Anomaly Detection: A Tutorial
Theory and Applications

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• Introduction and Overview

• Theory
  • Statistical Methods
  • Distance and Density Based Methods
  • Addressing Scalability
  • Anomalies in Complex Data
  • Evaluation Methods

• Applications
  • Network Intrusion Detection
  • Fraud Detection
  • Epidemiological Studies
  • Climate and Weather Data Analysis
Anomaly Detection - Overview

• In Data Mining, anomaly or outlier detection is one of the four tasks.
  • Classification
  • Clustering
  • Pattern Mining
  • Anomaly Detection

• Historically, detection of anomalies has led to the discovery of new theories. Famous examples include
  • El Nino and Southern Oscillation Index (SOI).
  • The discovery of the planet Neptune.
  • The use of fluoride in toothpaste!

• Anomalies often lead to “surprise” - a form of inference known as abduction (different from induction and deduction).
• Hawkins: “an outlier is an observation, which deviates so much from other observations as to arouse suspicions that it was generated by a different mechanism.” [15]
Statistical Methods

- Lets begin with the univariate Normal distribution

\[ f(x) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \]

- Notice exponent measures square of deviation from mean and normalized by standard deviation

\[ \left(\frac{x - \mu}{\sigma}\right)^2 = (x - \mu)(\sigma^2)^{-1}(x - \mu) \]

- For d dimension, the exponent is called (square of) **Mahalanobis distance**

\[ (x - \mu)'\Sigma^{-1}(x - \mu) \]

where \( \Sigma \) is the \( d \times d \) variance-covariance matrix.
The key observation is that if data $x$ follows a $d$ dimensional Gaussian distribution then:

$$(x - \mu)'\Sigma^{-1}(x - \mu) \approx \chi^2_d$$

Anomalies can be found in the tail of the distribution.

There are three major weaknesses of the above approach.

- Data may not follow a Normal distribution or be a mixture of distributions.
- Both mean and variance of $\chi^2$ is $d$. For high-dimensional data this is a problem.
- Mean and thus variance are extremely sensitive to outliers - and we are using them to find anomalies - often leads to false negatives.
• Mahalanobis normalizes for variance

<table>
<thead>
<tr>
<th>Point Pairs</th>
<th>Mahalanobis</th>
<th>Euclidean</th>
</tr>
</thead>
<tbody>
<tr>
<td>(14,29)</td>
<td>5.07</td>
<td>11.78</td>
</tr>
<tr>
<td>(16,61)</td>
<td>4.83</td>
<td>6.84</td>
</tr>
</tbody>
</table>

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Distance-based anomalies

- Intuition: A data point which is far away from its nearest neighbors is a candidate anomaly.
- Several definitions which capture the above intuition.

\[ DB(p, D) \text{ anomaly [20]}: \text{ an object } o \text{ in a data set } T \text{ is a } DB(p, D) \text{ anomaly if at least a fraction } p \text{ of objects in } T \text{ have distances greater than } D \text{ from } o. \]

- Generalizes the notion of “three standard deviation from the mean.”
- This definition had a huge influence on subsequent development in outlier detection.
To build some intuition, consider data generated from the Normal distribution $N(0, 1)$. Then if $O$ is a $DB(p, D)$ outlier:

$$
\frac{1}{(2\pi)^{\frac{1}{2}}} \int_{O-D}^{O+D} e^{-\frac{x^2}{2}} \, dx \leq 1 - p
$$

Example: If $O$ is 3 (3 standard deviations away from the mean) then it is a $DB(0.1, 0.999)$ outlier.

Thus for particular settings of $D$ and $p$, $DB(p, D)$ captures standard outliers.

But much more general (e.g., any distance metric).
Distance-based methods \((DB(k, N))\)

- \(DB(k, N)\) anomaly [28]: top \(N\) data instances whose distances to its \(k\)-th nearest neighbor are largest.
- Several advantages. Ranking for anomalies is more intuitive. Setting of parameters generally easier.
- A Simple Nested Loop (SNL) algorithm can be used to select the top \(N\), \(DB(k, N)\) outliers. Time complexity is \(O(n^2d)\) where \(n\) is the database size and \(d\) is the dimensionality.
Pruning rule

- \textit{DB}(k, N)\ anomaly [3]: a data instance is not an anomaly if its distance to its \(k\)-th current nearest neighbor is less than the score of the weakest anomaly among top \(N\) anomalies found so far.
- A large number of non-anomalies can be pruned without carrying out a full data search.
- Complexity: nearly \(O(n)\)
Examples of pruning technique

- Non-anomalies are pruned earlier.

<table>
<thead>
<tr>
<th>Index</th>
<th>Distance to knn</th>
<th>Comparisons</th>
<th>Weakest anomaly</th>
<th>Weakest score</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Anomaly has first ordering (No. of comparisons = 10)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>

| Anomaly has last ordering (No. of comparisons = 12) |
| 1     | 1               | 3           | 1               | 1             |
| 2     | 1               | 3           | 1               | 1             |
| 3     | 1               | 3           | 1               | 1             |
| 4     | 2               | 3           | 4               | 2             |

| The best case (No. of comparisons = 8) |
| 1     | 1               | 3           | 1               | 1             |
| 2     | 2               | 3           | 2               | 2             |
| 3     | 1               | 1           | 2               | 2             |
| 4     | 1               | 1           | 2               | 2             |

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Strengths and weaknesses - Distance-based techniques

- Do not make any assumption about the distribution of the data
- Scalable for large dataset \( (O(n)) \)
- Capable of finding only global anomalies
- Can lead to non-intuitive results in Top-k situations
Density-based anomaly

- Calculate the density of an object based on the density of its $k$ nearest neighbours.

$$density(p) = \frac{1}{\left(\sum_{q \in N_k(p)} \frac{dist_k(p, q)}{|N_k(p)|}\right)}$$

$$relative\text{-}density(p) = \frac{density(p)}{\frac{1}{|N_k(p)|} \sum_{q \in N_k(p)} density(q)}$$

$$anomaly\text{-}score(p) = \frac{1}{relative\text{-}density(p)}$$

- LOF: indicates a degree of local outlier-ness [6]
Strengths and Weaknesses

- Can detect global and local anomalies
- Cannot use pruning technique and has a complexity of $O(n^2)$
- Require a method combining the strengths of distance and density based approaches? A distance based approach which can capture density?
Commute time

- Commute time between $i$ and $j$ is the expected number of steps that a random walk starting at $i$ will take to reach $j$ once and go back to $i$ for the first time.
- Commute time can capture both the distance between points and the data densities.

\[
\hat{\text{Commute time}} \quad \text{between} \quad i \quad \text{and} \quad j \quad \text{is the expected number of steps that a random walk starting at} \quad i \quad \text{will take to reach} \quad j \quad \text{once and go back to} \quad i \quad \text{for the first time.}
\]

\[\hat{\text{Commute time}} \quad \text{can capture both the distance between points and the data densities.}\]

\[
\begin{array}{c|c|c|c|c|c}
\text{Euclidian Distance} & \text{Commute Distance} \\
\hline
\text{Index} & 1 & 2 & 3 & 4 & 5 \\
\hline
1 & 0 & 1.00 & 1.85 & 1.85 & 2.41 \\
2 & 1.00 & 0 & 1.00 & 1.00 & 1.41 \\
3 & 1.85 & 1.00 & 0 & 1.41 & 1.00 \\
4 & 1.85 & 1.00 & 1.41 & 0 & 1.00 \\
5 & 2.41 & 1.41 & 1.00 & 1.00 & 0 \\
\end{array}
\]

\[
\begin{array}{c|c|c|c|c|c}
\text{Euclidian Distance} & \text{Commute Distance} \\
\hline
\text{Index} & 1 & 2 & 3 & 4 & 5 \\
\hline
1 & 0 & 12.83 & 19.79 & 19.79 & 20.34 \\
2 & 12.83 & 0 & 6.96 & 6.96 & 7.51 \\
3 & 19.79 & 6.96 & 0 & 7.51 & 6.96 \\
4 & 19.79 & 6.96 & 7.51 & 0 & 6.96 \\
5 & 20.34 & 7.51 & 6.96 & 6.96 & 0 \\
\end{array}
\]
Computation of commute time

- Commute time can be computed using graph Laplacian matrix $L$

$$c_{ij} = V_G(e_i - e_j)^T L^+(e_i - e_j)$$

$L^+$: pseudo-inverse of $L$

$V_G$: graph volume

$e_i$: $i$-th column of the identity matrix

- Commute time is Euclidean distance in the space spanned by eigenvectors of $L$.

$$c_{ij} = V_G[(S^{-1/2}V^T)(e_i - e_j)]^T[(S^{-1/2}V^T)(e_i - e_j)]$$

$V, S$: eigenvectors and eigenvalues of $L$
Anomaly detection using commute time (CDOF)

- Construct the mutual $k$ nearest neighbor graph $G$ from the dataset
- Compute the Laplacian matrix $L$ of $G$ and its eigensystems
- Find top $N$ anomalies using the distance-based technique in commute time with pruning rule
- Complexity: $O(n^3)$
- Commute time method can detect global, local, and group anomalies.
Fast estimation of commute time

- Speilman and Srivastava [31] combined random projection and a linear time solver to build a structure where we can compute the compute time between two nodes in $\tilde{O}(\log n)$ time.
- Complexity of CDOF: $O(n^3) \rightarrow O(n \log n)$
- Uses a near linear time solver for a linear system of equation $Ax = b$
- Spielman and Teng solvers. Also see work by Iannis Koutis from CMU.
Scalability for Density-based method

- The pruning rule for Distance-based methods does not apply to Density-based approaches.
- We can go from $O(n^2)$ to nearly $O(n \log n)$ by using an index.
- One solution for the curse of high dimensionality is to use of random projections.
PINN Algorithm (ICDM 2010)

Find $ck$-nearest-neighbours
candidate neighbour set

Find $k$-nearest-neighbours from within the candidate set

$k$-nn Result

For each point

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Anomaly Detection
PINN Guarantee

- The PINN Algorithm provides probabilistic guarantees.
- Under certain assumptions about intrinsic dimensionality \( c \) with high probability
  \[
  \frac{1 - \epsilon}{1 + \epsilon} \cdot LOF(p) \leq \overline{LOF}(p) \leq \frac{1 + \epsilon}{1 - \epsilon} \cdot LOF(p).
  \]
- In practice we do not know the intrinsic dimensionality of data. However random projections are quite robust.
Examples: high-dim distance-based outliers

- On a large database of images, the bright images show up as distance based outliers
Examples: high-dim density-based outliers

- On a large database of images, occluded images show up as density based outliers
Examples: local density-based outliers

- Examples of images ranked by LOF
Addressing Scalability
- Well suited for **data parallel** algorithms
  - Using CUDA - *Compute Unified Device Architecture* (Nvidia)
- Need to re-engineer existing algorithms
  - Utilization of device memory
  - Minimize CPU⇔GPU transfer of data
  - Keep threads homogeneous
- Most model based algorithms are naturally setup for the testing phase
- Model building needs careful redesign
- What about unsupervised algorithms?
Implementing $DB(k, N)$ on GPUs

- Return top N data instances whose distances to $k$-th nearest neighbor are largest (Serial $DB(k, N)$ is $O(n^2)$)

- Involves computing pairwise distances

- Load block $i$ and block $j$ to shared memory
  - Data layout in memory should be optimized

- Each thread computes distance between a pair of instances
  - Can utilize this time to load next chunk of data from host to device memory

- Writes results to corresponding output block

- Sorting can be done efficiently in CUDA [29]
Moving Beyond Multi-dimensional Record Data

### Categorical (Mixed)
- Fraud Detection
- Cyber Networks

### Discrete Sequences
- Genomic
- System Calls

### Spatio-temporal
- Remote sensing
- Climate

### Time Series
- Sensor Networks
- Healthcare

### Spatial
- GIS
- Image analysis

### Graphs
- Social networks
- Epidemiology

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Anomaly Detection
Handling Categorical Data

- Each attribute can belong to one of many categories.
- No ordering between categories
- Mixed data (categorical and continuous attributes)?

<table>
<thead>
<tr>
<th>cap-shape</th>
<th>cap-surface</th>
<th>···</th>
<th>habitat</th>
<th>type</th>
</tr>
</thead>
<tbody>
<tr>
<td>convex</td>
<td>smooth</td>
<td></td>
<td>urban</td>
<td>poisonous</td>
</tr>
<tr>
<td>convex</td>
<td>smooth</td>
<td></td>
<td>grasses</td>
<td>edible</td>
</tr>
<tr>
<td>bell</td>
<td>smooth</td>
<td></td>
<td>meadows</td>
<td>edible</td>
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<tr>
<td>convex</td>
<td>scaly</td>
<td></td>
<td>urban</td>
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<tr>
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<td>grasses</td>
<td>edible</td>
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<tr>
<td>···</td>
<td></td>
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</tr>
</tbody>
</table>

Table: Mushroom Data Set [2].
Approaches to Identify Categorical Anomalies

Using Association Analysis [24]

- **Binarize** data
- Learn **rules** \((X \Rightarrow Y)\)
  - Choose high confidence rules \((P(Y|X))\)
- For test record \(Z = \langle X, Y \rangle\) find rules of the form \(P(!Y|X)\)
  - \(Y\) is not observed when \(X\) is observed

Using Bayesian Networks [33]

- Learn Bayesian network structure and parameters
- Compute \(P(Z)\) for test data record \(Z\)
- Flag anomaly if \(P(Z) < \delta\)

Using Similarity Metrics [10]

- Use a similarity measure \((S(X_1, X_2))\)
- Apply distance/density/clustering based method (e.g. lof)
Conditional Probability Test [18]

- Identify unusual combinations of attribute values
  \[ r(a_t, b_t) = \frac{P(a_t, b_t)}{P(a_t)P(b_t)} \]
- \( A \cap B = \emptyset \)
- **Assumption**: If \( r(a_t, b_t) \) is low and is observed in test record \( t \), then \( t \) is anomalous
- For a test record \( t \):
  - For each *mutually exclusive* pair of attribute sets \( \{A, B\} \)
    compute \( r(a_t, b_t) \)
  - Score \( t \) based on all \( r \)-values:
    - Assign minimum \( r \)-value as score
    - Take product of all \( r \)-values
- Need to compare exponential pairs of subsets!!!
  - Only consider subsets up to size \( k \)
  - Ignore subsets with frequency less than a threshold \( \alpha \)
  - Avoid comparing *independent* subsets of attributes
  \[ \mu(A, B) \geq \beta_\mu \]
Estimating Probabilities for CPT \[18\]

- **Maximum Likelihood Estimation**

\[
\frac{P(a_t, b_t)}{P(a_t)P(b_t)} = \frac{C(a_t, b_t)}{N} \times \frac{N}{C(a_t)} \times \frac{N}{C(b_t)}
\]

- $C(a_t)$: Number of training instances with $A = a_t$
- $N$: Total number of training instances

- **Laplace Smoothing:**

\[
E(p) = \frac{C(p) + 1}{N + 2}
\]

\[
r(a_t, b_t) = \frac{E(a_t, b_t)}{E(a_t) \times E(b_t)}
\]

**Speedup Tricks**

- Replace rare attribute values with generic attribute (reduce *arity*)
- Use efficient data structure to querying for counts(AD Trees [26])
  - ADTrees work faster for low arity attributes
Finding Anomalies in Discrete Sequences

• Many problem formulations:
  1. **Anomalous symbols** in a sequence
  2. **Anomalous subsequence** in a sequence
  3. **Anomalous sequence** in a database of sequences


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Treating Sequences as Points

- Utilize a distance/similarity measure
  - Plug into a distance/density/clustering based method
- Simplest: *Hamming Distance*
  \[
  h(A_i, B_i) = \begin{cases}
  1, & A_i \neq B_i \\
  0, & A_i = B_i
  \end{cases}
\]

  \[
  H(A, B) = \sum_{i=1}^{n} h(A_i, B_i)
\]

- Issues: Unequal lengths, misalignment
- Normalized Length of Longest Common Subsequence

  \[
  D(A, B) = 1 - \frac{|LCS(A, B)|}{\sqrt{|A||B|}}
\]

  - Standard Dynamic Programming method is slow
  - Faster versions available (*Hunt Szymnaski* method [7])

- Weaknesses:
  - Cannot *localize anomalies* within a sequence
  - Weak anomaly signals might get lost
Using Sliding Windows

- Slide a window of size $k$
- Extract all windows from a sequence $(n - k + 1)$
- Training (Creating a normal dictionary): Store all unique windows in all normal sequences and their counts
- Testing:
  - For each window find the frequency in normal dictionary
  - Anomaly score is inverse of the aggregate frequencies for all windows (normalized by length)
- Many variants exist:
  - For each window find the hamming distance to the closest window in the normal dictionary [16]
- Issues:
  - Penalizes low frequency windows in the normal dictionary
  - Rewards high frequency windows that might not be relevant
  - Can construct anomalous sequences that will escape detection
Using Probabilistic Models

- Probability of occurrence of sequence $S$
  \[ P(S) = \prod_{i=1}^{n} P(S_i|S_1, \ldots, S_{i-1}) \]

- Short memory property of sequences:
  \[ P(S_i|S_1, \ldots, S_{i-1}) = P(S_i|S_{i-k}, \ldots, S_{i-1}) \]

- Conditional probability estimates for a symbol $S_i$:
  \[ P(S_i|S_{i-k}, \ldots, S_{i-1}) = \frac{f(S_i|S_{i-k}, \ldots, S_i)}{f(S_i|S_{i-k}, \ldots, S_{i-1})} \]
  - $f$ is estimated from the normal dictionary
  - Anomaly score for a test sequence is inverse of the normalized probability of occurrence
  - Issues: What if the suffix occurs very infrequently in the normal data (or not at all)?
    - Replace with the longest suffix that occurs sufficient number of times [32] - Probabilistic Suffix Trees
    - Significantly reduces the size of the model

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Finding Contextual Anomalies

- Sometimes *contextual information* is available about data
  - Not used directly as a feature
  - Are well understood, no anomalies in the context
  - Can reduce false positives and yield interesting anomalies
- Example adapted from [30]
  - **Contextual anomalies** - Anomalous with respect to a *context*
  - Context is defined using *environmental* variables
    - Spatial (*Latitude, Longitude*)
    - Graph context (*Edges, Weights*)
    - Temporal location
    - Domain specific (*Demographic, other*)
  - How to incorporate context?
    - Reduce to traditional anomaly detection (subset on context)
    - Explicitly model contextual information (time series, spatial)
Conditional Anomaly Detection

- **Data instance** $d \Rightarrow u_1, u_2, \ldots, u_{d_U}, v_1, v_2, \ldots, v_{d_V}$
  - $d_U$ environmental attributes
  - $d_V$ indicator attributes

- **Algorithm [30]**:
  1. Learn a Gaussian Mixture Model (GMM) $U = U_1, U_2, \ldots, U_{n_U}$, each with dimensionality $d_U$
  2. Learn a set of Gaussians $U = V_1, V_2, \ldots, V_{n_V}$, each with dimensionality $d_V$
  3. Learn a probabilistic mapping function $p(V_j | U_i)$
  4. Score a test instance $d = [u, v]$:

$$S = \sum_{i=1}^{n_U} p(u | U_i) \sum_{j=1}^{n_V} p(v | V_j)p(V_j | U_i)$$
Finding Collective Anomalies

- Find a collection of data points
- Each point by itself is normal
- The collection *as a whole* is anomalous
- Relevant when data has inherent structure, and
- When domain definition of anomalies cannot be described as point anomalies

**A Simple Solution**

1. Break data into groups
2. Compute features for each group
3. Apply traditional anomaly detection

**Examples**

1. Time series
2. Image
3. Spatial clusters of galaxies
Using Latent Dirichlet Allocation for Group Anomalies

- Find **anomalous groups** in data [34]
- Example: Spatial clusters of galaxies
  - **topics**: red, green, emissive
  - **words**: continuous features

**Flexible Genre Model (FGM)**

- For each **group**:
  1. Draw a genre $1, 2, \ldots, T \ni y_m \sim \mathcal{M}(\pi)$
  2. Draw topic distribution for $y_m : S^K \ni \theta_m \sim \text{Dir}(\alpha y_m)$
  3. Draw $K$ topics
     $$\{\beta_{mk} \sim P(\beta_{mk} | \eta_k)\}_{k=1,2,\ldots,K}$$
  4. For each **point** in group:
     1. Draw topic membership: $z_{mn} \sim \mathcal{M}(\theta_n)$
     2. Generate point
        $$x_{m,n} \in P(x_{m,n} | \beta_{mk}, z_{mn})$$

**Model Parameters**

- $\mathcal{M}(\pi)$ - Multinomial
- **Genre** - $\text{Dir}(\alpha_t)$
- Topic generators $P(\cdot | \eta_k)$ - GIW
- Point generators $P(x_{mn} | \beta_{nk})$ - Multivariate Gaussian
Inference and Learning Parameters

- Approximate inference of latent variables (*Gibbs Sampling*)
- Use samples to learn parameters (*Single step Monte Carlo EM*)

Anomaly Detection

- Infer the topic distribution $\theta_m$
- Compute negative log likelihood w.r.t. $\alpha_t$
- Rationale: An anomalous group will be unlikely to be generated from any genre
- Geometric interpretation: Mapping each group into a $T$ dimensional space and finding anomalies
Evaluating Anomaly Detection Methods - Labels

- Labeled *validation data set* exists
  - Confusion matrix
  - Traditional evaluation metrics
    - *Class imbalance?*
  - ROC Curve
- *Validation set* does not exist
  - Use *domain expertise* to find $TP$ and $FP$
  - $FN$ is harder to estimate
    - Pseudo false negative estimation techniques [25]

<table>
<thead>
<tr>
<th>Actual</th>
<th>Predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$a$</td>
</tr>
<tr>
<td>$a$</td>
<td>$TP$</td>
</tr>
<tr>
<td>$n$</td>
<td>$FP$</td>
</tr>
</tbody>
</table>

$$
\text{Acc} = \frac{TP + TN}{\sum TP}
$$

$$
\text{Rec (R)} = \frac{TP}{TP + FN}
$$

$$
\text{Prec (P)} = \frac{TP}{TP + FP}
$$

$$
F = \frac{2 \times R \times P}{R + P}
$$
Evaluating Anomaly Detection Methods - Scores

- Convert to binary output
  - Use threshold $\delta$ on score (Scale issues? [21])
  - Take top $x\%$ as anomalies
- ROC curve by varying $x$ or $\delta$
- Quality of output
  - Does the output “suggest” $x$ or $\delta$?
  - Which output is better?
Unifying Scores

- Different methods assign scores in different ranges
  - $kNN$-based scores $[0, 1]$
  - $Lof$ scores $[1, 6]$
  - $ABOD$ scores $[0, 80000]\!!$
    - Anomalies have lower scores
  - Direct scaling to $[0, 1]$ might lose distinction between normal and anomalies
  - Desired scaling: Stretch *interesting* ranges and shrink irrelevant ones

- Generalized Procedure for Normalizing Outlier Scores [21]
  - **Regularity:** $\Rightarrow S(o) \geq 0, \forall o$, $S(o) \approx 0$ if $o$ is normal and $S(o) \gg 0$ if $o$ is anomalous
  - **Normality:** $S$ is regular and $S(o) \in [0, 1], \forall o$
Regularization and Normalization of Scores

**Regularization**

1. \( R(o) := \max\{0, S(o) - \text{base}_S\} \)
2. \( R(o) := S_{\text{max}} - S(o) \)
3. \( R(o) := -\log \frac{S_{\text{max}}}{S(o)} \)

**Normalization**

1. \( N(o) := \frac{S(o)}{S_{\text{max}}} \)
2. \( N(o) := \max\left(0, \text{erf}\left(\frac{S(o) - \mu_S}{\sigma_S \sqrt{2}}\right)\right) \) (*Gaussian Scaling*)
   - Suited for high dimensional data
3. \( N(o) := \max\left(0, \frac{\text{cdf}_S^\gamma(o) - \mu_\gamma}{1 - \mu_\gamma}\right) \) (*Gamma Scaling*)
   - Where, \( \text{cdf}_S^\gamma(o) := P(k, S(o), \theta) \)
   - \( P \) is the regularized Gamma function
   - Suited for low dimensional data
Generating Labeled Data for Validation

Generating Both Normal and Anomalous Data

- Use generative models for normal and anomalous behavior
- Several generators available
  - Multivariate continuous data [27]
  - Multivariate categorical data [5]
  - Discrete sequences using HMM [12]
- Drawbacks: Might not capture the domain characteristics

Injecting Anomalies - Random Perturbation [30]

- Given data point $z = \{x, y\}$, $x$ and $y$ are partitions of feature space
- Take a random sample $D$ of the entire data set
- Let $z' = \{x', y'\} \in D$, such that distance between $y$ and $y'$ is maximum
- Replace $x$ with $x'$ and add $z$ back to data set
Applications: Overview

- How to set up an anomaly detection solution for a given application domain?
  - Available data?
  - Define anomalies, define normal behavior
  - Identify requirements and constraints (online, real-time, limited resources)
  - What domain knowledge available
    - Feature identification
    - Defining normal and anomalous behavior
    - Tuning parameters
  - Available ground truth (training, validation)
Anomaly Detection or Intrusion Detection?

Traditional Intrusion Detection Systems (IDS): finding attacks corresponding to predefined pattern data set known as signatures, therefore system is absolutely vulnerable against zero-day attacks.

Network Anomaly Detection Systems (NADS): to detect zero-day attacks without any pre-identified signature besides profile normal behavior of the network and address suspected incidents.

- **Network Anomaly Detection**: finding unusual and large changes in the network traffic.
- **Examples**: intentional attacks (e.g. Distributed Denial of Service - DDoS) or unusual network traffic (e.g. flash crowds).
Motivation: How Much Serious?

- According to Symantec report, released in early 2011, more than 286 million new threats have been detected in 2010 which is a huge number.
Network Topology

- A Typical network

- Origin-Destination (OD) flow is the traffic that enters at an origin node and exits at a destination node of a backbone network: $x_{1,t}$, $x_{1,t}$.

- Link measurement is the traffic enters at an node during an interval: $y_{1,t}$

- Relationship between link traffic and OD flow traffic is captured by the routing matrix $A$. 

Chawla and Chandola Anomaly Detection
Network Anomalies Detection: Problem

\[ y_{1,t} = x_{2,t} + x_{3,t} \]  

Only measure at links

1.
2.
3.
router

\[
\begin{pmatrix}
  y_{1,t} \\
  y_{2,t} \\
  y_{3,t}
\end{pmatrix} =
\begin{pmatrix}
  0 & 1 & 1 \\
  1 & 0 & 1 \\
  1 & 1 & 0
\end{pmatrix}
\begin{pmatrix}
  x_{1,t} \\
  x_{2,t} \\
  x_{3,t}
\end{pmatrix}
\]

\[ Y_t = A_t x_t \quad (t=1,\ldots,T) \]

\( A \) has size (No of links) x (no of OD flows), \( A_{ij} = 1 \) if OD flow j traverses through link i

\[ Y = AX \]

Time-invariant \( A_t (= A) \), \( Y=[y_1\ldots y_T] \), \( X=[x_1\ldots x_T] \)

Typically massively under-constrained!
Every sudden change in an OD flow \( X \) is formally considered to be a volume anomaly...

\[
\begin{pmatrix}
OD_1 & \ldots & \ldots & OD_j & \ldots & \ldots & OD_m
\end{pmatrix}
\]

Each time bin:

\[
\begin{pmatrix}
x_{1,1} & \ldots & \ldots & x_{j,1} & \ldots & \ldots & x_{m,1}
\end{pmatrix}
\]

\[
\vdots
\]

\[
\begin{pmatrix}
x_{1,t} & \ldots & \ldots & x_{j,t} & \ldots & \ldots & x_{m,t}
\end{pmatrix}
\]

\[
\vdots
\]

\[
\begin{pmatrix}
x_{1,n} & \ldots & \ldots & x_{j,n} & \ldots & \ldots & x_{m,n}
\end{pmatrix}
\]

**A network with \( m \) node will have \( m^2 \) OD flows.**

- Thus OD flows are high dimensional data.
  - 20 node will result in 400 dimensions.

**However, quite intuitively OD flows are correlated.**

- Hence they can be represented with far fewer dimensions.
Why care about OD Flows

- Volume anomaly typically arises on an OD flow (traffic arriving at one node and destined for another node)
- If we only monitor traffic on network links, volume arising from an OD flow may not be noticeable. Thus, naive approach won’t work if OD flow info is not available

Figure source [22]
If data along the $p$ dimensions are correlated (high positive or negative covariance), then it can be represented with fewer dimensions ($k$).

Only 5-10 dimensions are sufficient to capture $95+\%$ of the traffic, Chawla and Chandola (SIGMETRICS’04).

Data mapped onto the $k$ dimensions are usually called the normal component, remaining data is called the residual component.

$$Z = \hat{Z} + \tilde{Z}$$

Traffic vector of all links at a particular point in time

Normal traffic vector

Residual traffic vector

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Anomaly Detection
Subspace Method Algorithm

- **Step 1**: Determine the PCs based on eigenvalue decomposition of the covariance matrix of the dataset.
- **Step 2**: Choose first top $k$ principle components with the highest eigenvalues as matrix $P$.
- **Step 3**: Normal traffic subspace called $\hat{Z}$:
  \[ \hat{Z} = PP^T Z = CZ \]
- **Step 4**: Abnormal traffic subspace called $\tilde{Z}$:
  \[ \tilde{Z} = (I - PP^T)Z = \tilde{C}Z \]
- **Step 5**: If the norm of a vector is large then it is an “anomaly”.

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Subspace Analysis Results

- Note that during anomaly, normal component does not change that much while residual component changes quite a lot.
- Thus, anomalies can be detected by setting some threshold.

Figure source [22]
Discussion: Typical Characteristics of Anomaly

- Most Anomalies induce a change in distributional aspects of packet header fields (called features).

- Most important features include 5-tuple: Source & destination IP addresses, Source and destination port numbers, and IP protocol.
  - DOS attack – multiple source IP address concentrated on a single destination IP address
  - Network scan – dispersed distribution of destination addresses
  - Most worms/viruses also induce some change in distribution of certain features
  - However these changes can be very subtle and mining them is like searching for needles in a haystack

- Unlike many previous approach, this paper aims to detect events which disturb the distribution of traffic features rather than traffic volume
Limitation of Volume

- Figure source [22]

- Port scan anomaly (traffic feature changes, however traffic volume remains more or less the same)

We can use entropy to capture the variations in the traffic feature

\[ H(X) = - \sum_{i=1}^{N} \left( \frac{n_i}{S} \right) \log_2 \left( \frac{n_i}{S} \right) , \]

- Takes value 0 when distribution is maximally concentrated.
- Takes value \( \log_2 N \) when distribution is maximally dispersed.

Port scan dwarfed in volume metrics...

But stands out in feature entropy, which also reveals its structure
**Entropy Based versus Volume Based**

- **DoS/DDoS Attacks** - a spike in traffic data toward a dominant destination IP.
- **Scan anomaly** - a spike in traffic data from a dominant source IP.
- **Flash Crowd anomaly** - again a spike in traffic data to a dominant destination IP.
- **Worm anomaly** - a spike in traffic with a dominant port.

<table>
<thead>
<tr>
<th>Anomaly Label</th>
<th># Found in Volume</th>
<th># Additional in Entropy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha Flows</td>
<td>84</td>
<td>137</td>
</tr>
<tr>
<td>DOS</td>
<td>16</td>
<td>11</td>
</tr>
<tr>
<td>Flash Crowd</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>Port Scan</td>
<td>0</td>
<td>30</td>
</tr>
<tr>
<td>Network Scan</td>
<td>0</td>
<td>28</td>
</tr>
<tr>
<td>Outage Events</td>
<td>4</td>
<td>11</td>
</tr>
<tr>
<td>Point to Multipoint</td>
<td>0</td>
<td>7</td>
</tr>
<tr>
<td>Unknown</td>
<td>19</td>
<td>45</td>
</tr>
<tr>
<td>False Alarm</td>
<td>23</td>
<td>20</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>152</strong></td>
<td><strong>292</strong></td>
</tr>
</tbody>
</table>

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Anomaly Detection
Fraud Detection

- **Domain Question:** Identify fraudulent activities or *players* from observed *transaction* data

- **Data**
  - Transactions between different players in the system
  - Meta information about the individuals
  - An underlying graph structure

- **Challenges:**
  - Track and model human behavior
  - Anomalies caused by *adaptive* human adversaries
  - Massive data sizes

- **Insurance (auto, health*)**
  - Claimant, Provider, Payer

- **Telecommunications**
  - Customer, Provider

- **Credit Cards**
  - Customer, Supplier, Bank

- **Web Advertising**
  - User, Advertiser, Publisher

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[1] Chawla and Chandola

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A Generic Fraud Detection Method

- **Activity Monitoring** [13]
  1. Build profiles for individuals (customers, users, etc.) based on historic data
     - User X makes $n$ calls on an average in January
  2. Compare current behavior with historical profile for *significant deviations*

- **Clustering based** [4]
  1. Cluster historical profiles of customers
  2. Identify small clusters or outlying profiles as anomalies

- **Strengths**
  - Anomaly detection is fast (good for real time)
  - Results are easy to explain

- **Weaknesses**
  - Need to create and maintain a large number of profiles
  - Not *dynamic*
  - Adequate historical data might not be available
  - Too many false positives
Exploiting Graph Structure - Weighted Graphs

- Represent data as a weighted graph
  - Communication networks (phone, email, SMS)
  - Provider referral networks

- Objective: *Identify anomalous nodes*

- For each node, extract several features based on the properties of the induced sub-graph (*egonet*) of neighboring nodes [1]

- Choose features that can highlight anomalous nodes
  1. $N_i$: degree of node
  2. $E_i$: number of edges in egonet
  3. $W_i$: total weight of egonet
  4. $\lambda_i$: principal eigen vector of weighted adjacency matrix of egonet

- Data is transformed into a point in a multi-dimensional space
Identifying Anomalies

- Traditional anomaly detection (lof)
  - Can be slow but can identify any type of anomalous structure
- Faster method to identify specific types of anomalous structures:
  - Identify relevant feature pairs and power law relationship

- E.g., Egonet Density Power Law: \( N_i \) vs. \( E_i \) - detect near cliques and stars

\[
E_i \propto N_i^\alpha, 1 \leq \alpha \leq 2
\]

- Anomaly score for node \( i \) w.r.t. a pair of features \( (y = Cx^\theta) \)

\[
S_i = \frac{\max(y_i, Cx_i^\theta)}{\min(y_i, Cx_i^\theta)} \star \log (|y_i - Cx_i^\theta| + 1)
\]
Represent data as a bipartite graph
- Healthcare Data (Beneficiaries vs. Providers)
- Insider trading (Traders vs. Stocks)

Objective: Identify anomalous links

Given a query node $a \in V_1$ find the “relevance” of all other nodes in $V_1$ to $a$
- $RelevanceScore(a, b) \propto$ Number of times a “random walk” from $a$ reaches $b$

Use the relevance scores to compute the normality scores for a node $t \in V_2$
- Find set $S_t = \{a | \langle a, t \rangle \in E\}$
- Compute $|S_t| \times |S_t|$ similarity matrix using relevance vectors for $a \in S_t$
- Normality Score = mean of non-diagonal entries of similarity matrix
Detecting Disease Outbreaks

- **Domain Question:**
  - Early detection of disease outbreaks
    - Anthrax attack?

- **Data:**
  - Emergency department visits
  - Grocery data (*Example* [14])
  - Clinical visits
  - Weather/climate data

- **Challenges:**
  - Weak signals in the data
    - ED cases involving cough ⇒ *Flu* or *SARS*
  - Integration of multiple signals (*lag analysis*)
  - Account for spatial and temporal correlations

---

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  - ED cases involving cough ⇒ *Flu* or *SARS*
- Integration of multiple signals (*lag analysis*)
- Account for spatial and temporal correlations
What’s Significant About Recent Events (WSARE)?

1. Learn Bayesian network from historical data
   - *Environmental* and *response* variables

2. Sample from the BN ($DB_{baseline} | \text{Current Environment}$)
3. Compute contingency table for *rules* for $DB_{baseline}$ and $DB_{current}$
   - Rules are single assignment rules ($X_i = Y^j_i$) or conjunctions
4. Find $p$-value for rules using $\chi^2$-test
   - *Null Hypothesis*: Rows and columns of tables for $DB_{baseline}$ and $DB_{current}$ are independent
5. Find rule with largest $p$-value. Repeat Step 2.
Incorporating Spatial and Temporal Relationships

- WSARE does not explicitly model the spatial and temporal relationships
  - What happened yesterday?
  - What happened in the adjoining neighborhood (yesterday)?

- **Bayesian Network Spatio-Temporal (BNST) modeling framework** [17]
  - Add nodes for temporal and spatial dependencies
    - Need more data to train!!
Anomaly Detection in Climate and Weather

- **Science Questions:**
  - Identify natural and anthropogenic disasters.
  - Identify long time scale events - droughts, atmospheric rivers, cold fronts, etc.

- **Data:**
  - Ground observations, Remote sensing data (satellites, air-borne), Climate model simulation outputs
  - Multiple variables, spatio-temporal (often has height dimension as well)

- **Challenges:**
  - Model spatio-temporal relationships across multiple variables
  - Explain the cause of anomalies
  - Massive data sizes

---

Climate and weather extreme events are well defined

Key challenge is to find significant events and explain the cause.
Anomalies are Widely Used in Climate!

- Most analysis done on “anomaly” time series
- Difference from a “base period” (Too simplistic?)
- Brings spatial smoothness (e.g., a mountain top and nearby valley can have very different temperatures), Removes seasonality
- Understand climate and weather phenomenon
- *Southern Oscillation Index (SOI)*
  - Difference between Sea Level Pressure (SLP) anomalies for Tahiti and Darwin, Australia.

*Figure:* Global Average Temperature Anomaly (1975 - 2007) Src: [www.metoffice.gov.uk](http://www.metoffice.gov.uk)
Constructing Anomalies from Raw Data

- Anomaly time series for a given location, \( i \):

\[
v_i' = v_i - b_i
\]

where \( b_i \) is the base (reference).

- How to choose \( b_i \)?
  - Mean of all data for location \( i \)
  - Monthly mean values (account for seasonality)
  - Monthly \( z \)-score values
  - Median (more robust)
  - Using a shorter “reference period”
    - 30 year moving window

- Different methods show statistically significant differences\[19\]
  - What is the right strategy?
  - Weighted mean of different strategies (Pick weights using Monte Carlo sampling)
Anomaly Detection for Identifying Droughts

• **Science question:** Identify significant drought patterns using historical observation data or future simulation data or both

• Find persistent spatiotemporal anomalies in precipitation data

• A two step approach:
  1. Find precipitation anomalies using thresholds
  2. Find large **connected components** across space and time
     - Matlab - `bwlabel`, `bwlabeln`

• **Followup Science question:** Explain cause?

**Figure:** Video courtesy Dr. Arindam Banerjee

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Atmospheric Rivers [8]

- Water Vapor Content
- Anomalies using a threshold
- Connected components

Cold Fronts [23]

- Surface winds and Potential temperature fields
- Methodology:
  1. Compute features for every grid
  2. Cluster grids into $K$ clusters
  3. Label clusters as anomalous or not using thresholds
  4. Filter out false positives using domain knowledge

Chawla and Chandola Anomaly Detection
• How useful are the anomalies from the domain perspective?
• Common pitfalls:
  • Anomalies are algorithmically correct but are not relevant (bad data, noise, simplistic)
  • Anomalies are not actionable
    • Not identified in timely fashion
    • Resolution is not fine enough
    • Cause not explained
  • Anomalies lost among false positives
• Solution?
  • Good validation data during design
  • Clear definition of a domain anomaly and distinction from other potential competitors
Introduction

Data Mining Methods

Density-based anomaly

Commute Time Approach

Addressing Scalability

Anomalies in Complex Data

Evaluating Anomaly Detection Methods

Applications

Problem solutions

PCA and Subspace Method

Subspace Method Algorithm

Subspace Analysis

Results Discussion

Typical Characteristics of Anomaly Detection Methods

Based Fraud Detection Epidemeology

Anomaly Detection in Climate and Weather

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