

# Advances in Anomaly Detection

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# Outline

- Defining the Anomaly Detection Problem
- Benchmarking Current Algorithms for Unsupervised Anomaly Detection
- PAC Theory of Rare Pattern Anomaly Detection
- Incorporating Analyst Feedback
- Applications
  - Weather network anomaly detection
  - Open Category detection

# Defining Anomaly Detection

- Data  $x_1, \dots, x_N$ , each  $x_i \in \Re^d$
- Mixture of “nominal” points and “anomaly” points
- Anomaly points are generated by a different process than the nominal points
- Anomaly detector:  $A(x) = \text{anomaly score}$
- Goals:
  - Find all of the anomalies in the training data
  - Determine whether a new query point  $x_q$  is an anomaly

# Three Settings

- Supervised
  - Training data labeled with “nominal” or “anomaly”
- Clean
  - Training data are all “nominal”, test data contaminated with “anomaly” points.
- Unsupervised
  - Training and test data consist of mixture of “nominal” and “anomaly” points

# 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



[Emmott, Das, Dietterich, Fern, Wong, 2013; KDD ODD-2013]

[Emmott, Das, Dietterich, Fern, Wong. 2016; arXiv 1503.01158v2]

# Benchmarking Methodology

- Select 19 data sets from UC Irvine repository
- Choose one or more classes to be “anomalies”; the rest are “nominals”
- Manipulate
  - Relative frequency
  - Point difficulty
  - Irrelevant features
  - Clusteredness
- 20 replicates of each configuration
- Result: 25,685 Benchmark Datasets

# Metrics

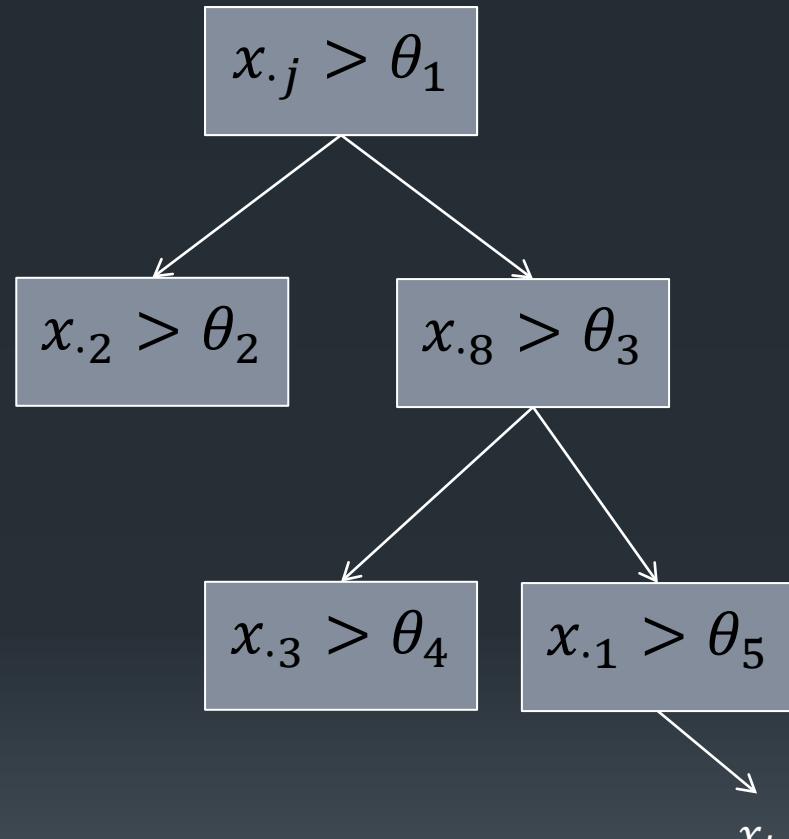
- AUC (Area Under ROC Curve)
  - ranking loss: probability that a randomly-chosen anomaly point is ranked above a randomly-chosen nominal point
  - transformed value:  $\log \frac{AUC}{1-AUC}$
- AP (Average Precision)
  - area under the precision-recall curve
  - average of the precision computed at 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 Models (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)

# Isolation Forest [Liu, Ting, Zhou, 2011]

- Construct a fully random binary tree
  - choose attribute  $j$  at random
  - choose splitting threshold  $\theta_1$  uniformly from  $[\min(x_j), \max(x_j)]$
  - until every data point is in its own leaf
  - let  $d(x_i)$  be the depth of point  $x_i$
- repeat 100 times
  - let  $\bar{d}(x_i)$  be the average depth of  $x_i$
  - $score(x_i) = 2^{-\left(\frac{\bar{d}(x_i)}{r(x_i)}\right)}$ 
    - $r(x_i)$  is the expected depth



# Analysis

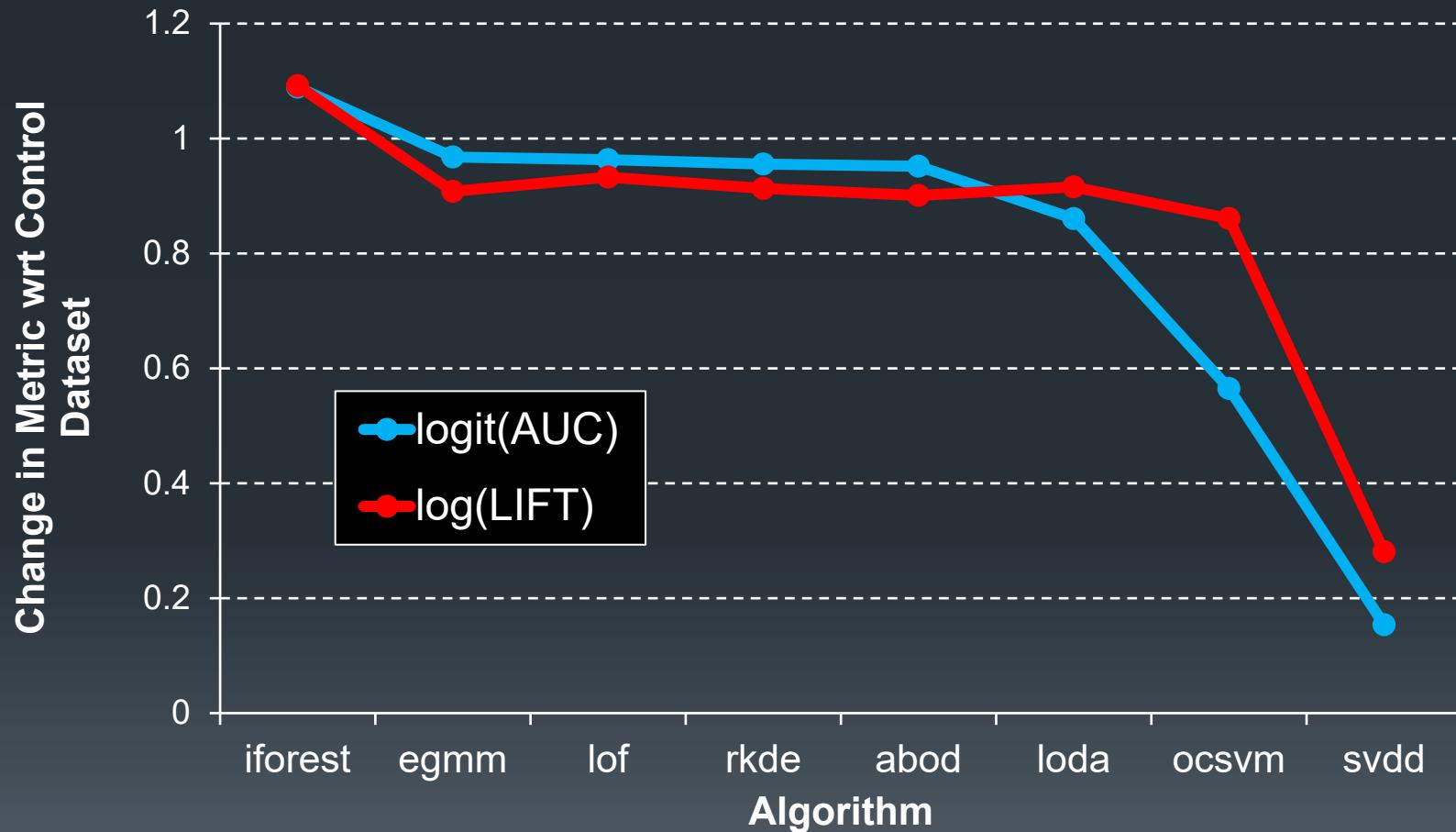
- Linear ANOVA
  - $metric \sim rf + pd + cl + ir + mset + algo$ 
    - rf: relative frequency
    - pd: point difficulty
    - cl: normalized clusteredness
    - ir: irrelevant features
    - mset: “Mother” set
    - algo: anomaly detection algorithm
- Validate the effect of each factor
- Assess the *algo* effect while controlling for all other factors

# What Matters the Most?



- Problem and Relative Frequency!
- Choice of algorithm ranks third

# Algorithm Comparison



# iForest Advantages

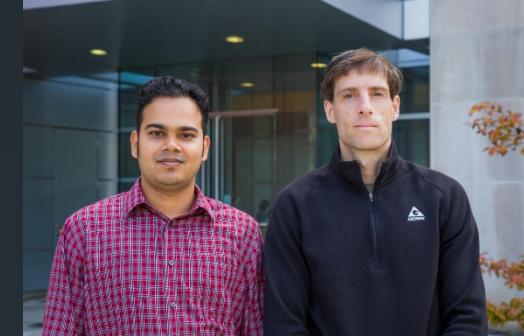
- Most robust to irrelevant features
  - for both AUC and LIFT
  - Hypothesis: effect of irrelevant features can be averaged out by computing a large forest
- Second most robust to clustered anomaly points
  - for AUC
  - Why?

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# Towards a Theory of Anomaly Detection [Siddiqui, et al.; UAI 2016]

- 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  $\Re^d$ 
  - Typical choices:
    - uniform over  $[-1, +1]^d$
    - standard Gaussian over  $\Re^d$
- $\mu(h)$  is the measure of the pattern defined by  $h$
- Let  $p$  be the “nominal” probability density defined on  $\Re^d$  (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 for

- pattern space  $\mathcal{H}$ ,
  - measure  $\mu$ ,
  - parameters  $\tau, \epsilon, \delta$

if for any probability density  $p$  and any  $\tau$ ,  $\mathcal{A}$  draws a sample from  $p$  and with probability  $1 - \delta$  detects all  $\tau$ -rare points 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
- Running time: polynomial in  $\frac{1}{\epsilon}$ ,  $\frac{1}{\delta}$ , and  $\frac{1}{\tau}$ , and some measure of the complexity of  $\mathcal{H}$

# RAREPATTERNDTECT

- 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  $\mathcal{H}$ , RAREPATTERNDTECT 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  $\mathcal{V}_{\mathcal{H}}$ , RAREPATTERNDTECT is PAC-RPAD with sample complexity

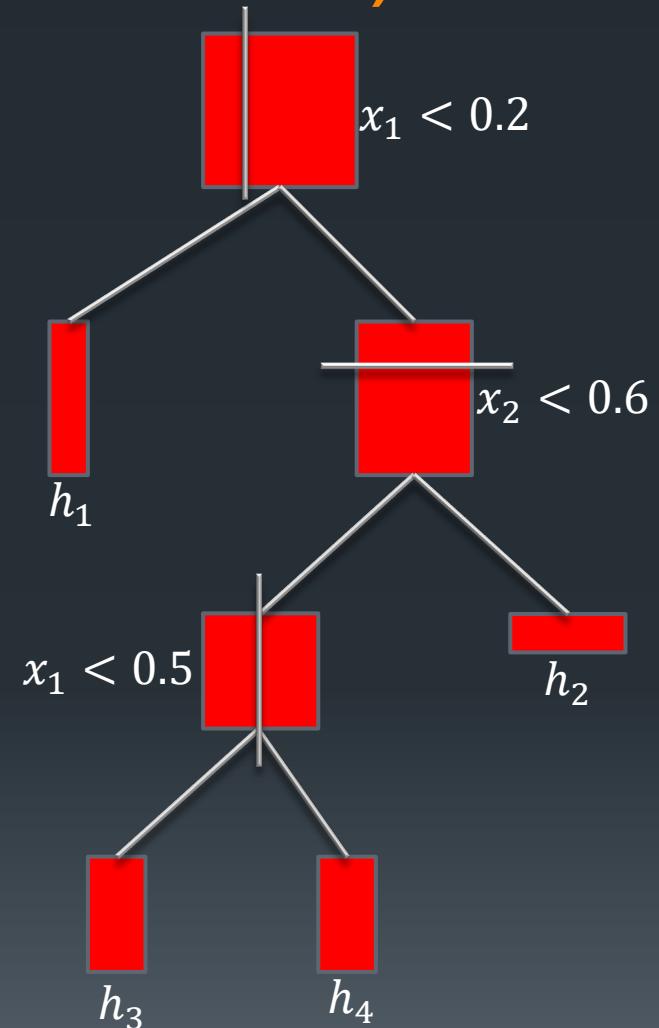
$$N(\epsilon, \delta) = O\left(\frac{1}{\epsilon^2} \left( \mathcal{V}_{\mathcal{H}} \log \frac{1}{\epsilon^2} + \log \frac{1}{\delta} \right)\right)$$

# Examples of PAC-RPAD $\mathcal{H}$

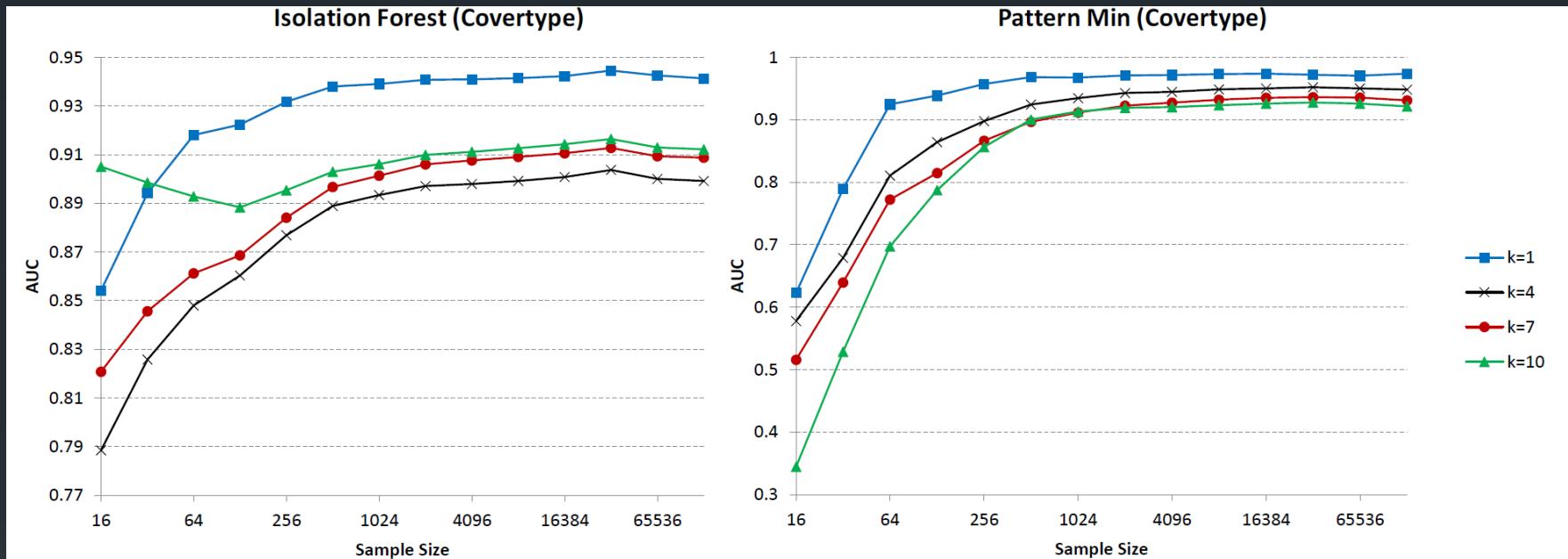
- Half spaces
- Axis-aligned hyper-rectangles (related to iForest leaves)
- Stripes (equivalent to LODA's histogram bins)
- Ellipsoids
- Ellipsoidal shells (difference of two ellipsoidal level sets)

# 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)

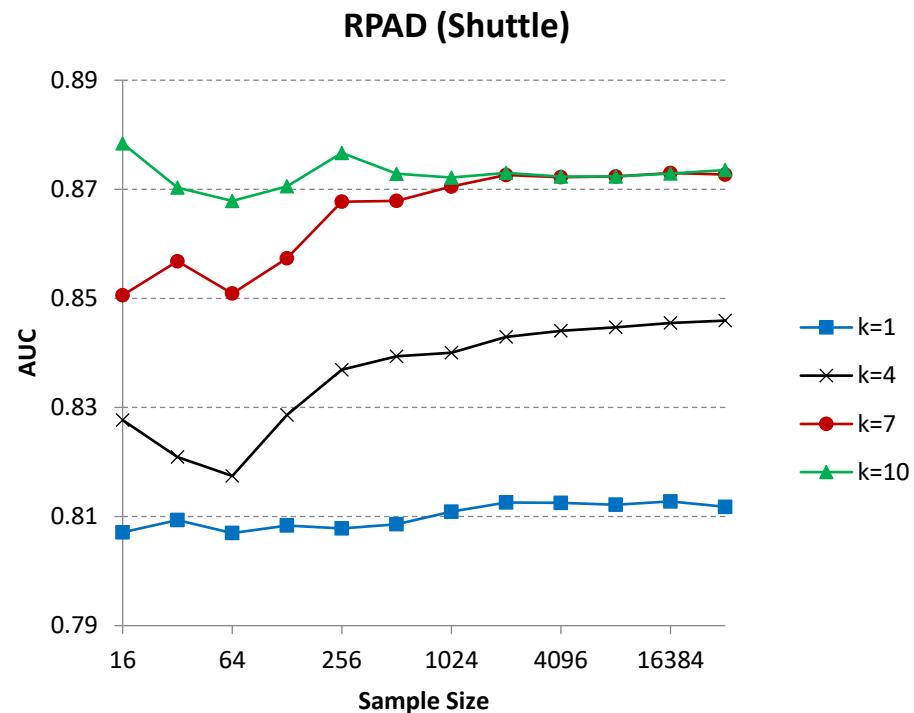
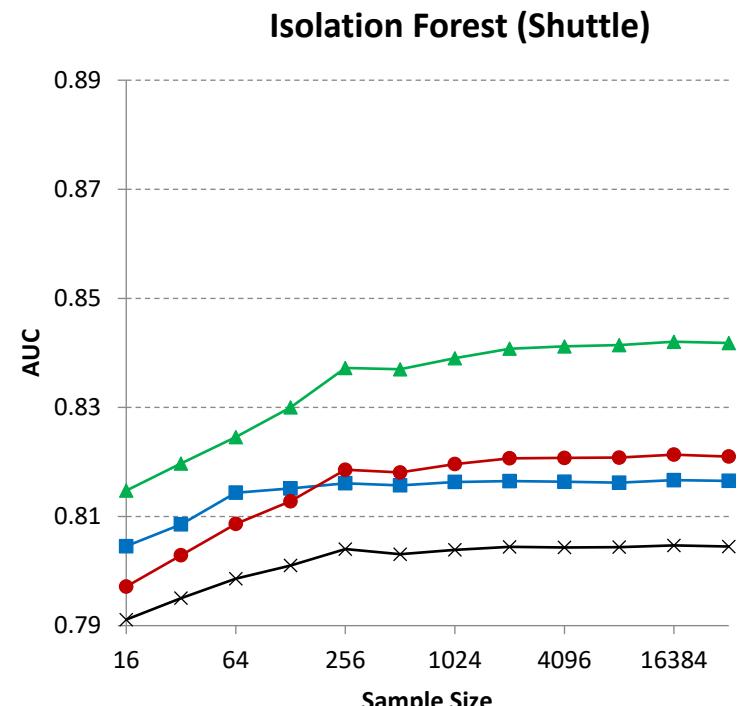


# Results: Covertype



- PatternMin learns more slowly, but eventually beats IFOREST

# Results: Shuttle



- PatternMin consistently beats iForest for  $k > 1$

# RPAD Conclusions

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

# Outline

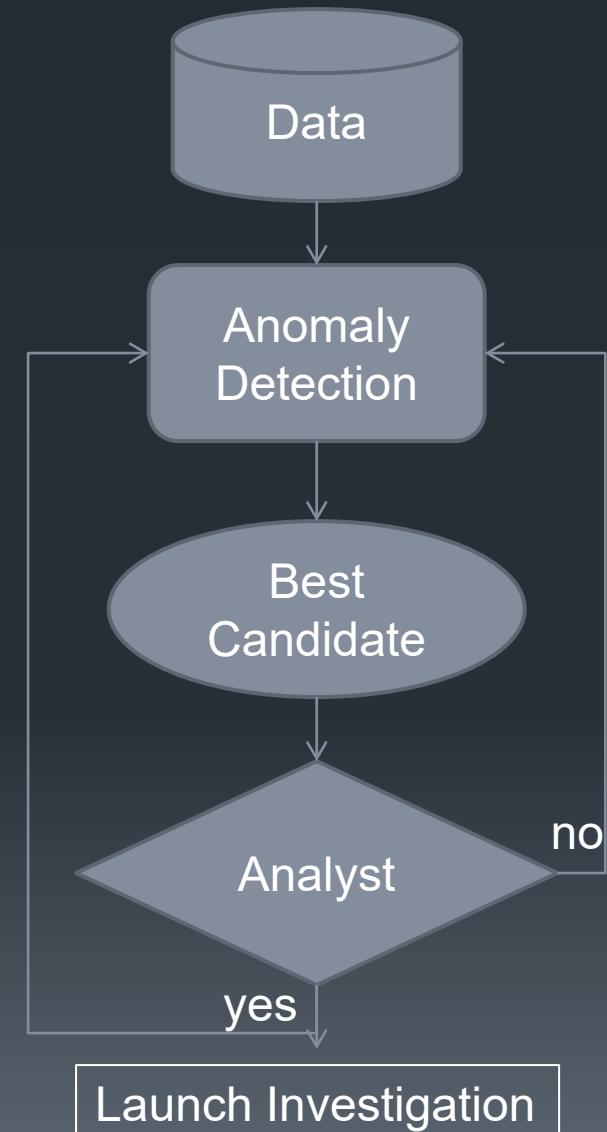
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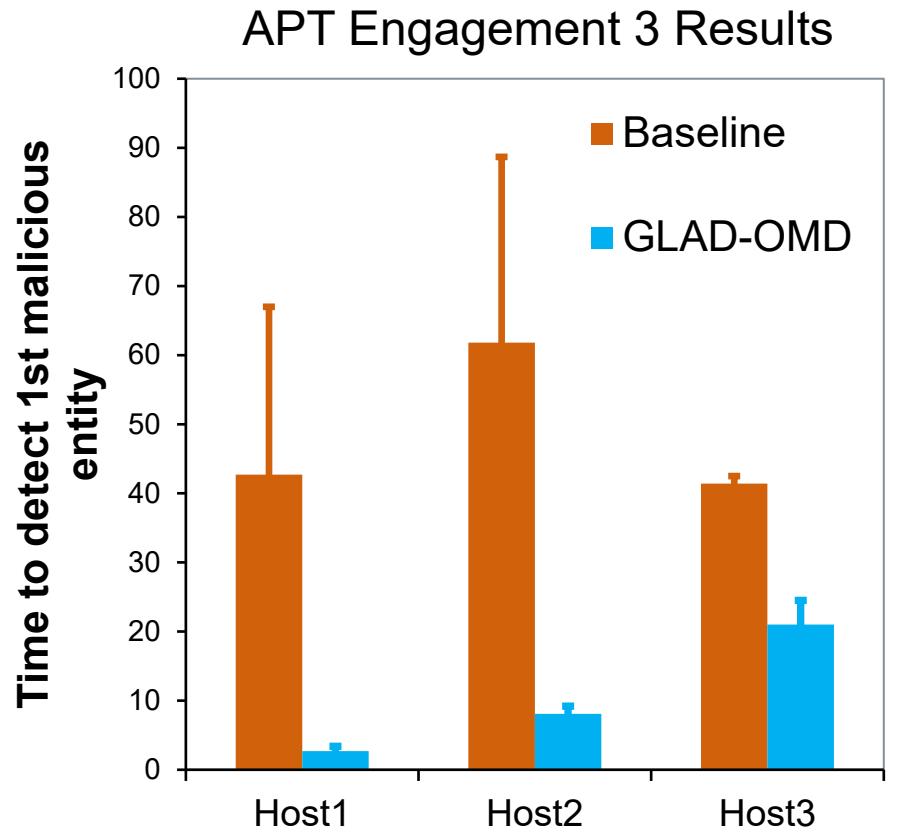
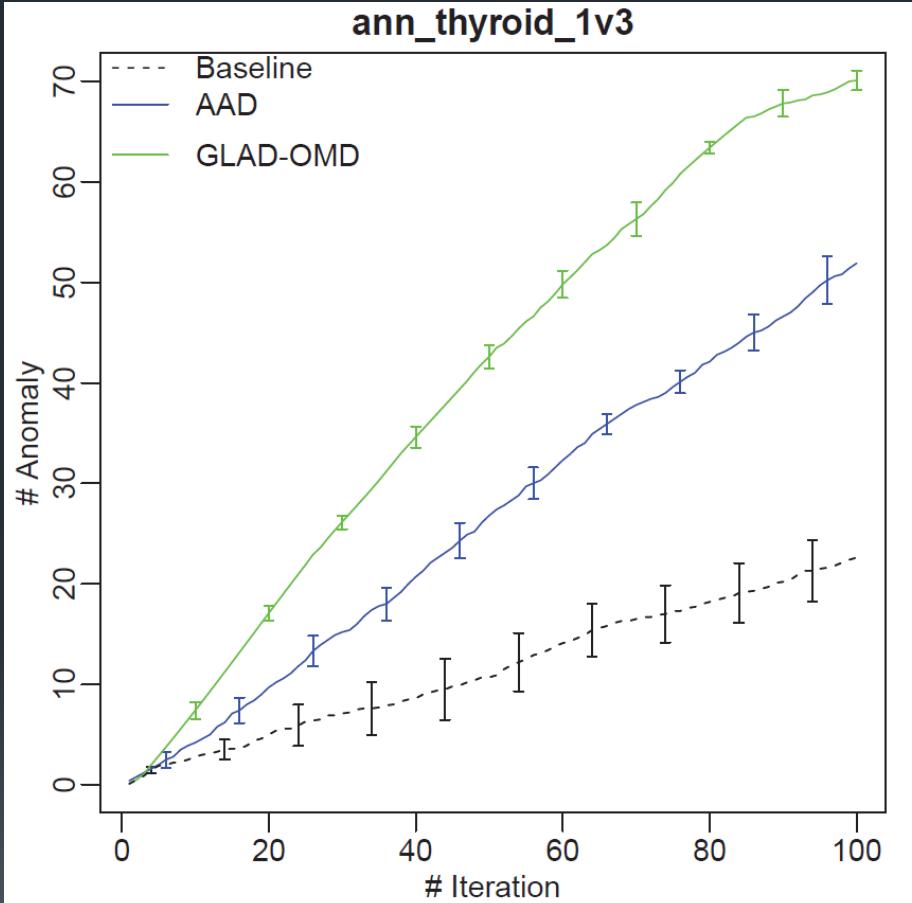
# Incorporating Analyst Feedback

- Show top-ranked (unlabeled) candidate to the Analyst
- Analyst labels candidate
- Label is used to update the anomaly detector



[Das, et al, ICDM 2016]  
[Siddiqui, et al., KDD 2018]

# Analyst Feedback Yields Huge Improvements in Anomaly Discovery



# Method

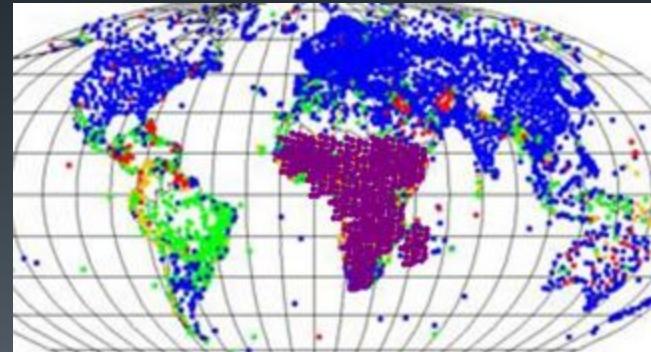
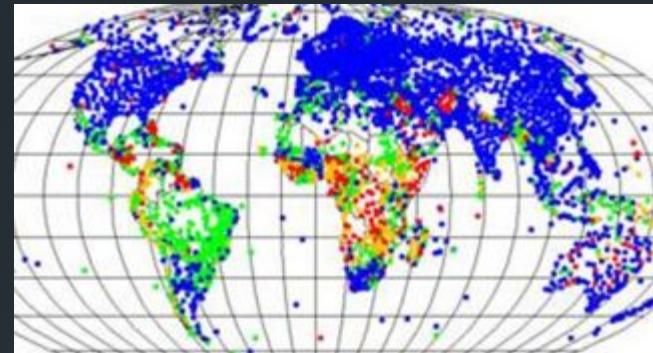
- Transform the Isolation Forest into a gigantic linear model
  - Each node in each tree becomes a Boolean feature that is 1 if  $x_q$  visits that node
  - Initial weight of each feature is 1.0, so that the weighted sum == sum of isolation depths in the forest
- Apply online convex optimization algorithms to learn from analyst feedback
  - Online Mirror Descent adjusts the weights to reduce the score of anomalies and increase the score of nominals

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# TAHMO: Trans-Africa Hydro-Meteorological Observatory

- Africa is very poorly sensed
  - Only a few dozen weather stations reliably report data to WMO (blue points in map)
  - Poor sensing → No crop insurance → Low agricultural productivity
  - Goal: Make Africa the best-sensed continent & improve agriculture
- Project TAHMO ([tahmo.org](http://tahmo.org))
  - TU-DELFT & Oregon State University
  - Design low-cost weather station
  - Deploy 20,000 such stations across Africa
  - Create data products (e.g., drought assessments, inundation estimates)
- Automated Data Quality Control
  - Detect broken sensors as anomalies



# SENSOR-DX Architecture: Design and Training

- Define a set of views of the TAHMO data
  - A view involves 1 or more sensors from 1 or more stations over 1 or more time points
  - Each view defines a set of view tuples  $\nu$
- Fit an anomaly detector to the view tuples
- Introduce a state variable  $s$  for each sensor at each station and time point
- Fit probabilistic models  $P(A(\nu)|\text{parents}(\nu))$
- Hypothesis: It is easier to model the anomaly score distribution than it is to model the sensor readings

# Example View

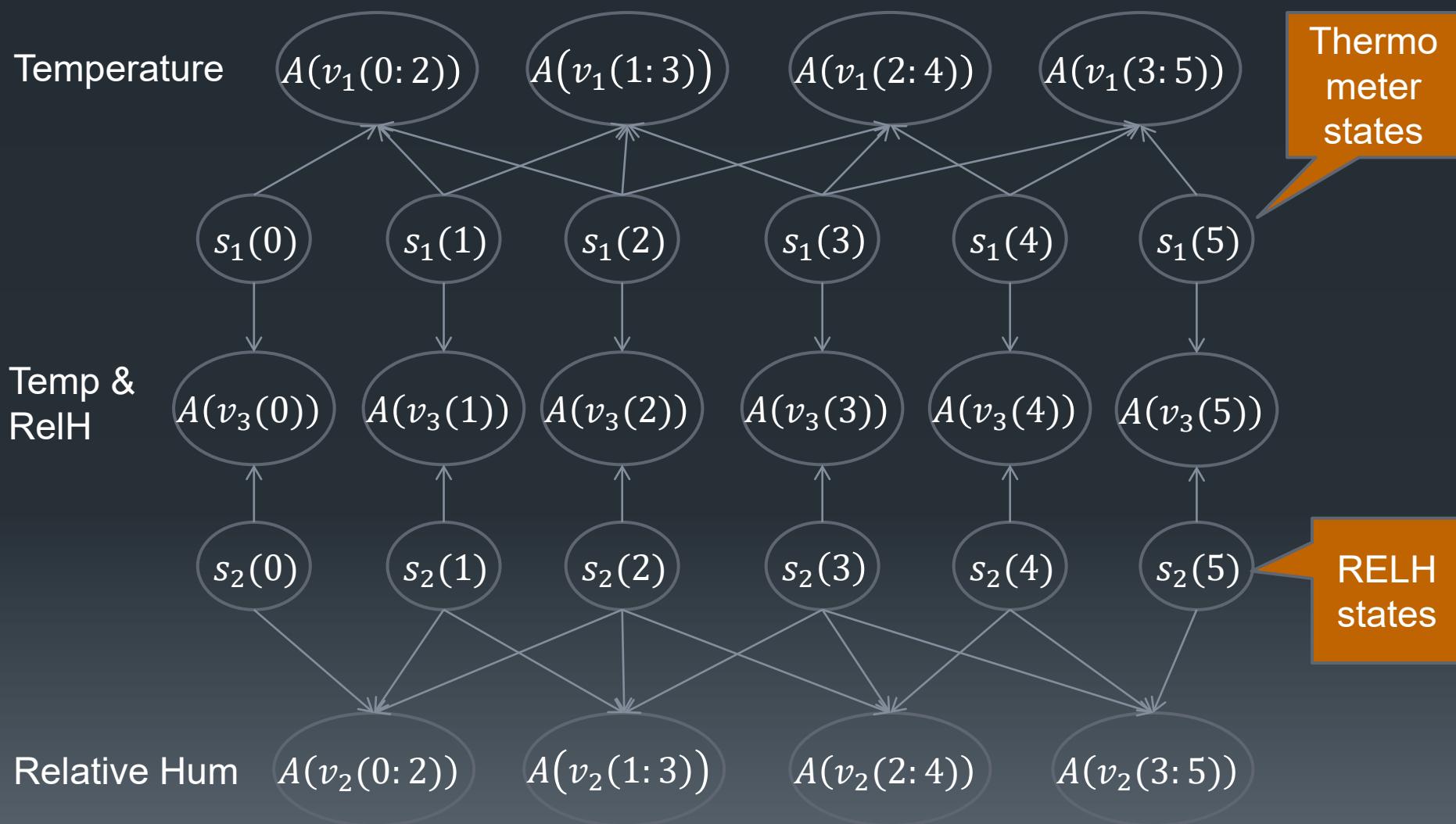
- Temperature  $T$  at times  $t - 2, t - 1, t$

0	1	2	3	4
15	15.5	16.2	17	16.5

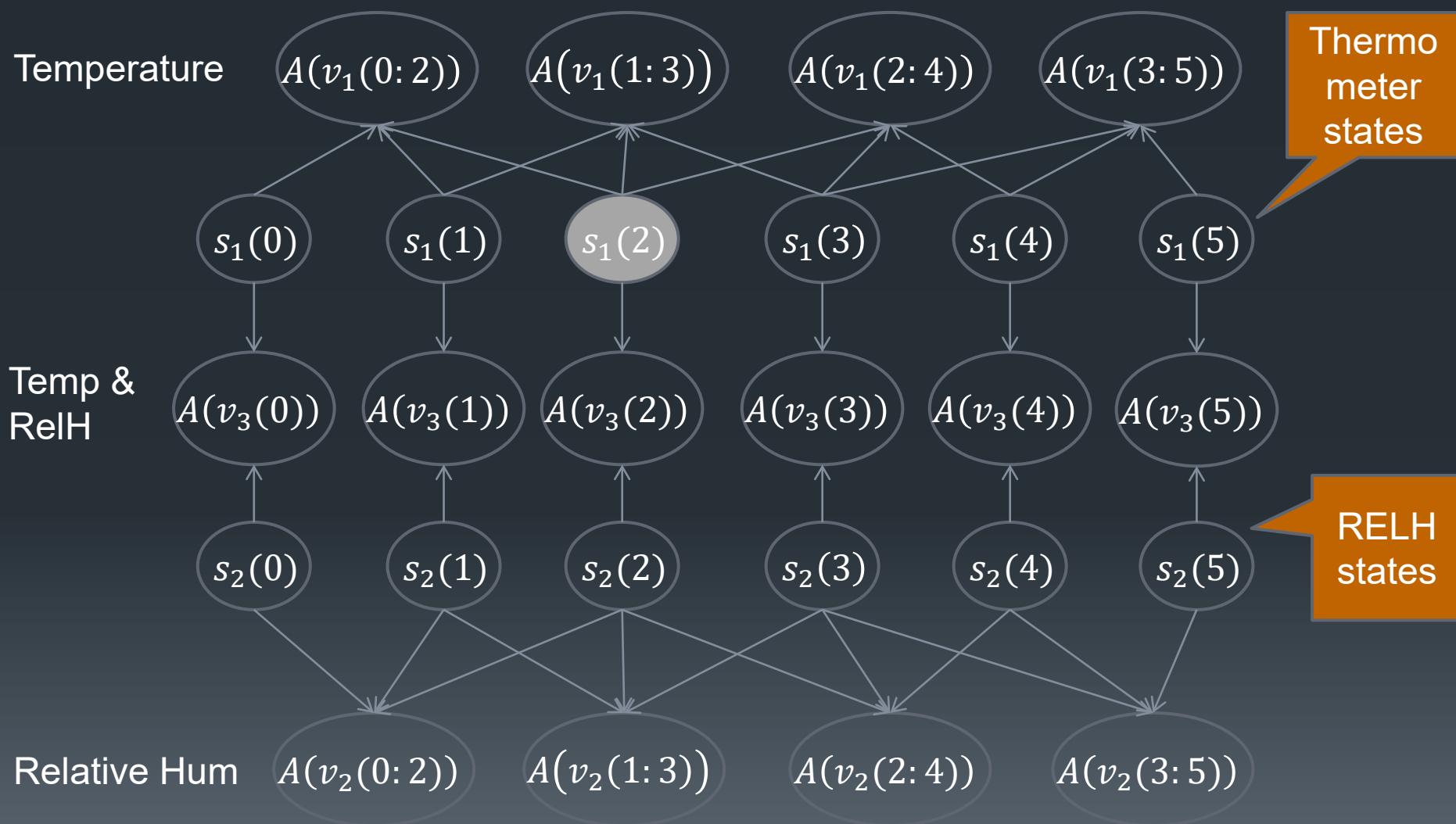
- View tuples

	$t - 2$	$t - 1$	$t$
$v_1(0: 2)$	15	15.5	16.2
$v_1(1: 3)$	15.5	16.2	17
$v_1(2: 4)$	16.2	17	16.5

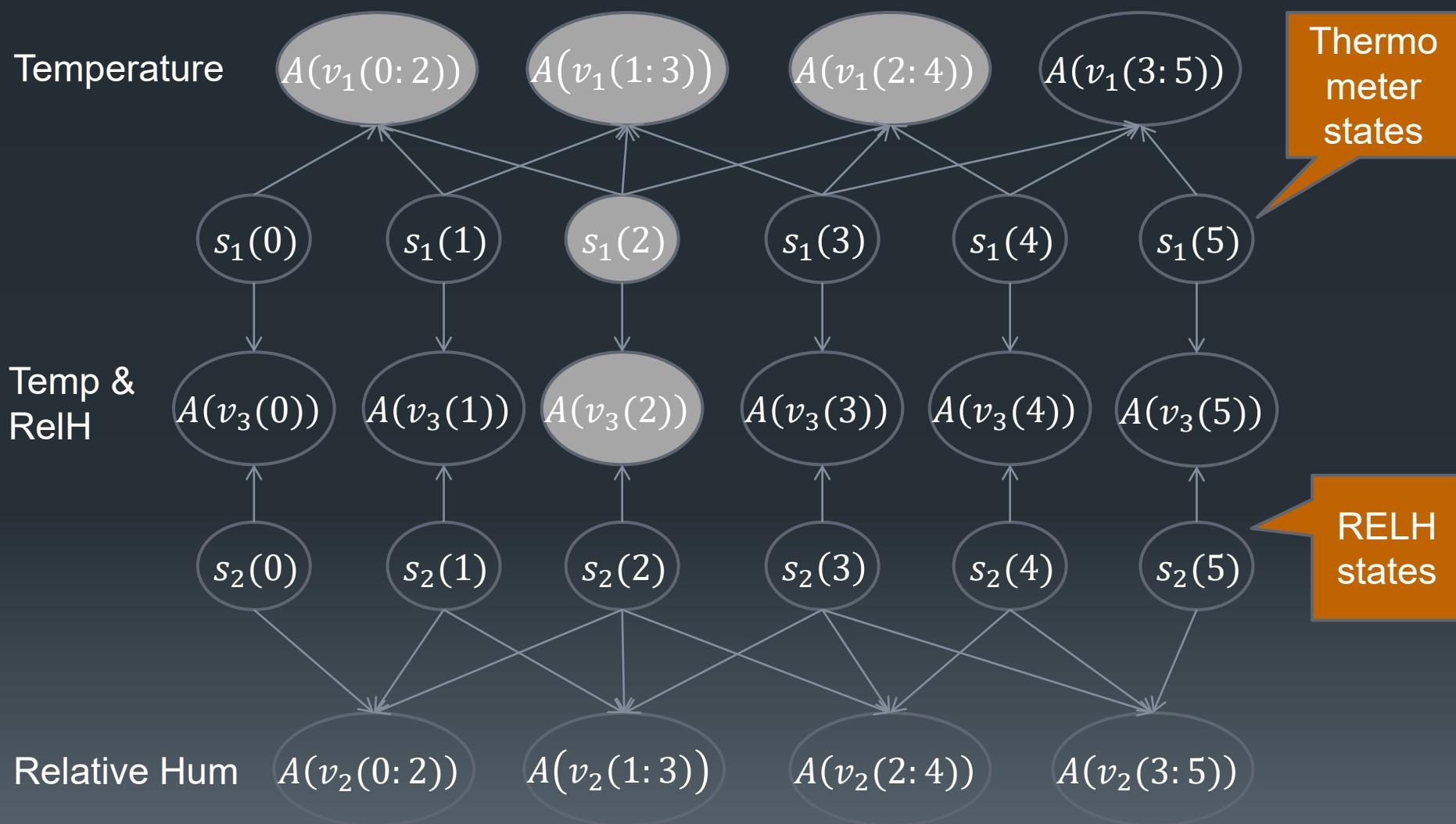
# Diagnostic Model



# Diagnostic Model



# Diagnostic Model



# Run Time Quality Control

- Assemble incoming data into view tuples
- Compute anomaly score for each view tuple
- Perform probabilistic inference to determine which sensor states best explain the observed anomaly scores:

$$\arg \max_S P(S|A(V))$$

# Experimental Evaluation

[Tadesse Zemicheal]

- Data: Oklahoma Mesonet

- 1 year for training, 1 year for testing
- 5 minute reporting interval; 20-day blocks
- Hourly sensor state variable
- Sensors:
  - Temperature (TAIR), relative humidity (RELH), atmospheric pressure (PRES), and Solar Radiation (SRAD)
- Stations:
  - OKCE, OKCN, OKCW, NRMN

- Synthetic faults

- spike noise, flatline, offset

- Isolation Forest

- Baseline:

- Single sensor view

- SENSOR-DX:

- Four views

- Metrics:

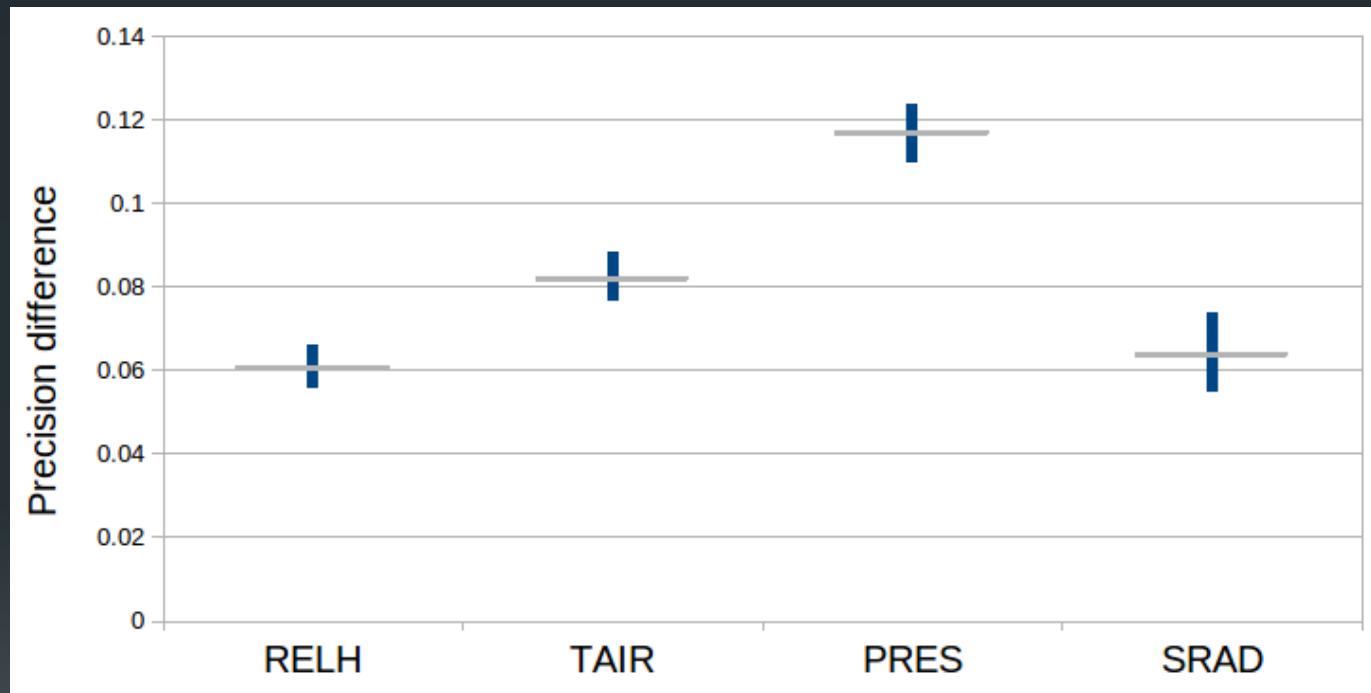
- Precision and recall



View type	State/period	Total #views
Single sensor view	1	16
Same sensor two station view	2	24
Two sensor single station view	2	24
Single sensor three hour view	3	14
<b>Total views per block</b>		<b>80</b>

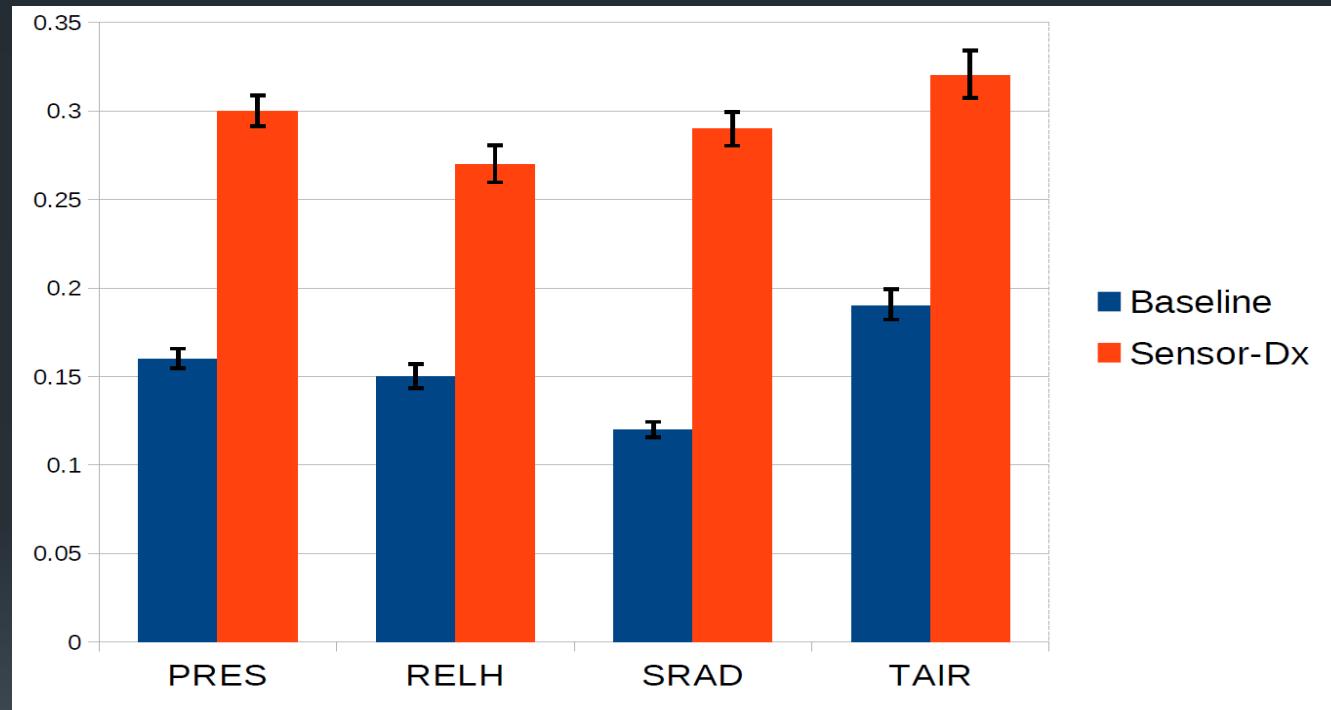
# Result: SENSOR-DX improves precision

Difference in precision of multi-view method versus single-view baseline



95% two-sided  
paired differences  
bootstrap confidence  
intervals

# Precision at Matching Recall Level



95% confidence intervals

Sensor-DX  
improves precision,  
but the false alarm  
rate will still be quite  
high

# Status

- Deployment on TAHMO network is in progress
- Integrated with
  - Network Manager dashboard
  - Trouble ticket system

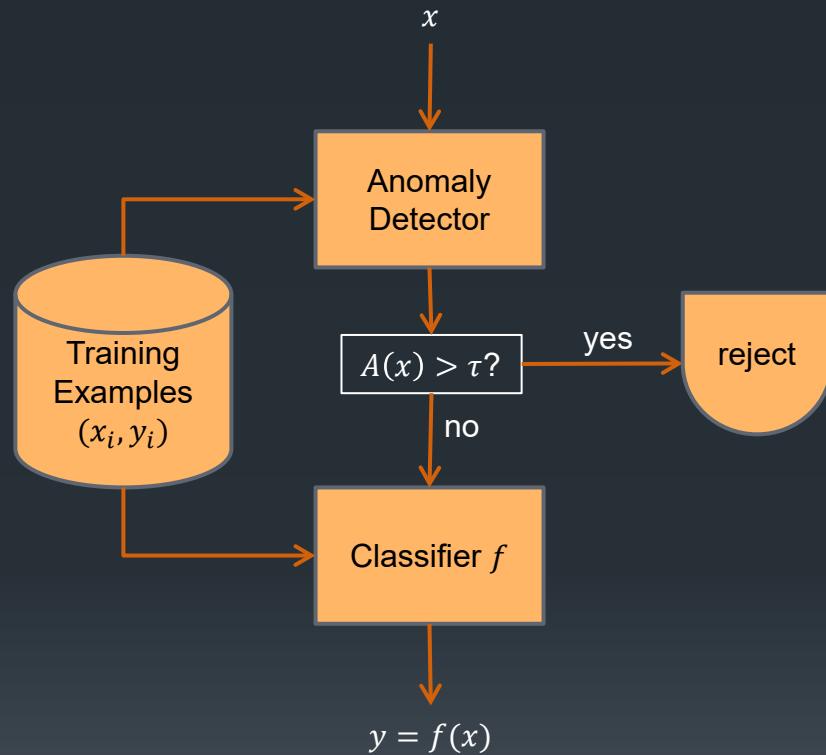
# Open Category Classification

[Liu, Garrepalli, Fern, Dietterich, ICML 2018]

- Training data for classes  $\{1, \dots, K\}$
- Test data may contain queries corresponding to additional classes
- Can we detect them?

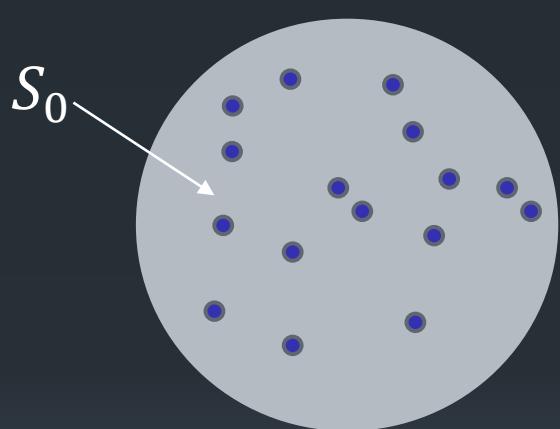


# Prediction with Anomaly Detection

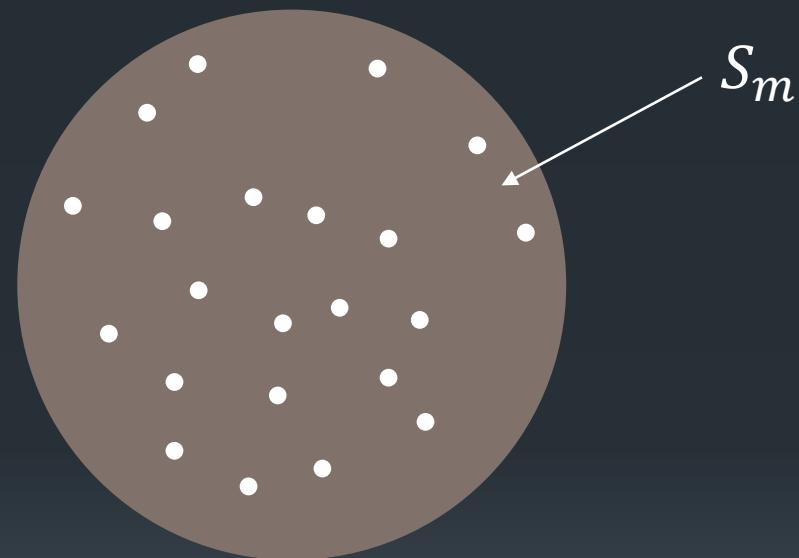


# Training Data

$P_0$   
Nominal Distribution



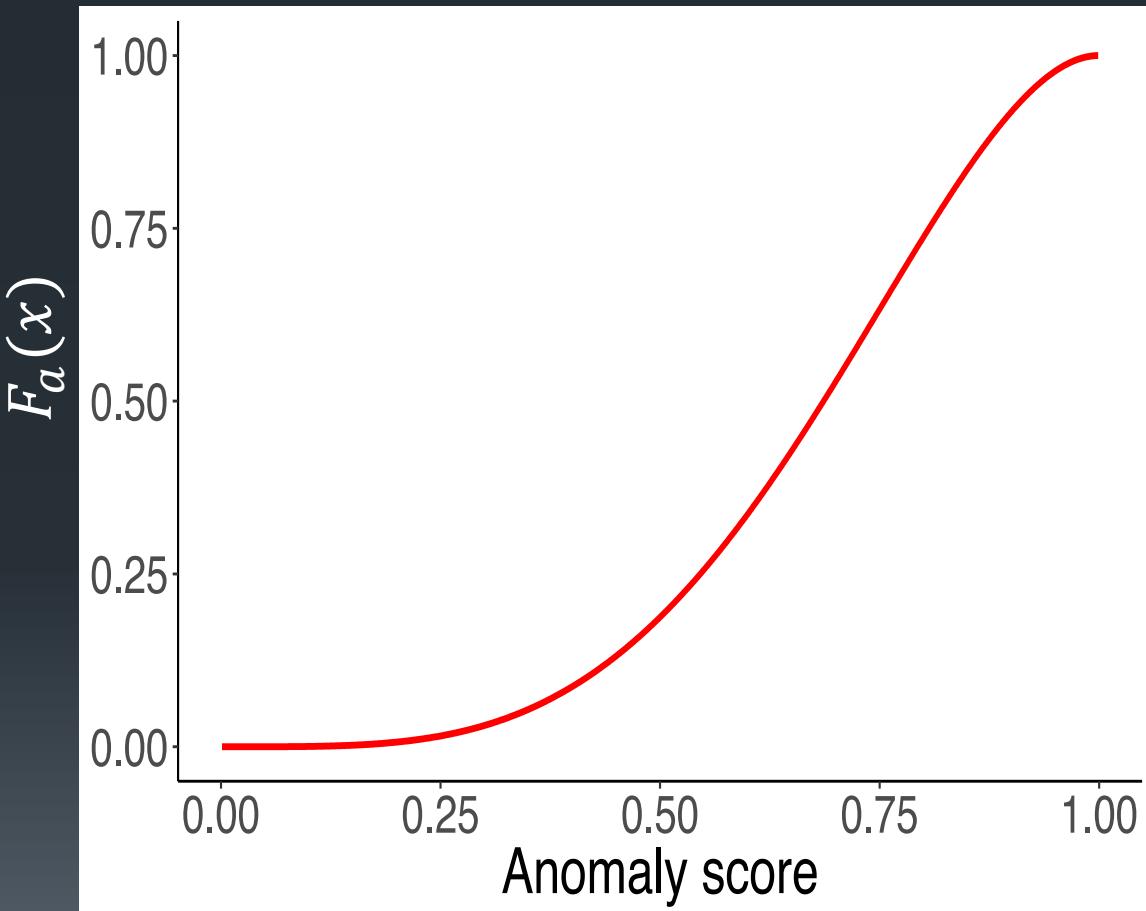
$P_m$   
Mixture Distribution



Proportion of Aliens =  $\alpha$

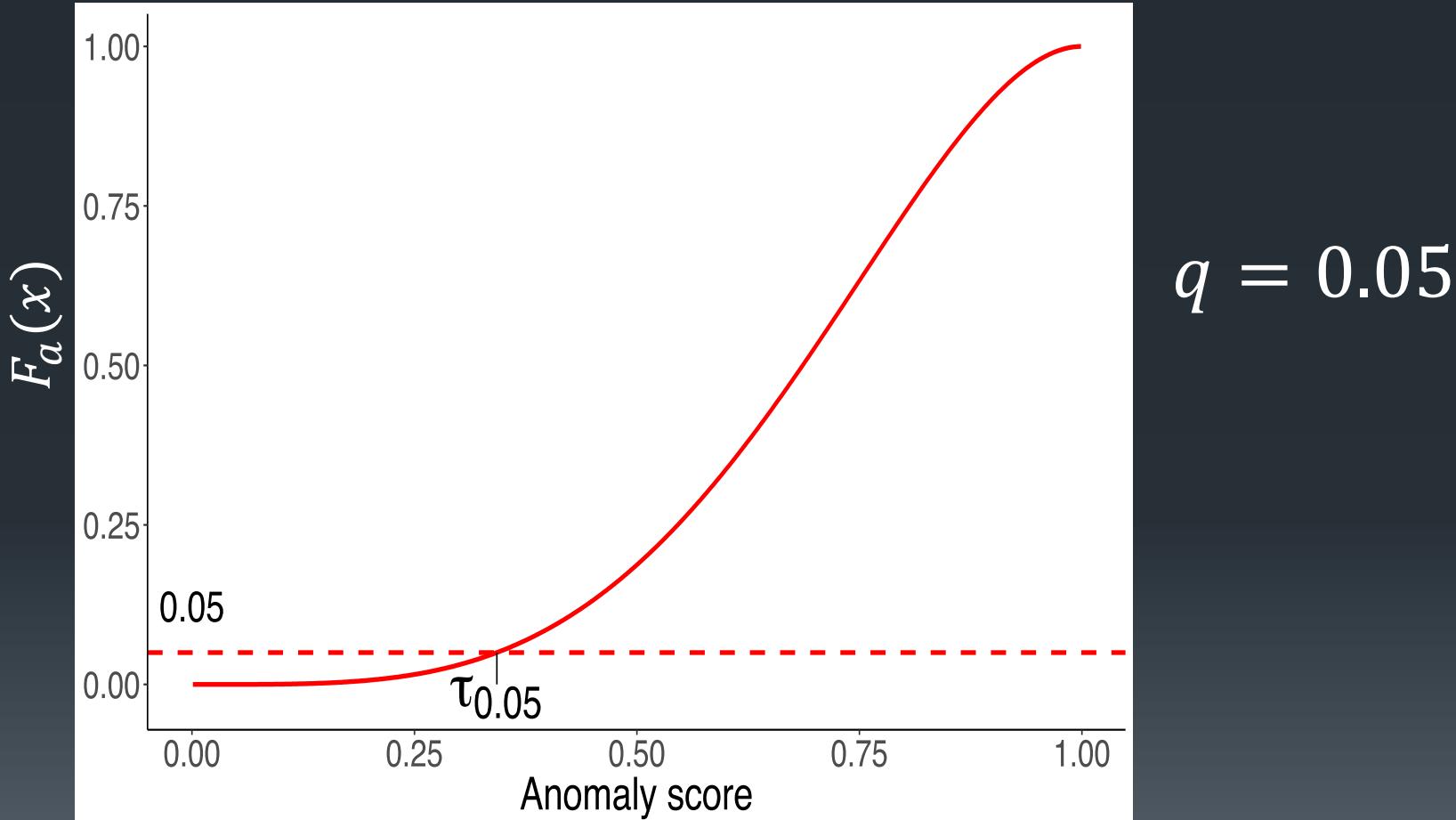
$$P_m = (1 - \alpha)P_0 + \alpha P_a$$

# CDF of Alien Anomaly Scores: $F_a$



Want to have  
recall =  $1 - q$

# Choosing $\tau$ for target quantile $q$

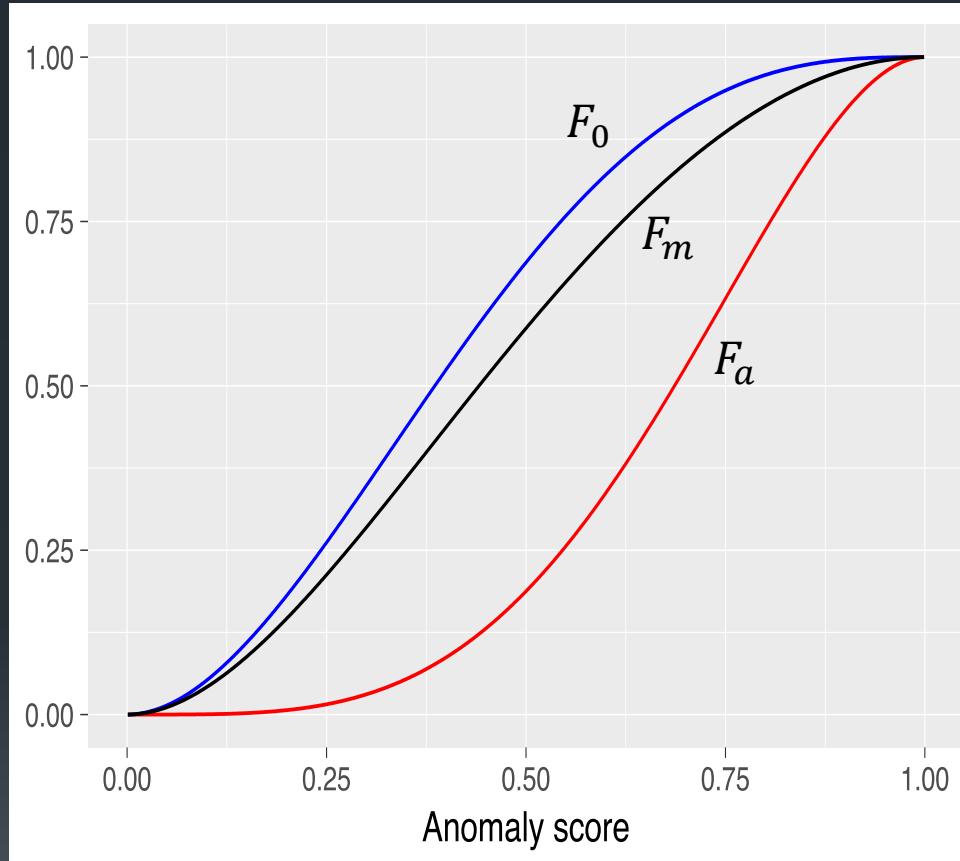


$$P_m = (1 - \alpha)P_0 + \alpha P_a$$

implies that

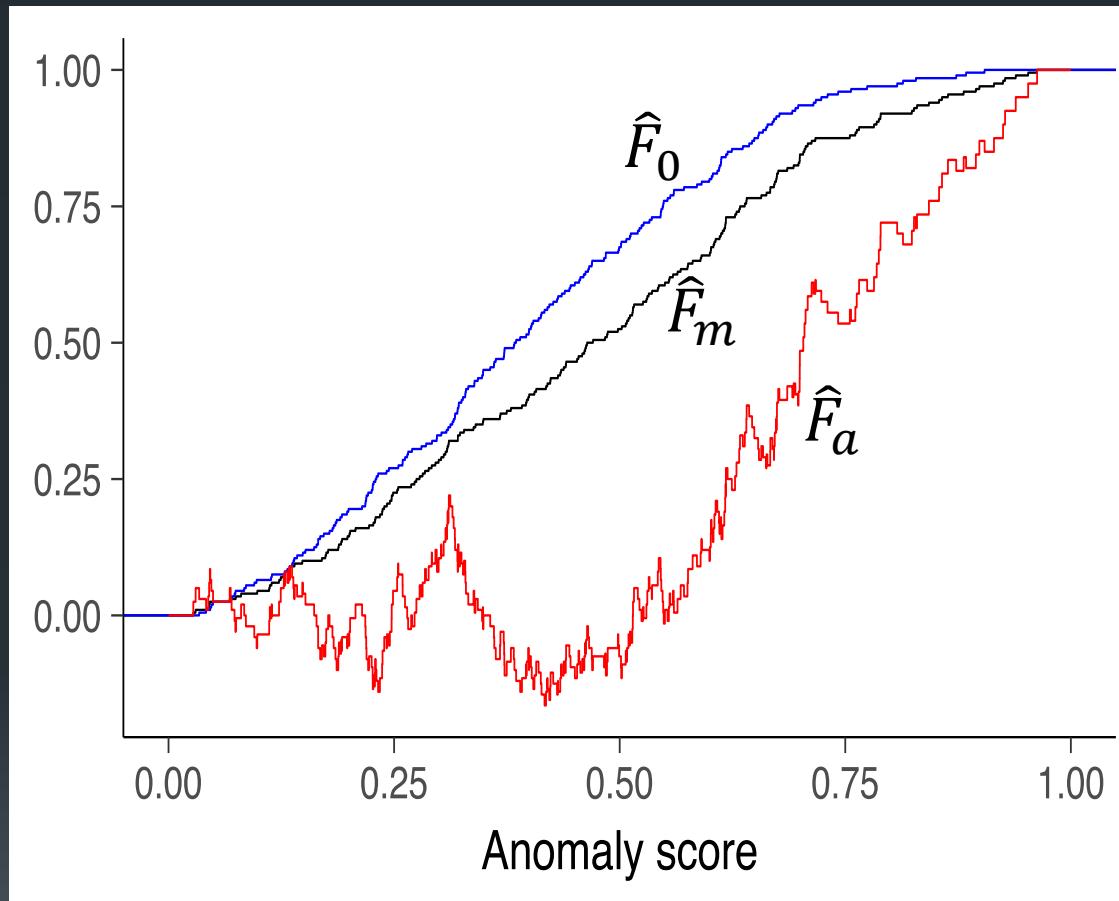
$$F_m(x) = (1 - \alpha)F_0(x) + \alpha F_a(x)$$

# CDFs of Nominal, Mixture, and Alien Anomaly Scores



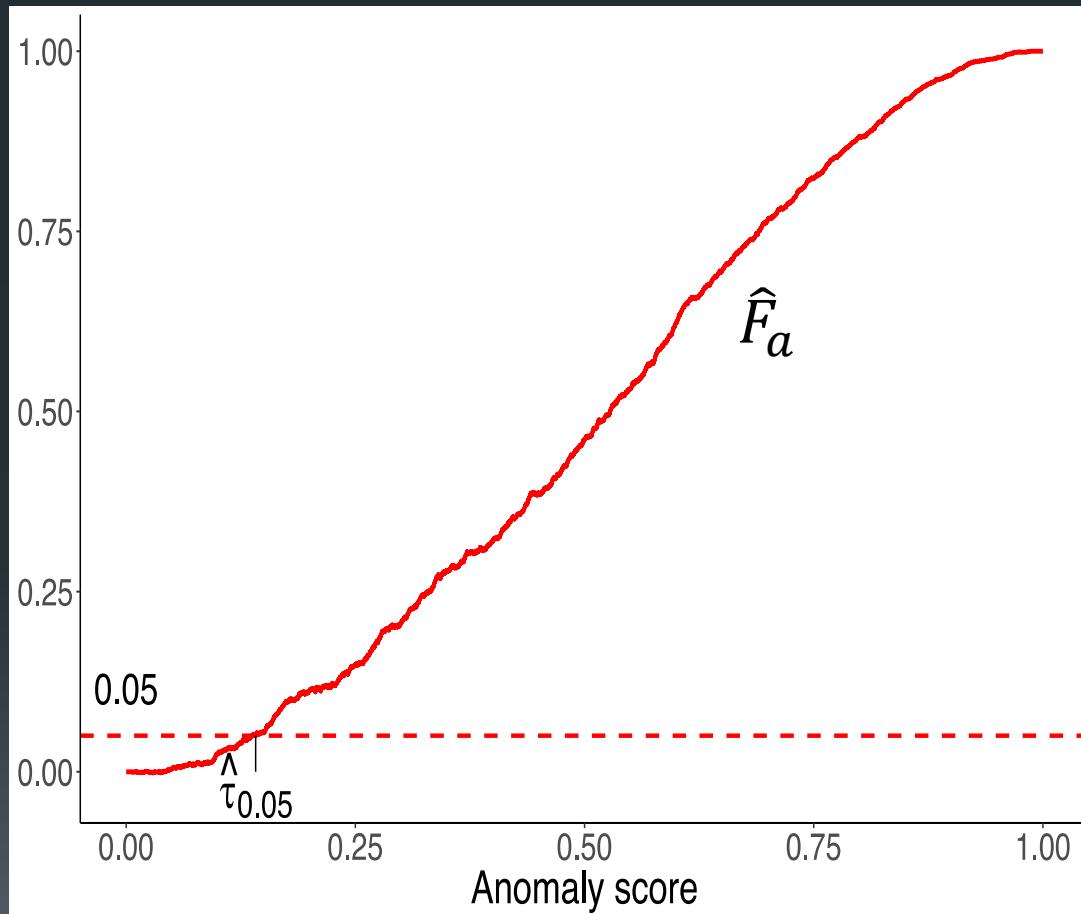
$$F_a(x) = \frac{F_m(x) - (1 - \alpha)F_0(x)}{\alpha}$$

# What We Have Are Empirical CDFs



$$\hat{F}_a(x) = \frac{\hat{F}_m(x) - (1 - \alpha)\hat{F}_0(x)}{\alpha}$$

# We Use the Empirical Estimate $\hat{\tau}_{0.05}$



# EstimateTau( $S_0, S_m, q, \alpha$ )

- 1: Anomaly scores of  $S_0$ :  $x_1, x_2, \dots, x_k$
- 2: Anomaly scores of  $S_m$ :  $y_1, y_2, \dots, y_m$
- 3: Compute empirical CDFs  $\hat{F}_0$  and  $\hat{F}_m$ .
- 4: Calculate  $\hat{F}_a$  using

$$\hat{F}_a(x) = \frac{\hat{F}_m(x) - (1 - \alpha)\hat{F}_0(x)}{\alpha}.$$

- 5: Output detection threshold

$$\hat{\tau}_q = \max_{u \in S} \hat{F}_a(u) \leq q,$$

where  $S = \{x_1, x_2, \dots, x_k, y_1, y_2, \dots, y_m\}$ .

# Theoretical Guarantee

[Liu, Garrepalli, Fern, Dietterich, ICML 2018]

- Theorem: If

$$n > \frac{1}{2} \ln \frac{2}{1 - \sqrt{1 - \delta}} \left( \frac{1}{\epsilon} \right)^2 \left( \frac{2 - \alpha}{\alpha} \right)^2$$

then with probability  $1 - \delta$  the alien detection rate will be at least  $1 - (q + \epsilon)$

Proof based on Massart (1990) concentration bound for empirical CDFs

# 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
- PAC-RPAD theory may account for the rapid learning of many anomaly detection algorithms
- Expert Feedback can double or triple the efficiency of detecting anomalies
- Anomaly detection can help find broken IoT sensors
- Anomaly detection can provide guarantees for open category detection

# Acknowledgements

- Partially supported by
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