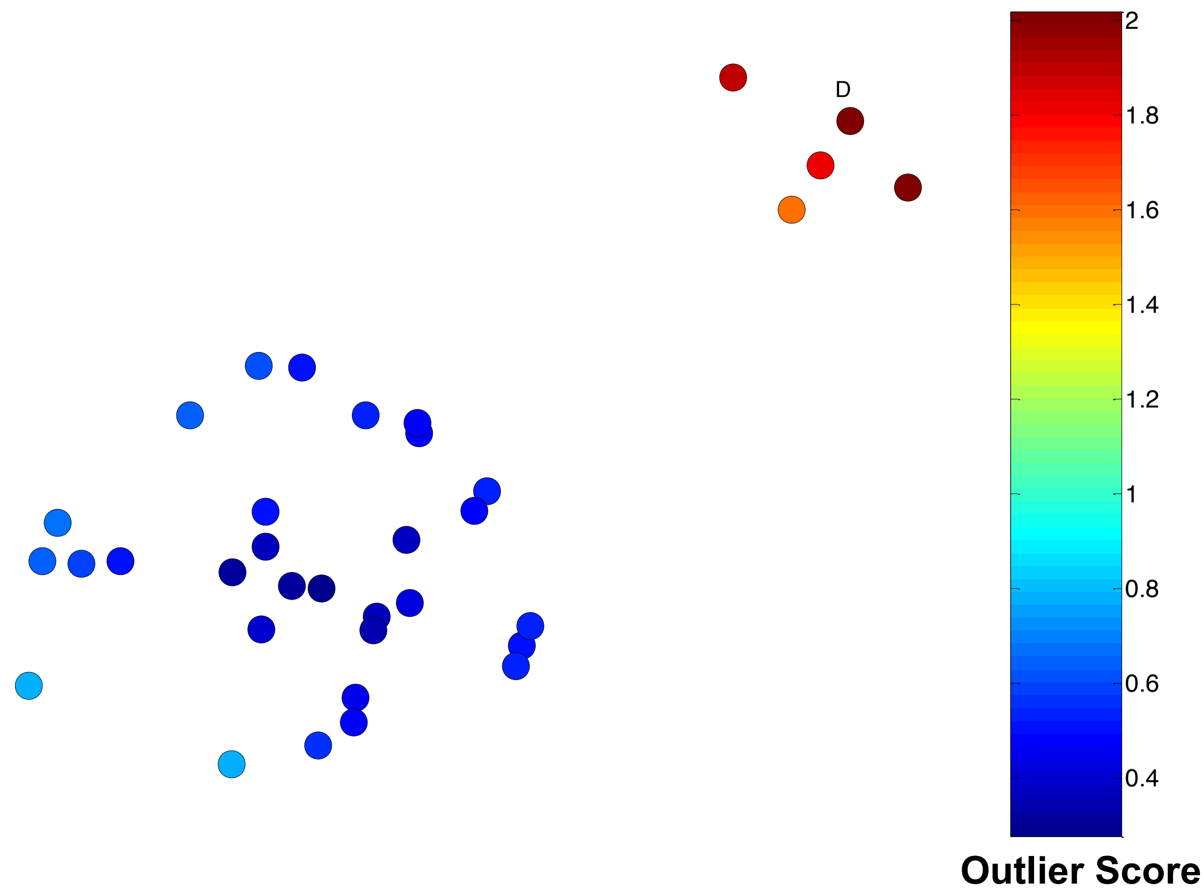
One Nearest Neighbor - One Outlier



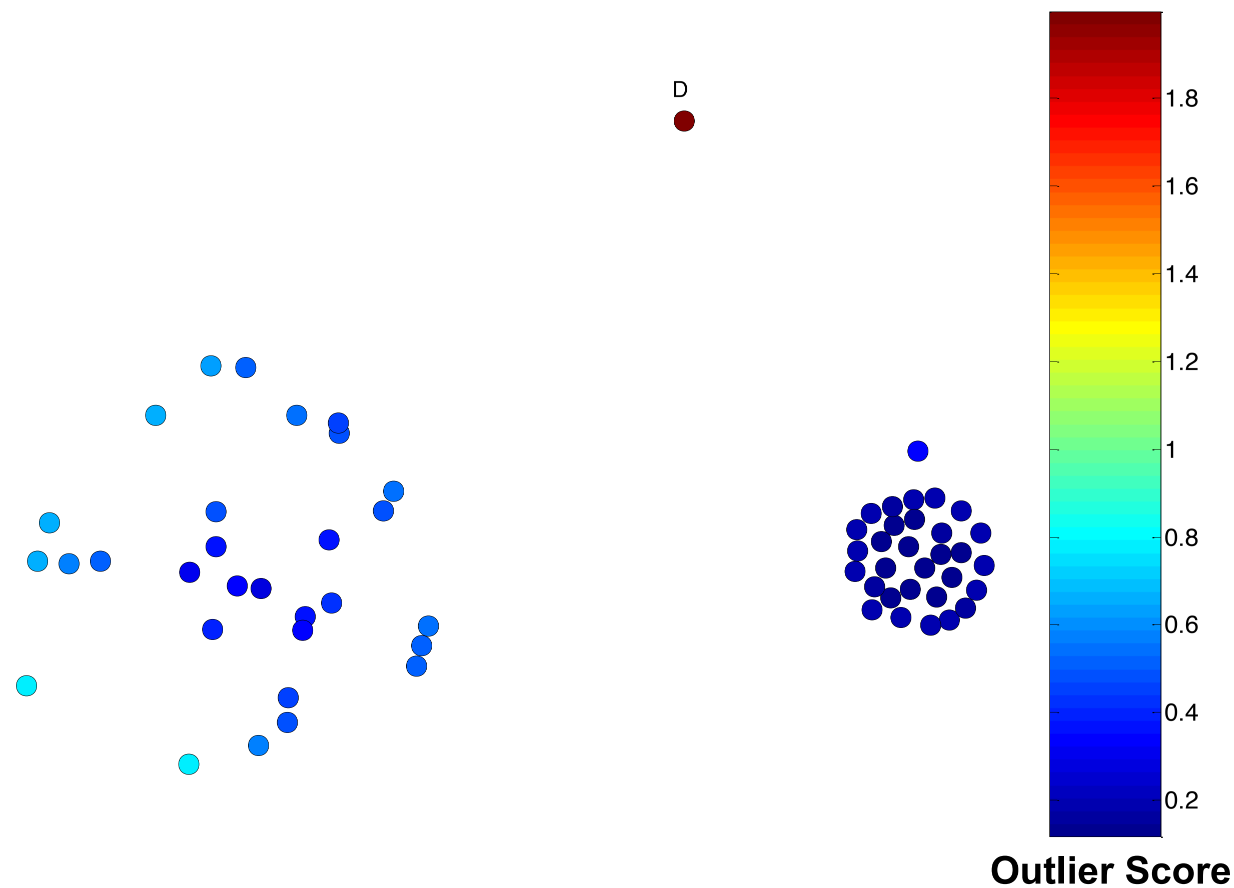
One Nearest Neighbor - Two Outliers



Five Nearest Neighbors - Small Cluster



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
- Let $y_1, \ldots, y_k$ be the k nearest neighbors of $\boldsymbol{x}$

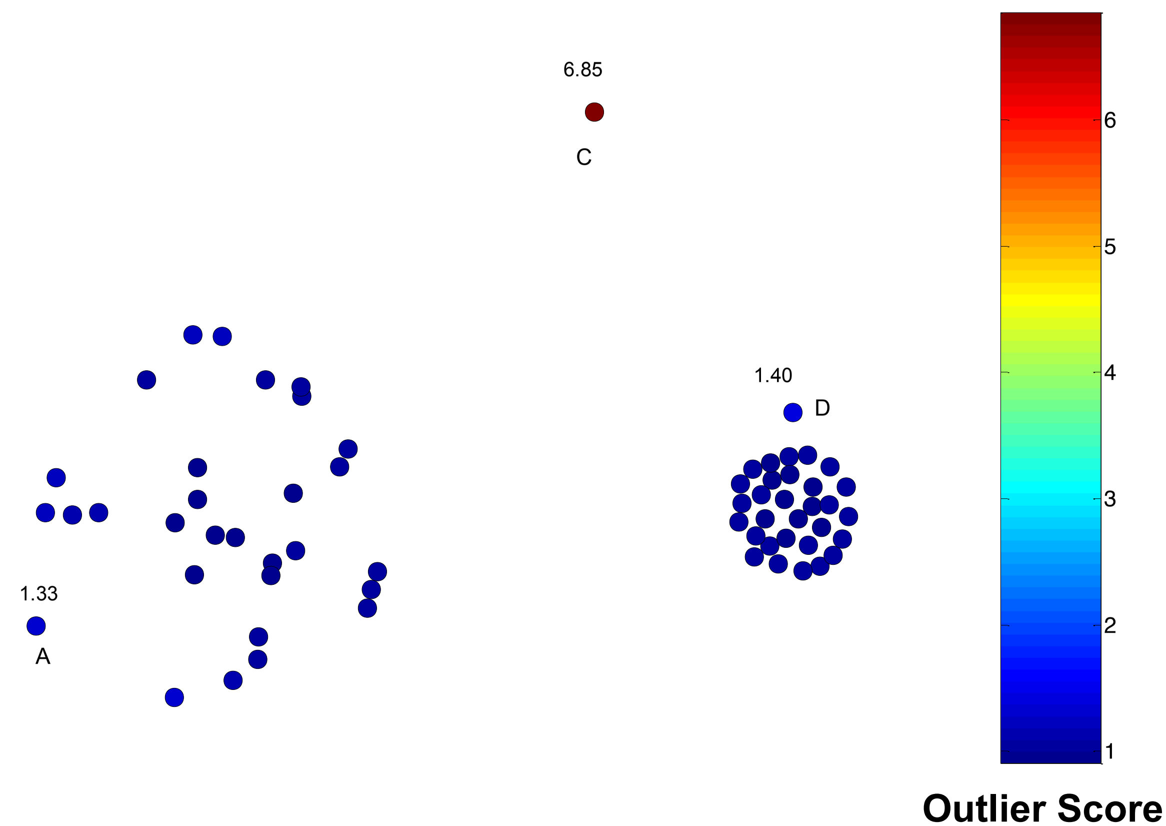
$$density(\boldsymbol{x}, k) = \frac{1}{dist(\boldsymbol{x}, k)} = \frac{1}{dist(\boldsymbol{x}, \boldsymbol{y}_k)}$$

$$relative\ density(\boldsymbol{x}, k) = \frac{\sum_{i=1}^{k} density(\boldsymbol{y}_i, k)/k}{density(\boldsymbol{x}, k)}$$

$$= \frac{dist(\boldsymbol{x}, k)}{\sum_{i=1}^{k} dist(\boldsymbol{y}_i, k)/k} = \frac{dist(\boldsymbol{x}, \boldsymbol{y})}{\sum_{i=1}^{k} dist(\boldsymbol{y}_i, k)/k}$$

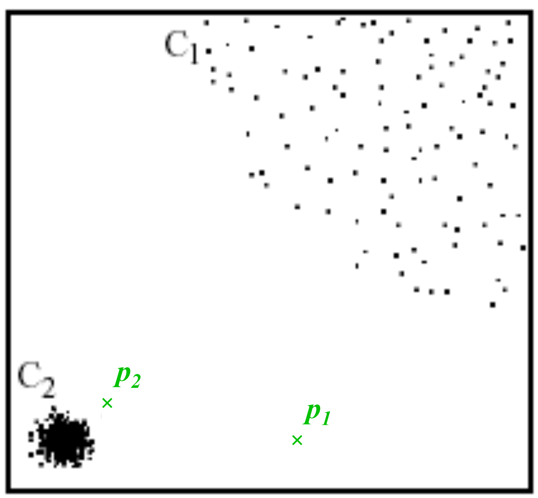
- Can use average distance instead

Relative Density Outlier Scores



Relative 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

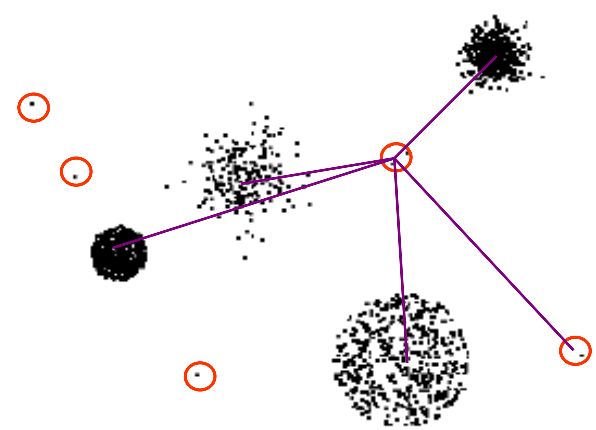
- Expensive – $O(n^2)$

- Sensitive to parameters

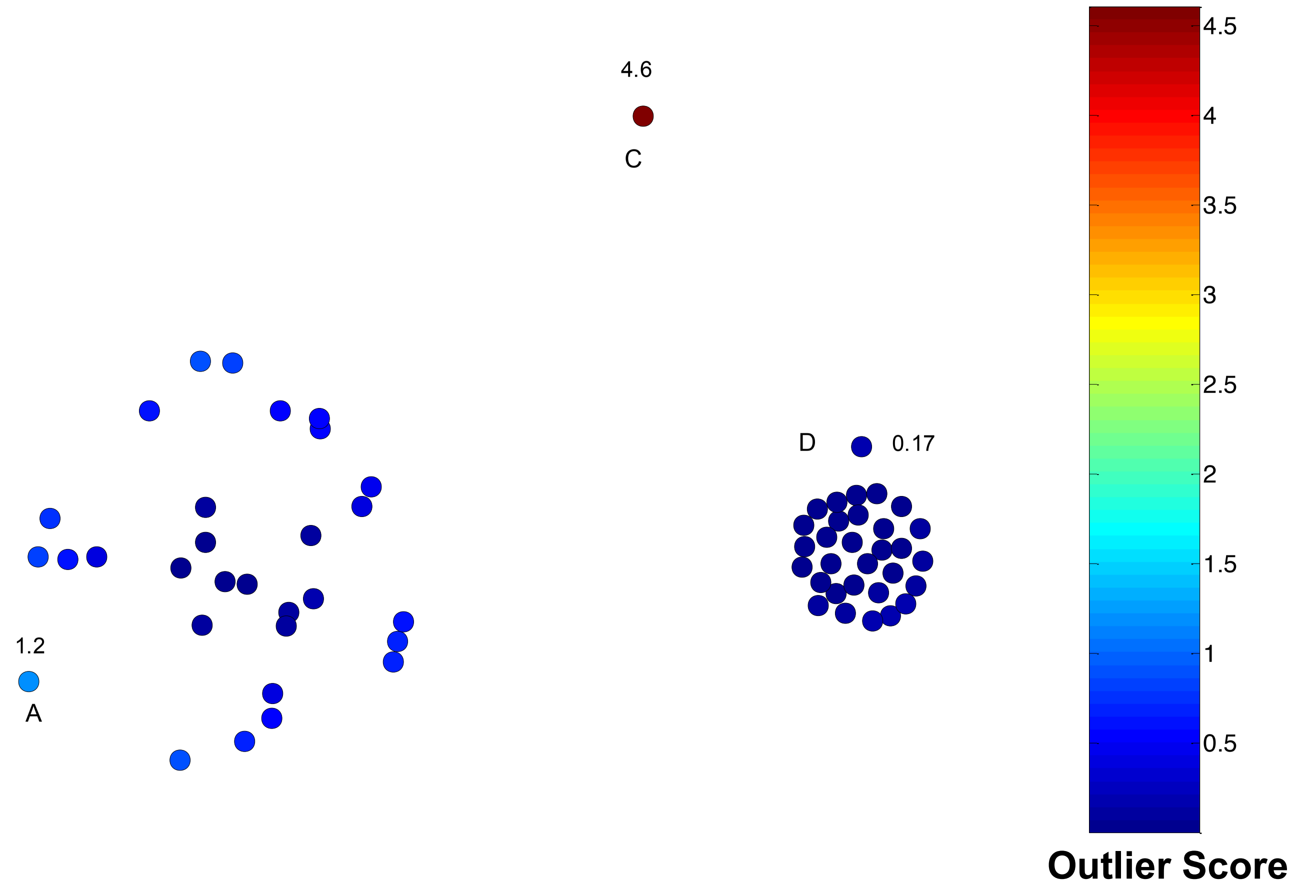
- Density becomes less meaningful in high-dimensional space

Clustering-Based Approaches

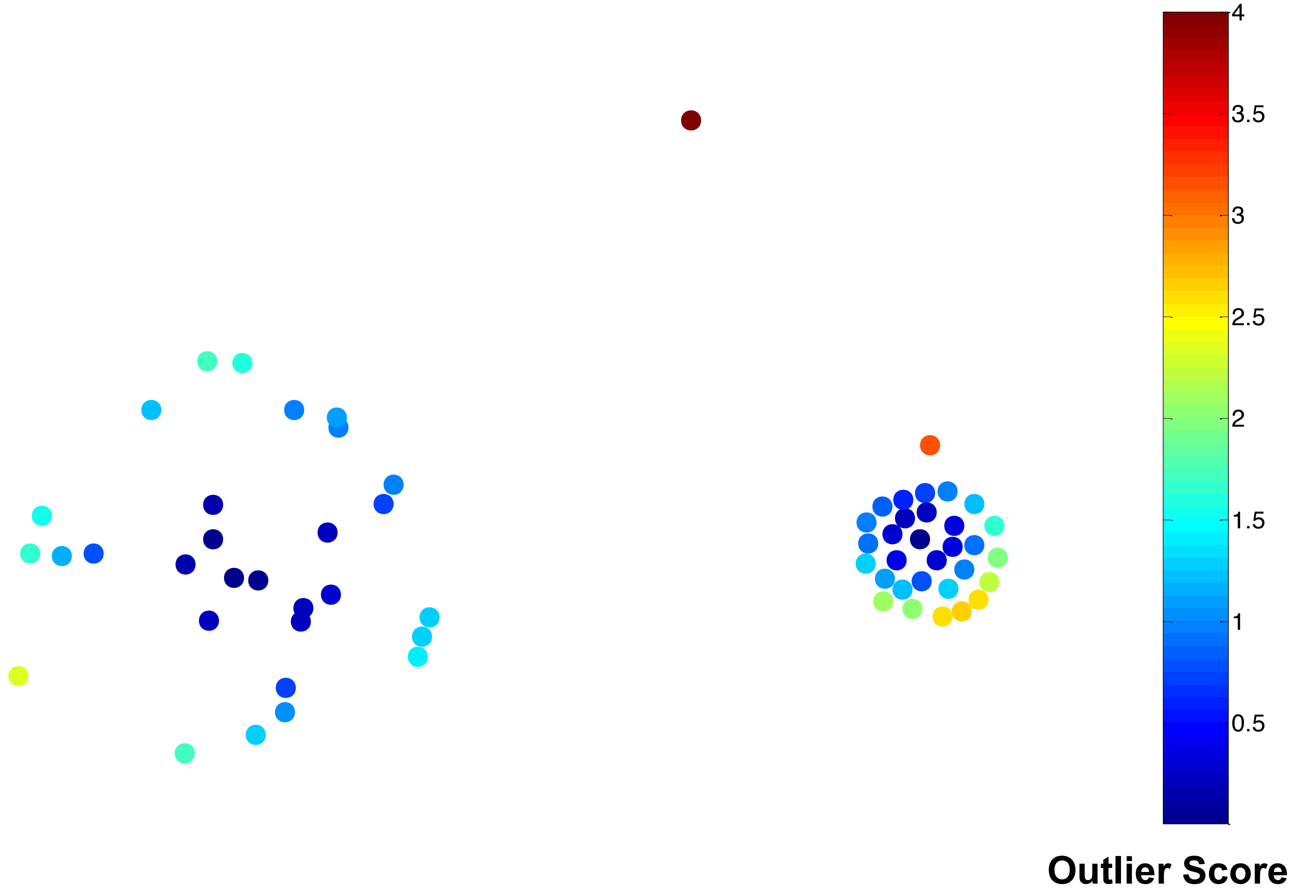
- An object is a cluster-based outlier if it does not strongly belong to any cluster
  - For prototype-based clusters, an object is an outlier if it is not close enough to a cluster center
    - Outliers can impact the clustering produced
  - For density-based clusters, an object is an outlier if its density is too low
    - Can't distinguish between noise and outliers
  - For graph-based clusters, an object is an outlier if it is not well connected



Distance of Points from Closest Centroids



Relative Distance of Points from Closest Centroid



Strengths/Weaknesses of Clustering-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

Reconstruction-Based Approaches

- Based on assumptions there are patterns in the distribution of the normal class that can be captured using lower-dimensional representations
- Reduce data to lower dimensional data
  - E.g. Use Principal Components Analysis (PCA) or Auto-encoders
- Measure the reconstruction error for each object
  - The difference between original and reduced dimensionality version

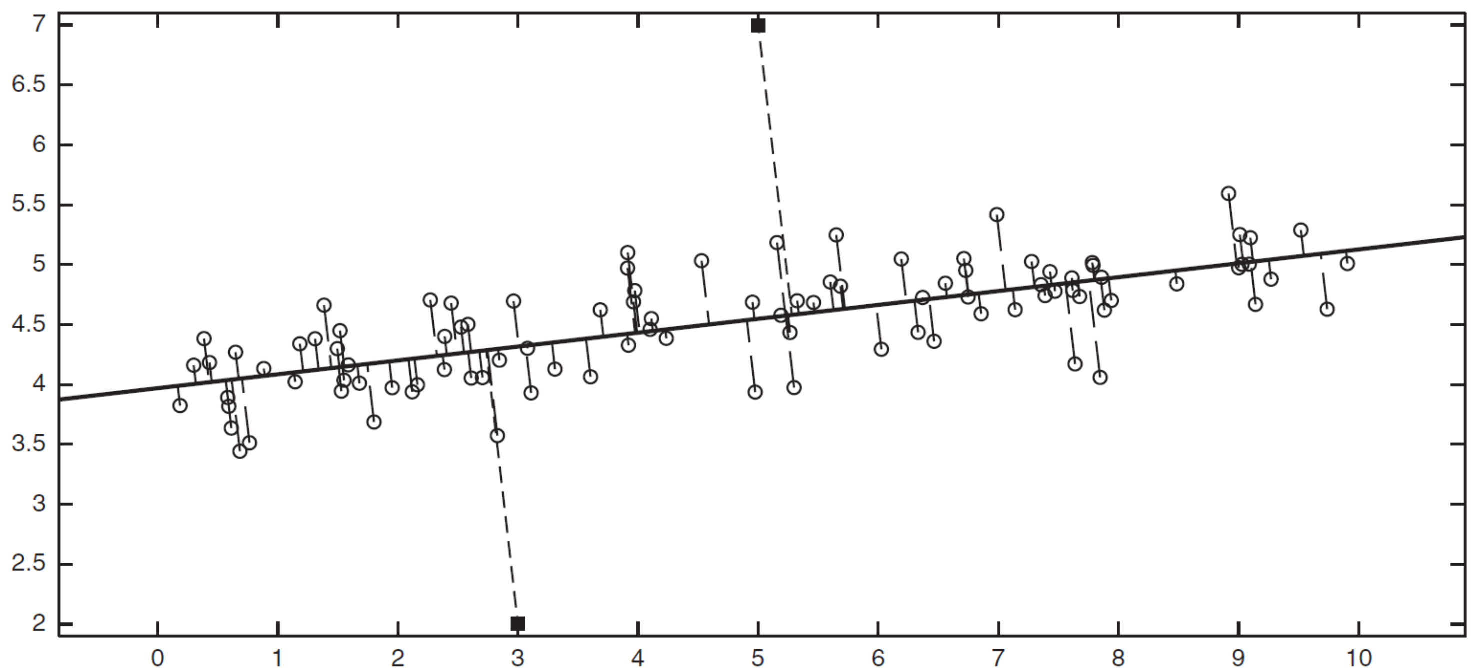
Reconstruction Error

- Let $\mathbf{x}$ be the original data object
- Find the representation of the object in a lower dimensional space
- Project the object back to the original space
- Call this object $\hat{\mathbf{x}}$

$$\text{Reconstruction Error}(\mathbf{x}) = \|\mathbf{x} - \hat{\mathbf{x}}\|$$

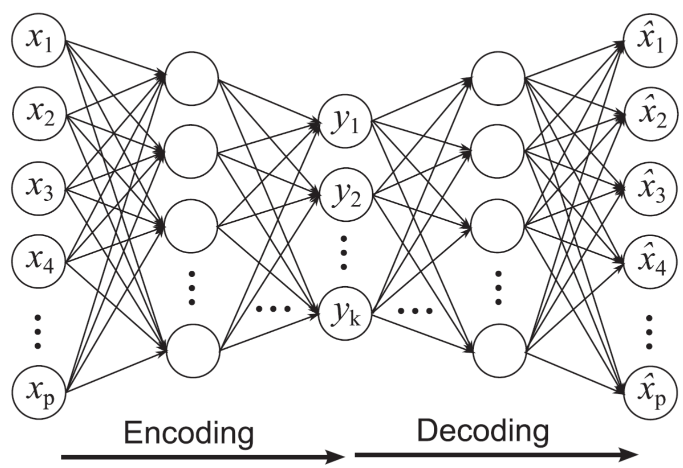
- Objects with large reconstruction errors are anomalies

Reconstruction of two-dimensional data



Basic Architecture of an Autoencoder

- An autoencoder is a multi-layer neural network
- The number of input and output neurons is equal to the number of original attributes.



Strengths and Weaknesses

- Does not require assumptions about distribution of normal class
- Can use many dimensionality reduction approaches
- The reconstruction error is computed in the original space
  - This can be a problem if dimensionality is high

One Class SVM

- Uses an SVM approach to classify normal objects
- Uses the given data to construct such a model
- This data may contain outliers
- But the data does not contain class labels
- How to build a classifier given one class?

How Does One-Class SVM Work?

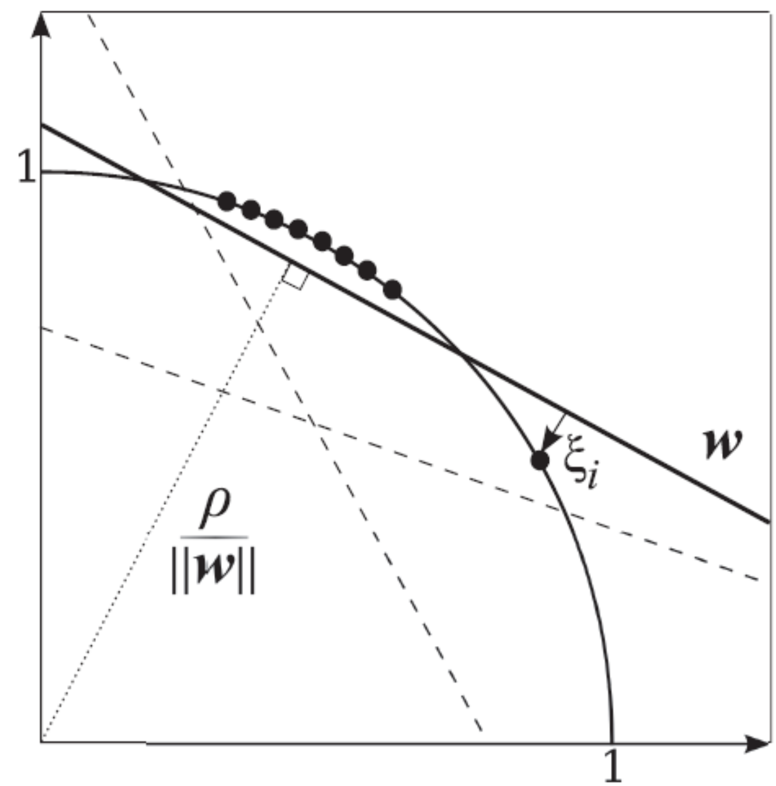
- Uses the “origin” trick
- Use a Gaussian kernel $\kappa(\mathbf{x}, \mathbf{y}) = \exp(-\frac{||\mathbf{x} - \mathbf{y}||^2}{2\sigma^2})$
  - Every point mapped to a unit hypersphere

    $$\kappa(\mathbf{x}, \mathbf{x}) = \langle \phi(\mathbf{x}), \phi(\mathbf{x}) \rangle = ||\phi(\mathbf{x})||^2 = 1$$
  - Every point in the same orthant (quadrant)

    $$\kappa(\mathbf{x}, \mathbf{y}) \ = \ \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle \ \geq \ 0$$

- Aim to maximize the distance of the separating plane from the origin

Two-dimensional One Class SVM



Equations for One-Class SVM

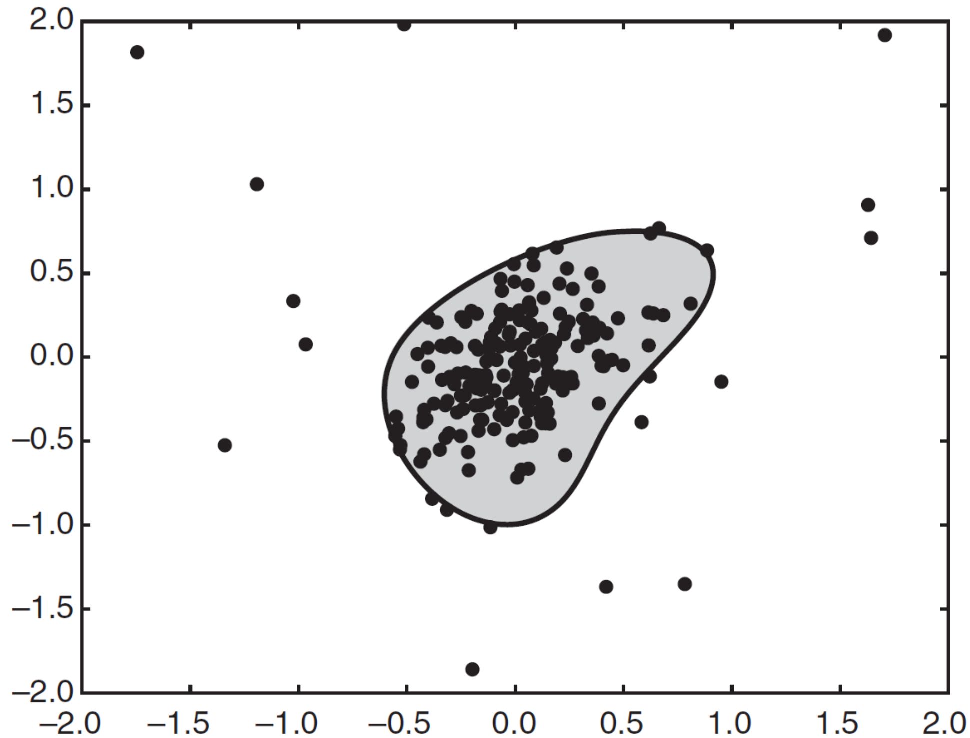
- Equation of hyperplane $\langle \mathbf{w}, \phi(\mathbf{x}) \rangle = \rho$
- ϕ is the mapping to high dimensional space
- Weight vector is $\mathbf{w} = \sum_{i=1}^{n} \alpha_i \phi(\mathbf{x_i})$
- ν is fraction of outliers
- Optimization condition is the following

$$\min_{\mathbf{w},\ \rho,\ \xi} \ \frac{1}{2}||\mathbf{w}||^2 - \rho + \frac{1}{n\nu}\sum_{i=1}^{n} \xi_i,$$

$$\text{subject to: } \langle \mathbf{w}, \phi(\mathbf{x_i}) \rangle \geq \rho - \xi_i, \ \ \xi_i \geq 0$$

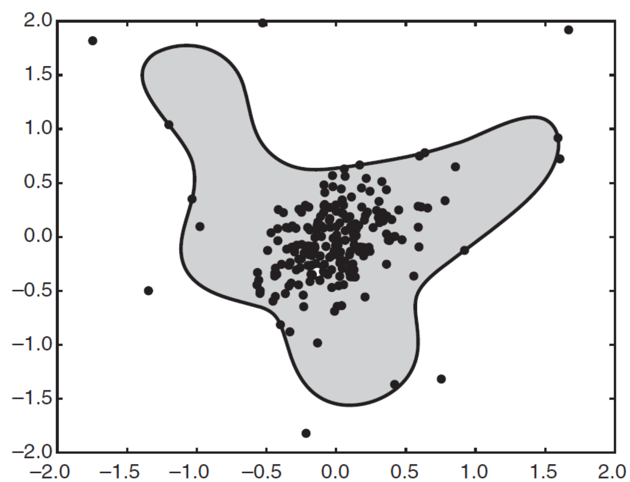
Finding Outliers with a One-Class SVM

- Decision boundary with $\nu = 0.1$

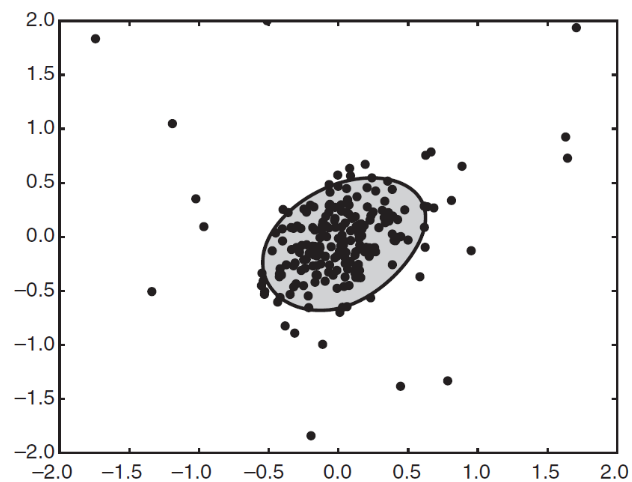


Finding Outliers with a One-Class SVM

- Decision boundary with $\nu = 0.05$ and $\nu = 0.2$



(a) $\nu = 0.05$.



(b) $\nu = 0.2$.

Strengths and Weaknesses

- Strong theoretical foundation
- Choice of ν is difficult
- Computationally expensive

Information Theoretic Approaches

- Key idea is to measure how much information decreases when you delete an observation

$$Gain(x) = Info(D) - Info(D \setminus x)$$

- Anomalies should show higher gain

- Normal points should have less gain

Information Theoretic Example

- Survey of height and weight for 100 participants

weight	height	Frequency
low	low	20
low	medium	15
medium	medium	40
high	high	20
high	low	5

- Eliminating last group give a gain of 2.08 − 1.89 = 0.19

Strengths and Weaknesses

- Solid theoretical foundation

- Theoretically applicable to all kinds of data

- Difficult and computationally expensive to implement in practice

Evaluation of Anomaly Detection

- If class labels are present, then use standard evaluation approaches for rare class such as precision, recall, or false positive rate
  - FPR is also know as false alarm rate

- For unsupervised anomaly detection use measures provided by the anomaly method
  - E.g. reconstruction error or gain

- Can also look at histograms of anomaly scores.

Distribution of Anomaly Scores

- Anomaly scores should show a tail

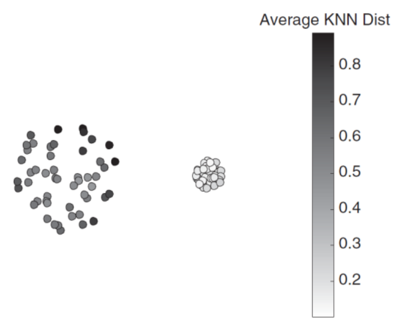


Figure 10.17. Anomaly score based on average distance to fifth nearest neighbor.

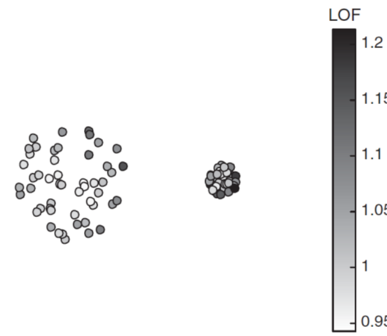


Figure 10.18. Anomaly score based on LOF using five nearest neighbors.