Machine Learning and Data Mining

Outlier Detection

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Outlier Detection in Machine Learning: Overview

- Outlier detection involves identifying data points that deviate significantly from the majority of the dataset
- Such anomalies can indicate:
  - Noise or errors in the data
  - Rare but important events (e.g., fraud, equipment failure)
  - Variability in the underlying process being studied
- Applications include fraud detection, predictive maintenance, healthcare, and finance

Key Techniques for Outlier Detection

- Statistical Methods
  - Identify outliers based on assumptions of the data distribution
  - Examples:
    - Z-Score: Measures the distance from the mean in standard deviations
    - IQR (Interquartile Range): Identifies outliers using quartiles
- Distance-Based Methods
  - Measure the distance of each point to its neighbors
  - Examples:
    - k-Nearest Neighbors (k-NN)
    - DBSCAN (Density-Based Spatial Clustering of Applications with Noise)
- Model-Based Methods
  - Train machine learning models to distinguish normal from abnormal data
  - Examples:
    - Isolation Forest
    - Autoencoders for anomaly detection

Challenges in Outlier Detection

- High Dimensionality
  - Outliers become harder to detect in high-dimensional spaces
  - Distance measures lose significance due to the curse of dimensionality
- Imbalanced Data
  - Outliers are rare, making standard classification approaches less effective
- Noise in Data
  - Differentiating between true outliers and random noise can be challenging
- Dynamic Datasets
  - Continuous data streams may introduce new patterns over time

Evaluation Metrics for Outlier Detection

- Precision
  - Fraction of detected outliers that are true outliers
- Recall
  - Fraction of true outliers that are successfully detected
- F1-Score
  - Harmonic mean of precision and recall
- Area Under Curve (AUC)
  - Evaluates model performance across various thresholds
- Execution Time
  - Important for real-time applications such as fraud detection or predictive maintenance

Applications of Outlier Detection

- Fraud Detection
  - Identify unusual patterns in transactions that indicate fraud
- Predictive Maintenance
  - Detect anomalies in sensor data to predict equipment failures
- Healthcare
  - Identify rare disease cases or anomalies in medical imaging data
- Finance
  - Detect unusual trading activity or financial irregularities
- Network Security
  - Identify abnormal network traffic patterns signaling potential attacks

Significance of Outlier Detection

- Enhancing Data Quality
  - Removing or correcting outliers improves model accuracy
- Critical Insights
  - Detecting rare events can lead to significant operational improvements
- Preventing Losses
  - Early detection of anomalies reduces financial, operational, or reputational damage

Anomaly detection

- Find objects that are different from most other objects
- How to measure such dissimilarity/exceptionality/inconsistency?
- How to explore the data set to find outliers?
- Anomaly does not imply necessarily a small number
- An anomaly can also be caused by errors in data collection

Synonim

anomaly $\leftrightarrow$ outlier

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Focus on some applications of anomaly detection - I

- Fraud detection

  Example Change in purchasing behaviour for credit card customers

- Network intrusion detection

  Example Monitor packets in communication networks to discover attacks

- Ecosystem disturbances

  Example Predict hurricanes, floods, etc. on the basis of metereological parameters

Focus on some applications of anomaly detection - II

- Medical diagnosis

  Example Unusual sympthoms can indicate potential health problems

- Public health

  Example Anomalous diseases can indicate problems in vaccination campaign

Causes of anomalies - I

Data from different classes

- Most item of the previous slide are examples of anomalies that represent a different class of objects
- Hawkins' definition of an Outlier
  - An outlier is an observation that differs so much from other observations as to arouse suspicion that it was generated by a different mechanism

Causes of anomalies - II

Natural variation
: When data can be modeled by a normal distribution, most objects are near a center, extreme values have low likelihood, nevertheless they can be interesting

Data measurement and Collection errors
: Incorrect recordings due to human errors, device-related errors, noise; removal of such errors is usually named Data Cleaning

Approaches to Anomaly Detection - I

Model–based techniques

Build a model of the data (e.g. estimate the parameters of a probability distribution): outliers will fit poorly in the model

- if the model is a set of clusters, then the outlier will not fit well to any cluster
- if the model is a regression then the outlier will be far from the predicted value
- classification-based techniques could fail, because it is difficult to build a model of the, relatively rare, anomalies

Approaches to Anomaly Detection - II

Proximity–based techniques
: Anomalous objects are those that are distant from most of the other objects In two or three dimension, scatter plots allow visual identification of anomalies

Density–based techniques
: Density follows straightforwardly from the proximity measure. Object in low-density regions can be considered outliers. Density can be measured extensively or estimated with some approximation

The use of class labels - I

Supervised: There exists a training set with both anomalous and normal objects
- objects labelled as normal or anomalous
- problem of imbalanced classes

Unsupervised: Labels are not available
- learn from the training set a way to assign to each object a score reflecting the degree of anomaly
- anomalies should be different one from the other

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The use of class labels - II

Semi–supervised The training set contains only normal objects

- compute the anomaly score from the information available for normal objects
- in this case a relation among anomalies does not affect the result
- a.k.a. one class classification

Issues - I

Number of attributes used

- single attribute values can be anomalous, e.g. person's height of mt0.40
- common values can be anomalous when considered together, e.g. a person with (height=mt1.50,weight=kg120)

Global versus Local Perspective

An object may seem unusual w.r.t. all object, but usual w.r.t. its neighborhood

Degree of Anomaly

Instead of a binary decision, the degree allows to set a threshold that can be adjusted in a tuning step

Issues - II

Operation

Discover one-anomaly-at-a-time versus many-anomalies-at-once

- find the most anomalous object, remove it from the data set and loop
- find a set of anomalous objects
- the latter is prone to the problem of masking, e.g. several similar anomalies mask each other
- and also to the problems of swamping, e.g. the anomalies distort the data model and normal objects seem to be anomalous

Issues - III

Evaluation
: Usual measures for the evaluation of classifiers (precision, recall, ...) are uneffective due to the unbalancing of normal and anomalous class

Efficiency
: Classification and statistical methods are usually expensive to set up but lightweight run–time; proximity methods in principle should compare each object with all the others, and tend to have $O(n^2)$ complexity

Probabilistic definition of an Outlier

Definition

An object that has a low probability w.r.t. a probability distribution model of the data

- Probability distribution model created from the data by estimating the parameters for a user–specified distribution
- Statistical tests to identify discordant observations

Issues in probabilistic definition

Identifying the specific distribution

E.g. Gaussian, Poisson, Binomial, ..., a wrong model invalidates the results

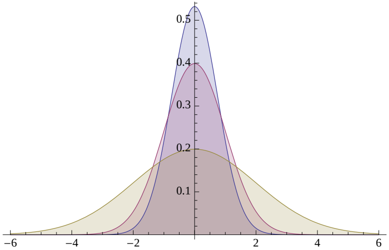
Number of attributes used

There are techniques available for multi–variate data

Mixtures of distributions

Model the data as a mixture of different distributions, usually of the same type but with different parameters (e.g. mixture of Gaussians and Expectation Maximization algorithm)

Detecting Outliers in a Univariate Normal Distribution



Normal PDF for $\sigma = 0.75, 1, 2$

Definition

An object with an attribute value x from a Normal distribution $Nb(0, 1)$ is an outlier if $|x| \geqslant c$, where $prob(|x|) \geqslant c = \alpha$

α is the probability of false positive, i.e. that a regular object is labeled as outlier

Strengths and Weaknesses

- strong theoretical foundations, well established techniques, such as parameter estimation
- plenty of methods for "outlierness" tests for univariate data
- fewer methods available for multivariate data
- bad performance with high-dimensional data

Proximity-based Outlier Detection

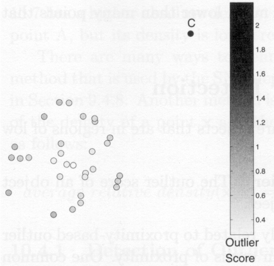
- An object is anomalous if it is distant from most points
- Relies on a proximity measure
- For each object, make (in principle) a sorted list of its neighbors, according to proximity

Distance to k–Nearest Neighbor

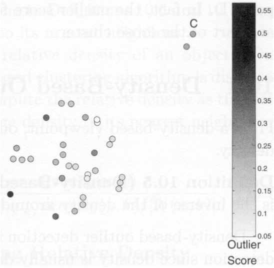
The outlier score of an object is the distance to its k–nearest neighbor

- Highly sensitive to the value of k

Outlier score - I

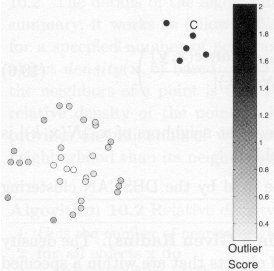


Outlier score based on 5–th nearest neighbor

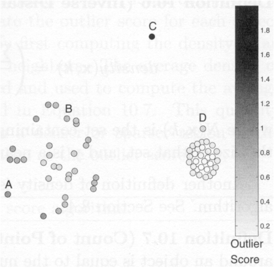


Outlier score based on 1-st nearest neighbor. Nearby outliers have low outlier scores

Outlier score - II



Outlier score based on
5–th nearest neighbor
A small cluster becomes
a set of outliers



Outlier score based on
5–th nearest neighbor
Clusters of different density

Another definition

Definition - *distance–based outlier* [Knorr and Ng.(1998)]

Given a positive real number R and a positive integer k
an object is a *distance–based outlier* if
less than k objects lie within distance R from the object

Proximity–based solutions

- Problem: finding the top m outliers in a data set
- Based on the notion of distance of the k-th Nearest Neighbors
- Brute force solution has complexity $\mathcal{O}(N^2)$
- There exists much more efficient algorithms

The Bay's algorithm [Bay and Schwabacher(2003)]

A simple nested loop with simple pruning

- For each example in $\mathcal{X}$ keep track of the k nearest neighbors found so far
- Determine the cutoff value of the score as the distance of the k-th nearest neighbor of the top m-th outlier found so far
- When an example achieves a score lower than the cutoff it is removed, because it can no longer be an outlier
- Later iterations find increasing scores, and the efficiency of pruning is increasing
- If data are in random order the average complexity is near linear
- Worst case complexity is $\mathcal{O}(N^2)$

Density-based Outlier Detection

Intuition

Outliers are found in low-density areas

Definition - Density–based outlier

The outlier score of an object is the inverse of the density around the object

Definition - Inverse distance

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

where $Nb(\mathrm{x}, k)$ is the set containing the k–nearest neighbors of x

In practice, this is the inverse of the average distance
to the objects in its neighborhood

Alternative definition of density

Definition - Count of Points within a Given Radius

The density around an object is defined as the number of objects that are within a specified distance d from the object

Issues in the choice of d

If d too small the density can be underestimated, with an effect similar to the choice of k too large in distance-based methods

Average Relative Density

- Problems in identification of outliers when data contains regions of different densities
- Find a definition relative to the neighborhood of the object
- Example: in slide 30, right, point D has higher absolute density than point A, but its density is lower relative to its nearest neighbors Jump to figure

$$\textit{average relative density}(\mathrm{x}, k) = \frac{\textit{density}(\mathrm{x}, k)}{\sum_{y \in N(\mathrm{x}, k)} \textit{density}(\mathrm{y}, k)/k}$$

It is the density normalized to the average density of the objects in the neighborhood

Detection of Outliers using Relative Density

k is the number of nearest neighbors
for objects x **do**
    Determine $Nb(\mathrm{x}, k)$, the k–nearest neighbors of x
    Determine $density(\mathrm{x}, k)$, the density of x using its nearest neighbors, i.e. the objects in $Nb(\mathrm{x}, k)$
for objects x **do**
    Set the $outlier\ score(\mathrm{x}, k) = average\ relative\ density(\mathrm{x}, k)$

Strengths and weaknesses

- works well when data has regions of different density
- natural complexity $O(N^2)$ in the number of objects
- can be reduced to $O(N \log N)$ for low–dimensional data with special data structures
- parameter selection quite difficult

Isolation Forest: Overview

- Isolation Forest (iForest) is an unsupervised anomaly detection algorithm
- It isolates anomalies by leveraging the fact that they are "few and different."
- Instead of profiling normal data, iForest directly isolates anomalies

Core Concept

- Isolation Principle
  - Anomalies are easier to isolate compared to normal points
  - Isolation is performed using random splits on data dimensions
- Tree Construction
  - Randomly select a feature and split value for each node
  - Continue splitting until:
    - A single data point remains in the partition
    - A maximum depth is reached
- Path Length
  - The depth of a point in the tree measures how quickly it gets isolated
  - Anomalies have shorter path lengths compared to normal points

Mathematical Details

- Path Length for a Point
  - Let $h(x)$ denote the path length of a point x in a tree
  - For n data points, the average path length $c(n)$ is approximated as:
    - $c(n) = 2H(n-1) - \frac{2(n-1)}{n}$,
    - where $H(i)$ is the i-th harmonic number $H(i) = \sum_{k=1}^{i} \frac{1}{k}$
- Anomaly Score
  - The anomaly score $s(x)$ is calculated as:
    - $s(x) = 2^{-\frac{E(h(x))}{c(n)}}$,
    - where $E(h(x))$ is the average path length of x across all trees
  - Interpretation:
    - $s(x) \rightarrow 1$: x is an anomaly
    - $s(x) \rightarrow 0.5$: x is a normal point

Computational Complexity

- Tree Construction
  - For n data points and t trees, the complexity is:
    - $O(t \cdot n \cdot \log(n))$,
    - as each tree requires $O(n \log(n))$ time
- Scalability
  - The algorithm scales well with large datasets due to its linear complexity in n
- Memory Efficiency
  - Each tree is built using a random subset of data (sub-sampling)
  - Reduces memory usage and improves efficiency

Advantages of Isolation Forest

- Unsupervised
  - No labels are required for training
- Efficient
  - Linear time complexity with respect to the number of samples
- Handles High Dimensions
  - Works well with datasets having many features
- Interpretability
  - Path lengths provide an intuitive understanding of anomalies

Limitations of Isolation Forest

- Random Splits
  - May lead to inconsistent results for small datasets
- Assumes Independent Features
  - Ignores correlations between features during splitting
- Suboptimal for Complex Data
  - May require fine-tuning for datasets with intricate patterns

Applications of Isolation Forest

- Fraud Detection
  - Identify fraudulent transactions based on behavioral patterns
- Predictive Maintenance
  - Detect sensor anomalies indicating potential equipment failures
- Network Security
  - Spot unusual network activity that could indicate cyberattacks
- Healthcare
  - Identify rare but critical events in patient monitoring data

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