Outline

- Analysis of the Anomaly Detection Problem
- Benchmarking Current Algorithms for Unsupervised AD
- Explaining Anomalies
- Incorporating Expert Feedback
- PAC Theory of Rare Pattern Anomaly Detection
Defining Anomaly Detection

- Data \( \{x_i\}_{i=1}^{N} \), each \( x_i \in \mathbb{R}^d \)
- Mixture of “nominal” points and “anomaly” points
- Anomaly points are generated by a different generative process than the nominal points
Three Settings

- **Supervised**
  - Training data labeled with “nominal” or “anomaly”

- **Clean**
  - Training data are all “nominal”, test data may be contaminated with “anomaly” points.

- **Unsupervised**
  - Training data consist of mixture of “nominal” and “anomaly” points
  - I will focus on this case
Well-Defined Anomaly Distribution Assumption

- WDAD: the anomalies are drawn from a well-defined probability distribution
  - example: repeated instances of known machine failures

- The WDAD assumption is often risky
  - adversarial situations (fraud, insider threats, cyber security)
  - diverse set of potential causes (novel device failure modes)
  - user’s notion of “anomaly” changes with time (e.g., anomaly == “interesting point”)
Strategies for Unsupervised Anomaly Detection

Let $\alpha$ be the fraction of training points that are anomalies

Case 1: $\alpha$ is large (e.g., > 5%)
- Fit a 2-component mixture model
  - Requires WDAD assumption
  - Mixture components must be identifiable
  - Mixture components cannot have large overlap in high density regions

Case 2: $\alpha$ is small (e.g., 1%, 0.1%, 0.01%, 0.001%)
- Anomaly detection via Outlier detection
  - Does not require WDAD assumption
  - Will fail if anomalies are not outliers (e.g., overlap with nominal density; tightly clustered anomaly density)
  - Will fail if nominal distribution has heavy tails
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Benchmarking Study

Andrew Emmott

- Most AD papers only evaluate on a few datasets
- Often proprietary or very easy (e.g., KDD 1999)
- Research community needs a large and growing collection of public anomaly benchmarks
Benchmarking Methodology

- Select data sets from UC Irvine repository
  - >= 1000 instances
  - classification or regression
  - <= 200 features
  - numerical features (discrete features ignored)
  - no missing values (mostly)
- Choose one or more classes to be “anomalies”; the rest are “nominals”
## Selected Data Sets

<table>
<thead>
<tr>
<th>Data Set</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel Plates Faults</td>
</tr>
<tr>
<td>Gas Sensor Array Drift</td>
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<tr>
<td>Image Segmentation</td>
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<tr>
<td>Landsat Satellite</td>
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<tr>
<td>Letter Recognition</td>
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<tr>
<td>OptDigits</td>
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<td>Page Blocks</td>
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<td>Shuttle</td>
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<td>Waveform</td>
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<tr>
<td>Yeast</td>
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<tr>
<td>Abalone</td>
</tr>
<tr>
<td>Communities and Crime</td>
</tr>
<tr>
<td>Concrete Compressive Strength</td>
</tr>
<tr>
<td>Wine</td>
</tr>
<tr>
<td>Year Prediction</td>
</tr>
</tbody>
</table>
Systematic Variation of Relevant Aspects

- **Point difficulty:** How deeply are the anomaly points buried in the nominals?
  - Fit supervised classifier (kernel logistic regression)
  - Point difficulty: \( P(\hat{y} = "nominal" | x) \) for anomaly points

- **Relative frequency:**
  - Sample from the anomaly points to achieve target values of \( \alpha \)

- **Clusteredness:**
  - Greedy algorithm selects points to create clusters or to create widely separated points

- **Irrelevant features**
  - Create new features by random permutation of existing feature values

- **Result:** 25,685 Benchmark Datasets
Metrics

- **AUC (Area Under ROC Curve)**
  - ranking loss: probability that a randomly-chosen anomaly point is ranked above a randomly-chosen nominal point
  - transformed value: $\log \frac{AUC}{1 - AUC}$

- **AP (Average Precision)**
  - area under the precision-recall curve
  - average of the precision computed at each ranked anomaly point
  - transformed value: $\log \frac{AP}{\mathbb{E}[AP]} = \log LIFT$
Algorithms

- **Density-Based Approaches**
  - RKDE: Robust Kernel Density Estimation (Kim & Scott, 2008)
  - EGMM: Ensemble Gaussian Mixture Model (our group)

- **Quantile-Based Methods**
  - OCSVM: One-class SVM (Schoelkopf, et al., 1999)
  - SVDD: Support Vector Data Description (Tax & Duin, 2004)

- **Neighbor-Based Methods**
  - LOF: Local Outlier Factor (Breunig, et al., 2000)
  - ABOD: kNN Angle-Based Outlier Detector (Kriegel, et al., 2008)

- **Projection-Based Methods**
  - IFOR: Isolation Forest (Liu, et al., 2008)
  - LODA: Lightweight Online Detector of Anomalies (Pevny, 2016)
Filtering Out Impossible Benchmarks

- For each algorithm and each benchmark
  - Check whether we can reject the null hypothesis that the achieved AUC (or AP) is better than random guessing
  - If a benchmark dataset is too hard for all algorithms, then we delete it from the benchmark collection
Analysis

- **Synthetic Control Data Set**
  - Nominals: standard $d$-dimensional multivariate Gaussian
  - Anomalies: uniform in the $[-4, +4]^d$ hypercube

- **Linear ANOVA**
  - $\text{metric} \sim \text{rf} + \text{pd} + \text{cl} + \text{ir} + \text{mset} + \text{algo}$
    - rf: relative frequency
    - pd: point difficulty
    - cl: normalized clusteredness
    - ir: irrelevant features
    - mset: “Mother” set
    - algo: anomaly detection algorithm

- Assess the *algo* effect while controlling for all other factors
Algorithm Comparison

![Algorithm Comparison Diagram]

Change in Metric wrt Control

Dataset

Algorithm

- iforest
- egmm
- lof
- rkde
- abod
- loda
- ocsvm
- svdd

logit(AUC)

log(LIFT)
More Analysis

- In a forthcoming paper, we provide much more detail
  - Mixed-effects model
  - Validation of the importance of each factor
  - Robustness of each algorithm to the factors
- Impact of different factors (descending order)
  - Choice of data set
  - Relative frequency
  - Algorithm
  - Point difficulty
  - Irrelevant features
  - Clusteredness
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Scenario: Explaining a Candidate Anomaly to an Analyst

- Need to persuade the expert that the candidate anomaly is real

- Idea:
  - Expose one feature value at a time to the expert
  - Provide appropriate visualization tools

- “Sequential Feature Explanation”

(arXiv:1503.00038)
Sequential Feature Explanation (SFE)
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Performance Metric: Minimum Feature Prefix (MFP). Minimum number of features that must be revealed for the analyst to become confident that a candidate anomaly is a true anomaly. In this example MFP = 4.
Let $S(x_1, ..., x_d)$ be the anomaly score for the vector $x = (x_1, ..., x_d)$.

Assume we have an algorithm that can compute a marginal score for any subset of the dimensions.

- Easy for EGMM, RKDE (score is $-\log \hat{P}(x)$)

Four Algorithms:

- Marginal Greedy
- Forward Selection: Independent Marginal Sequential Marginal
- Backward Elimination: Independent Dropout Sequential Dropout
Algorithms

- **Independent Marginal**
  - Compute $S(x_j)$ for each feature $j$
  - Order features highest $S(x_j)$ first

- **Sequential Marginal**
  - Let $L = \langle \rangle$ be the sequence of features chosen so far
  - Compute $S(L \cup x_j)$ for all $j \not\in L$
  - Add the feature $j$ to $L$ that maximizes $S(L \cup x_j)$

- **Independent Dropout**
  - Let $R$ be the set of all features
  - Compute $S(x_{R\setminus\{j\}})$ for each feature $j$ (delete one feature)
  - Sort features lowest $S(x_{R\setminus\{j\}})$ first

- **Sequential Dropout**
  - Let $L = \langle \rangle$ be the sequence of features chosen so far
  - Let $R$ be the set of features not yet chosen
  - Repeat: Add the feature $j \in R$ to $L$ that minimizes $S(x_{R\setminus\{j\}})$
Experimental Evaluations

(1) OSU Anomaly Benchmarks

- **Datasets**: 10,000 benchmarks derived from 7 UCI datasets
- **Anomaly Detector**: Ensemble of Gaussian Mixture Models (EGMM)
- **Simulated Analysts**: Regularized Random Forests (RRFs)
- **Evaluation Metric**: mean minimum feature prefix (MMFP) = average number of features revealed on outliers before the analyst is able to make a decision (exonerate vs. open investigation)
Results (EGMM + Explanation Method)

In these domains, an oracle only needs 1-2 features.

Dropout methods are often worse than marginal.

Random is always worst.

Often no benefit to sequential methods over independent methods.
Results
(Oracle Detector + Explanation Methods)

Sequential Marginal is better than Independent Marginal in most cases

Sequential Marginal is often tied with Optimal
Experimental Evaluations
(2) KDD 1999 (Computer Intrusion)

- Marginal much better than Dropout
- KDD 1999 is Easy

[95% Confidence Intervals]
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Incorporating Expert Feedback [Shubhomoy Das]

- Expert labels the best candidate
- Label is used to update the anomaly detector
Idea: Learn to reweight LODA projections

- LODA
  - $\Pi_1, \ldots, \Pi_M$ set of $M$ sparse random projections
  - $f_1, \ldots, f_M$ corresponding 1-dimensional density estimators
  - $S(x) = \frac{1}{M} \sum_m - \log f_m(x)$ average “surprise”

- Parameter $\tau$: quantile corresponding to number of cases analyst can label

- Goal: Learn to reweight the projections so that all known anomalies are above quantile $\tau$ and all known nominals are ranked below quantile $\tau$

- Method: Modification of Accuracy-at-the-Top algorithm (Boyd, Mohri, Cortes, Radovanovic, 2012)
## Experimental Setup

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Nominal Class</th>
<th>Anomaly Class</th>
<th>Total</th>
<th>Dims</th>
<th># anomalies(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abalone</td>
<td>8, 9, 10</td>
<td>3, 21</td>
<td>1920</td>
<td>9</td>
<td>29 (1.5%)</td>
</tr>
<tr>
<td>ANN-Thyroid-1v3</td>
<td>3</td>
<td>1</td>
<td>3251</td>
<td>21</td>
<td>73 (2.25%)</td>
</tr>
<tr>
<td>Covtype</td>
<td>2</td>
<td>4</td>
<td>286048</td>
<td>54</td>
<td>2747 (0.9%)</td>
</tr>
<tr>
<td>Covtype-sub</td>
<td>2</td>
<td>4</td>
<td>2000</td>
<td>54</td>
<td>19 (0.95%)</td>
</tr>
<tr>
<td>KDD-Cup-99</td>
<td>‘normal’</td>
<td>‘u2r’, ‘probe’</td>
<td>63009</td>
<td>91</td>
<td>2416 (3.83%)</td>
</tr>
<tr>
<td>KDD-Cup-99-sub</td>
<td>‘normal’</td>
<td>‘u2r’, ‘probe’</td>
<td>2000</td>
<td>91</td>
<td>77 (3.85%)</td>
</tr>
<tr>
<td>Mammography</td>
<td>-1</td>
<td>+1</td>
<td>11183</td>
<td>6</td>
<td>260 (2.32%)</td>
</tr>
<tr>
<td>Mammography-sub</td>
<td>-1</td>
<td>+1</td>
<td>2000</td>
<td>6</td>
<td>46 (2.3%)</td>
</tr>
<tr>
<td>Shuttle</td>
<td>1</td>
<td>2, 3, 5, 6, 7</td>
<td>12345</td>
<td>9</td>
<td>867 (7.02%)</td>
</tr>
<tr>
<td>Shuttle-sub</td>
<td>1</td>
<td>2, 3, 5, 6, 7</td>
<td>2000</td>
<td>9</td>
<td>140 (7.0%)</td>
</tr>
<tr>
<td>Yeast</td>
<td>‘CYT’, ‘NUC’, ‘MIT’</td>
<td>‘ERL’, ‘POX’, ‘VAC’</td>
<td>1191</td>
<td>8</td>
<td>55 (4.6%)</td>
</tr>
</tbody>
</table>
Algorithms

- Baseline: No learning; order cases highest $S(x)$ first
- Random: order cases at random
- AAD: Our method
- AI2: Veeramachaneni, et al. (CSAIL TR).
- SSAD: Semi-Supervised Anomaly Detector (Görnitz, et al., JAIR 2013)
Results: KDD 1999

![Graph showing the number of true anomalies against the number of queries for different methods: AAD, baseline, AI2, SSAD-MC, and SSAD-Top.](image)
Results: Abalone
Results: ANN-Thyroid-1v3
Results: Mammography
Summary: Incorporating Expert Feedback

- This can be very successful with LODA
  - Even when the expert labels the initial candidates as “nominal”
- AAD is doing implicit feature selection
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- Existing theory on sample complexity
  - Density Estimation Methods:
    - Exponential in the dimension $d$
  - Quantile Methods (OCSVM and SVDD):
    - Polynomial sample complexity

- Experimentally, many anomaly detection algorithms learn very quickly (e.g., 500-2000 examples)
- New theory: Rare Pattern Anomaly Detection
Pattern Spaces

- A pattern \( h: \mathbb{R}^d \rightarrow \{0,1\} \) is an indicator function for a measurable region in the input space
  - Examples:
    - Half planes
    - Axis-parallel hyper-rectangles in \([-1,1]^d\)

- A pattern space \( \mathcal{H} \) is a set of patterns (countable or uncountable)
Rare and Common Patterns

- Let $\mu$ be a fixed measure over $\mathbb{R}^d$
  - Typical choices:
    - uniform over $[-1, +1]^d$
    - standard Gaussian over $\mathbb{R}^d$
- $\mu(h)$ is the measure of the pattern defined by $h$
- Let $p$ be the “nominal” probability density defined on $\mathbb{R}^d$ (or on some subset)
- $p(h)$ is the probability of pattern $h$
- A pattern $h$ is $\tau$-rare if
  \[ f(h) = \frac{p(h)}{\mu(h)} \leq \tau \]
- Otherwise it is $\tau$-common
Rare and Common Points

- A point $x$ is $\tau$-rare if there exists a $\tau$-rare $h$ such that $h(x) = 1$
- Otherwise a point is $\tau$-common

- Goal: An anomaly detection algorithm should output all $\tau$-rare points and not output any $\tau$-common points
PAC-RPAD

- Algorithm $\mathcal{A}$ is PAC-RPAD with parameters $\tau, \epsilon, \delta$ if for any probability density $p$ and any $\tau$, with probability $1 - \delta$ over samples drawn from $p$, $\mathcal{A}$ draws a sample from $p$ and detects all $\tau$-outliers and rejects all $(\tau + \epsilon)$-commons in the sample.

- $\epsilon$ allows the algorithm some margin for error.

- If a point is between $\tau$-rare and $(\tau + \epsilon)$-common, the algorithm can treat it arbitrarily.
RAREPATTERNDETECT

- Draw a sample of size $N(\epsilon, \delta)$ from $p$
- Let $\hat{p}(h)$ be the fraction of sample points that satisfy $h$
- Let $\hat{f}(h) = \frac{\hat{p}(h)}{\mu(h)}$ be the estimated rareness of $h$
- A query point $x_q$ is declared to be an anomaly if there exists a pattern $h \in \mathcal{H}$ such that $h(x_q) = 1$ and $\hat{f}(h) \leq \tau$. 
Results

- Theorem 1: For any finite pattern space $\mathcal{H}$, RAREPATTERNDETECT is PAC-RPAD with sample complexity

\[ N(\epsilon, \delta) = O\left(\frac{1}{\epsilon^2} \left( \log |\mathcal{H}| + \log \frac{1}{\delta} \right) \right) \]

- Theorem 2: For any pattern space $\mathcal{H}$ with finite VC dimension $\nu_\mathcal{H}$, RAREPATTERNDETECT is PAC-RPAD with sample complexity

\[ N(\epsilon, \delta) = O\left(\frac{1}{\epsilon^2} \left( \nu_\mathcal{H} \log \frac{1}{\epsilon^2} + \log \frac{1}{\delta} \right) \right) \]
Examples of PAC-RPAD $\mathcal{H}$

- half spaces
- axis-aligned hyper-rectangles
- stripes (equivalent to LODA's histogram bins)
- ellipsoids
- ellipsoidal shells (difference of two ellipsoidal level sets)
Isolation RPAD (aka Pattern Min)

- Grow an isolation forest
  - Each tree is only grown to depth $k$
  - Each leaf defines a pattern $h$
  - $\mu$ is the volume (Lebesgue measure)
  - Compute $\hat{f}(h)$ for each leaf

Details

- Grow the tree using one sample
- Estimate $\hat{f}$ using a second sample
- Score query point(s)
Results: Shuttle

- PatternMin is consistently better for $k > 1$
RPAD Conclusions

- The PAC-RPAD theory seems to capture the behavior of algorithms such as IFOREST.
- It is easy to design practical RPAD algorithms.
- Theory requires extension to handle sample-dependent pattern spaces $\mathcal{H}$. 
Summary

- Outlier Detection can perform unsupervised or clean anomaly detection when the relative frequency of anomalies, $\alpha$ is small.
- Algorithm Benchmarking
  - The Isolation Forest is a robust, high-performing algorithm.
  - The OCSVM and SVDD methods do not perform well on AUC and AP. Why not?
  - The other methods (ABOD, LODA, LOF, EGMM, RKDE) are very similar to each other.
- Sequential Feature Explanations provide a well-defined and objectively measurable method for anomaly explanation.
- Expert Feedback can be incorporated into LODA via a modified Accuracy-at-the-Top algorithm with good results.
- PAC-RPAD theory may account for the rapid learning of many anomaly detection algorithms.