Time Series Anomaly Detection with label-free Model Selection

Deokwoo Jung, Nandini Ramanan, Mehrnaz Amjadi, Sankeerth Rao Karingula, Jake Taylor, and Claudionor Nunes Coelho Jr

ADVANCED APPLIED AI RESEARCH
PALO ALTO NETWORKS, USA
{djung,nramanan,mamjadi,skaringula,jataylor,ccoelho}@paloaltonetworks.com

Abstract

Anomaly detection for time-series data becomes an essential task for many data-driven applications fueled with an abundance of data and out-of-the-box machine-learning algorithms. In many real-world settings, developing a reliable anomaly model is highly challenging due to insufficient anomaly labels and the prohibitively expensive cost of obtaining anomaly examples. It imposes a significant bottleneck to evaluate model quality for model selection and parameter tuning reliably. As a result, many existing anomaly detection algorithms fail to show their promised performance after deployment.

In this paper, we propose LaF-AD, a novel anomaly detection algorithm with label-free model selection for unlabeled times-series data. Our proposed algorithm performs a fully unsupervised ensemble learning across a large number of candidate parametric models. We develop a model variance metric that quantifies the sensitivity of anomaly probability with a bootstrapping method. Then it makes a collective decision for anomaly events by model learners using the model variance. Our algorithm is easily parallelizable, more robust for ill-conditioned and seasonal data, and highly scalable for a large number of anomaly models. We evaluate our algorithm against other state-of-the-art methods on a synthetic domain and a benchmark public data set.

1 Introduction

As Internet of Things (IoT)-enabled devices and cloud infrastructure are increasingly available for critical data-driven applications such as cloud-based security services, there is an explosion of time series data that is now available [31]. There is an immense opportunity emerging to utilize time series data to extract actionable information for operations and maximize operational reliability and security. In particular, detecting anomalies during operations is critical for its immediate application to reduce unplanned service downtime and improve site reliability in cloud-based applications. A single hour of unplanned downtime or security breach in high-value/high-volume data applications can lead to millions of dollars operational losses [18]. Despite the need, it is highly challenging to develop anomaly detection or compare different models in an industrial setting that is reliably scalable for various applications due to the lack of data labels, system information, and poor data quality.

In many real-world data-driven applications, anomaly detection often does not perform as expected due to the following reasons. Firstly, labeled data sets are rarely available, expensive, and often impractical to obtain in significant quantities. Furthermore, there is usually no a priori knowledge about which points are normal or abnormal. There also can be ambiguity in the definition of an
anomaly. As a result, it needs to be learned from data without normal or abnormal examples (i.e., unsupervised learning). Inevitably, it imposes a significant limitation on optimizing model parameters since no validation dataset is available to test out-of-sample errors. In particular, using a more complex model (i.e., more parameters) often causes significant out-of-sample errors rendering the model highly unreliable over unseen data sets.

Secondly, time-series data from IoT devices and cloud infrastructures is often ill-conditioned, meaning that it contains a large number of missing, corrupted, and noisy training samples. Such data characteristic becomes more eminent for a higher dimensional sensor data as the average noise level, and missing value event per a training sample grows with its dimensionality. Learning reliable anomaly models from noisy data without labels is a highly challenging problem as there is no way to distinguish noise from a signal. Using a complex model tends to inadvertently employ its larger number of degrees of freedom in model parameters to fit the noise, which causes a significant model overfitting resulting in large out-of-sample errors.

Finally, learned anomaly models must be easily interpretable and trusted by users for advanced industrial analytics applications. Without the ability to explain why anomalies are detected, anomaly models are unlikely to be adopted for real industrial applications regardless of their accuracy. Anomalies that arise in industrial applications ultimately need to be explainable to field engineers or operators for further corrective or preventive actions. Hence, it is essential for a learning algorithm to obtain interpretable features in anomaly models from high-dimensional complex time series data.

In this paper, we propose a novel anomaly detection algorithm, Label-free Anomaly Detection or LaF-AD, for unlabeled times-series data. Proposed LaF-AD performs a fully unsupervised ensemble learning across a large number of candidate parametric models. We develop a model variance metric that quantifies the sensitivity of anomaly probability with a bootstrapping method. Then it makes a collective decision for anomaly events by model learners using the model variance. Our algorithm can be easily parallelizable, more robust for ill-conditioned data, and highly scalable for a large number of anomaly models. More importantly, it is highly interpretable to many feature sensors compared to other conventional approaches that use multivariate complex anomaly models. We evaluate our algorithm against synthetic and real-world public datasets.

The rest of the paper is organized as follows. Section 2 reviews the previous studies on data analytical techniques. Section 3 describes our proposed novel anomaly detection algorithm. Section 4 presents experimental results towards validation of the algorithm. Section 5 offers a summary and some concluding remarks.

2 Related Work

Anomaly detection has been studied and applied to time series data for decades [4]. Anomaly detection is cast into the three paradigms based on the nature of the data capturing anomalies; supervised, semi-supervised and unsupervised approaches [1]. In several scenarios, we can leverage previously known anomalies in the domain to label the data as non-anomalous or anomalous, paving the way for supervised or semi-supervised outlier detection. However, supervised approaches require high volumes of labeled instances of both non-anomalous and anomalous data to learn robust hypotheses from, making it impractical for real-world problems [13]. Semi-supervised algorithms are often derived from supervised anomaly detection methods by employing a bias term to handle the unlabeled data. [33][30].

More recently, unsupervised methods are preferred, which is also the concentration of this work. Most of the research under unsupervised anomaly detection can be categorized into statistical methods, distance-based, ensemble-based, and reconstruction-based techniques. Our proposed methodology combines concepts from each of these categories.

**Statistical methods:** Seminal probabilistic approaches focused on the marginal likelihood estimates \( p_\theta(X) \) of the data generation model to score the outliers [12][7][35][20]. A probabilistic algorithm by Dempster et al. employed the Gaussian Mixture Model (GMM) to fit a number of Gaussians to the data and employed expectation–maximization (EM) algorithm to estimate the parameters [11]. Blei & Jordan built upon this by using Dirichlet Process nonparametric models for adaptively determining the number of clusters based on the complexity of the data. Earlier work by Scholkopf et al. proposes One-class SVMs, nonparametric models in which an underlying probability density is assumed
(such as fitting GMMs) [29]. One of the drawbacks of the statistical methods is that they can only
detect anomalies w.r.t the global data distribution [32]. Generative models also suffer as they are
approximated as a simple linear model with conjugate priors to derive an analytical solution, due to
the complexity in computing marginal likelihoods $p_0(\mathbf{X}) = \int p_0(\mathbf{z})p_0(\mathbf{X}|\mathbf{z})d\mathbf{z}$, that often requires
computing very high dimensional integrals.

**Distance based methods:** The most popular method under the umbrella of distance-based anomaly
detection is proposed by Knorr et al. wherein a point $p$ is considered an $(\pi, \epsilon)$-outlier if at most $\pi\%$
of all points are less than $\epsilon$ away from $p$ [19]. More formally, $|\{q \in \mathcal{D} : \text{dist}(p, q) < \epsilon\}| \geq \pi|\mathcal{D}|$. This
approach was later extended by Ramaswamy et al., who proposed a highly efficient way to calculate
the anomaly score by computing the distance to the $k$th Nearest Neighbour of a point [27]. Then,
thresholds are used to classify a data point as anomalous or not. Another faster and scalable variant of
this effort is proposed by Angiulli & Pizzuti where a KNN based algorithm that takes the aggregate
distance of point $p$ overall its $k$ nearest neighbors as an anomaly score [3], i.e.,

$$
\text{NN}(p; k, \mathcal{D}) = \frac{1}{|\eta_k(p)|} \sum_{q \in \eta_k(p)} \text{dist}(p, q)
$$

where $\eta_k(p)$ returns the $k$ nearest neighbours of $p$ in $\{|\mathcal{D} \setminus \{p\}|\}$. Another popular method, local
outlier factor (LOF) by Breunig et al. computes the outlier score as a ratio of the average of densities
of the $k$ nearest neighbors to the density of the instance itself [5]. Both KNN and LOF have been
shown to do exceedingly well compared with state-of-the-art publicly available anomaly detection
methods in real problems. Still, both techniques do not scale well with large high-dimensional and
seasonal data. [8].

**Ensemble based methods:** The first ensemble learning approach to outlier detection runs on LOF
when they are learned with different sets of hyperparameters such that the resultant combination
is the anomaly scores [36]. Isolation Forest (IF) is another ensemble-based algorithm that builds a
forest of random binary trees such that anomalous instances have short average path lengths on the
trees [21, 22, 14].

**Reconstruction based methods:** Recent advent in anomaly detection compute synthetic reconstruc-
tion of the data. These approaches work because once projected to a lower-dimensional space,
anomalies lose information, which prevents them from being reconstructed effectively. This leads to
a higher reconstruction error for anomalous points. We compute the difference between an observed
value and its reconstruction as $1$.

**Nearest Neighbours:** $\langle \text{NN}(p; k, \mathcal{D}) \rangle = \frac{1}{|\eta_k(p)|} \sum_{q \in \eta_k(p)} \text{dist}(p, q)$

In LaF-AD we aim to provide an explainable approach by combining reconstruction-based method
LSTM-AE and ensemble methods for unsupervised anomaly detection, incorporating the advantages
of both models. In addition, we propose a model variance metric that quantifies the sensitivity of
anomaly probability with a bootstrapping method.

### 3 Learning Label-free Anomaly Model

This section formally describes algorithms for learning the anomaly models and provides a detailed
explanation of our proposed anomaly detection method. We use the following simplified matrix
notations. We use the notation $A_{n \times m} = [a_{ij}]_{i=1}^{n}_{j=1}^{m}$ for $n \times m$ matrix of $A$ where $i_1 \leq i \leq i_n$ and
$j_1 \leq j \leq j_m$. The $i$th row vector and the $j$th column vector of $A$ are denoted by $A_{i \cdot}$ and $A_{\cdot j}$. The
inner product of $a$ and $b$ is denoted by $\langle a, b \rangle$. The expectation of random variable $a$ is denoted by $\bar{a}$.
3.1 Algorithm Overview

Let us formally describe our problem formulation and overall approach of our algorithm. Suppose that we have $N$ samples of time series data set for training $X_{\text{train}} = \{(t_n, y_n)\}_{n=1}^{N}$ where $t_n$ and $y_n$ are a time stamp and time series data at sample index $n$. Similarly, let denote $X_{\text{val}} = \{(t_{n+k}, y_{n+k})\}_{k=N+1}^{K}$ for validation data set for model selection. Let define $x_i = (t_i, y_i)$ and $x$ denote a random variable of $x_i$.

Then anomaly detection algorithm $A$ is defined by $A : x_i \mapsto y_i \in \{0, 1\}$ where $y_i = 1$ represents an anomaly event and 0 for a normal event. The anomaly event is determined by setting a threshold 0.5 to anomaly probability $p_i$ such that $y_i = \mathbb{I}_{[p_i > 0.5]}$ where $\mathbb{I}$ is an indicator function. We aim to estimate $\mathbb{E}[\sigma^2_i | A]$, an expected out-of-sample variance for $y_i$ from $X_{\text{val}}$ given an anomaly algorithm $A$ where $\sigma^2_i = \text{Var}(y_i)$.

For ensemble method, we assume that $M$ anomaly models $f_1 \cdots f_M$ are learnt from their respective algorithm $A_m$ and a training data set $X_{\text{train}}$. Hence, anomaly ensemble model $\{f_m\}_{m=1}^{M}$ is learnt by $A_m : X_{\text{train}} \mapsto f^m$ and $f^m : x_i \mapsto \tilde{v}_i$. The the expected variance of anomaly model $m$ is formally described as following,

$$\mu^m := \mathbb{E}_x[\text{Var}(f^m(x))].$$

Let use a simplified notation $\tilde{v}^m := f^m(x)$. It is easily shown that $0 \leq \mu^m \leq 0.25$ since $\text{Var}(\tilde{v}^m) = \tilde{v}^m(1 - \tilde{v}^m)$ and $0 \leq \tilde{v}^m \leq 1$. Note that the model variance $\mu^m$ to 0.25 as out-of-sample anomaly prediction (i.e., predictions on $X_{\text{val}}$) becomes highly unstable $\tilde{v}^m \rightarrow 0.5$. Conversely, for more reliable anomaly prediction we have $\tilde{v}^m \rightarrow 1$ or 0 (i.e., $\mu^m = 0$).

To aggregate the anomaly models we derive ensemble weights of models $w^m_{\text{esm}} = \frac{1 - 4\mu^m}{\sum_{m=1}^{M} (1 - 4\mu^m)}$ that sets a zero weight for $\mu^m = 0.25$. The ensemble model output $\tilde{v}^*_i$ for ith sample is found by

$$\tilde{v}^*_i = \mathbb{I}_{[w_{\text{esm}}^T \cdot \mathbf{w}_{\text{esm}}^T > 0.5]}$$

where $\mathbf{v}_{\text{esm}} = (\tilde{v}_1, \ldots, \tilde{v}_N)$ and $\mathbf{w}_{\text{esm}} = (w^m_{\text{esm}})_{m=1}^{M}$. Therefore, $\mu^m$ is a sufficient statistic for the ensemble anomaly in [17]. Our proposed estimation algorithm for $\mu^m$ is inspired by jackknife+-after-bootstrap (J+aB) [17].

For bootstrap, our algorithm performs random downsampling of sampling rate $\alpha \in (0.5, 1]$, i.e., an ordered sub-sampling with replacement. Subsampling randomly selects data index for training with a fixed sampling ratio $\alpha$ for $B$ bootstrap models. The $j$th subsampled data is denoted by $\tilde{x}_j$ for $j = 0 \cdots B$ and $\tilde{x}_0 = (t_1, y_1)_{i=1 \cdots N}$ (i.e. the original dataset). Let $h_{ij}$ denote an indicator such that $h_{ij} = 1$ if ith sample selected for $j$th bootstrap, and 0 otherwise for $i = 1 \cdots N, j = 0 \cdots B$. Assume that 0th bootstrap uses all training samples (i.e., no subsampling) such that $h_{i0} = 1$ for $i = 1 \cdots N$. 

![Figure 1: Algorithm Overview](image)
Then the selected data index is represented as a hot-encoded binary matrix $H_{N \times B + 1} = [h_{ij}]_{i,j=1,0}^{N,B}$ such that $\sum_{i} h_{ij}/N \approx \alpha$ for a large $N$ and $B$. Let define an out-of-sample matrix denoted by $H^c$ such that $H^c = [h^c_{ij}]_{i,j=1,0}$ where $h_{ij}^c = [1 - h_{ij}]$ indicate an $i$th sample not seen by $j$th bootstrap.

We derive a weight matrix $W_{N \times B} = [w_{ij}]_{i,j=1,1}^{N,B}$ where $w_{ij} = h_{ij}/\sum h_{ij}^c$ which quantifies the credibility of $j$th bootstrap model for $i$th sample.

Our algorithm consists of two chained functions; embedding function $f_{emb}$ that learns a regular pattern (i.e., normal data) from unlabelled data to compute dissimilarity of samples from the learnt pattern and probability density function $g_{prob}$ that maps the dissimilarity into probability, that formally described by $f_{emb} : x_i \mapsto d_i$ and $g_{prob} : d_i \mapsto p_i$. Let $\theta^*_m(j)$ denote the optimal parameter of $m$th embedding model found by solving the optimization $\theta^*_m(j) = \arg\min_{\theta \in \Theta_{m}} \| f^m_{emb}(x_i^r; \theta^m) - y_j^i \|_2^2$ where $X^r_i = (x^r_i, y^i_n)$ and $y_j^i$ denote the out-of-sample error margin of anomaly probability for $m$th bootstrap and $m$th embedding model such that $g^m_j : d^m_{ij} \mapsto p^m_{ij}$. Assuming data contains two classes, the normal and the abnormal state we use GMM with $k = 2$ (i.e., two centroids) for the clustering algorithm $g$. The probability density function of $d^m_{ij}$ for GMM is defined by

$$g^m_j(x) = \sum_{k=0,1} \pi^m_{kj} N(x|\mu^m_{kj}, \Sigma^m_{kj})$$

where $0 \leq \pi_k \leq 1$ is the weight probability with $\sum_k \pi_k = 1$ and $N(x|\mu_k, \Sigma_k)$ is Gaussian distribution of the random variable $x$ with mean $\mu_k$ and covariance matrix $\Sigma_k$. The GMM model can be trained by Expectation-Maximization (EM) algorithm with training data $\{d_i\}_{i=1...n}$. Let us assume that $\mu_0 < \mu_1$. Then the anomaly state is voted to $v^m_{ij} = 1$ (i.e. abnormal) if $g^m_j(d_{ij}) = 1$, and 0 otherwise.

Let $r^m_i$ denote the out-of-sample error margin of anomaly probability for $i$th training sample and $m$th embedding model and $r^m = (r^m_i)_{i=1}^{N}$. Let $z^m_i$ denote the weighted average of anomaly probability over all bootstrappings given embedding model $m$. Then it can easily derived that $z^m_i = \langle P^m_i, W^m_i \rangle$ where $P^m_{N \times (B+1)} = [p^m_i]_{i=0,j=0}^{N,B}$ and $r^m = |z^m_i - p^m_i|$. Our algorithm is to estimate $\mu^m_k$ in (2) from anomaly probability samples with out-of-sample residual errors given $X_{val}$. Let us define $q^m_{ik} = z^m_{ki} \pm r^m_i$, its mean $\mu^m_k = \mathbb{E}[q^m_{ik}]$, and variance $(\sigma^m_k)^2 = \text{Var}[q^m_{ik}]$ for $k$th validation data. To estimate $\mu^m_k$, our algorithm draws $L$ samples of anomaly probability from the distribution (4).

$$p^m_k \sim N(\mu^m_k, (\sigma^m_k)^2)$$  \hspace{1cm} (4)

where $\epsilon$ is used to test anomaly model sensitivity on the anomaly threshold 0.5. Finally, we can compute the estimated anomaly model variance $\tilde{\mu}^m_\sigma$ in (5).

$$\tilde{\mu}^m_\sigma = \frac{1}{K} \sum_{k=1}^K \tilde{v}^m_k (1 - \tilde{v}^m_k)$$  \hspace{1cm} (5)

where $\tilde{v}^m_k = \sum_i^{L} \mathbb{I}_{(p > 0.5)}(p = p^m_{ik})$.

The overall algorithm architecture for our anomaly detection algorithm is shown in Fig. The figure illustrates the individual modules in the bootstrap model pipeline for our proposed method for model 1 to $M$: subsampling, embedding model, Gaussian mixture model, and model evaluation. In the figure, $i$th time series data $y_i$ comes with its corresponding time stamp $t_i$ for $i = 1 \ldots N$ where $N$ is the size of unlabelled dataset.

The aforementioned process are done independently by agents in parallel for all combinations of models and their bootstraps. Thus, $M \times B$ agents build a model and cast a vote for an observed sample, then the final voting score is computed their weighted average. The final decision on the anomaly is made by aggregating the anomaly probability matrix $P$ with residual error matrix $R$.  

\hspace{1cm}
3.2 Boosted Embedding Model

In order to decrease model variance $\mu_\sigma$ in (2), we leverage embeddings to learn seasonality (e.g., daily, weekly, monthly) or unknown cycles by multiple categorical features. Let’s assume $\theta^t$ to capture time-categorical features (e.g., months of the year, days of the week, and hours of the day) and $\theta^i$ to represent other independent categorical features. Then, the $m-th$ model can be formulated as $f^m := f^{emb}_m(x; \theta^t_m, \theta^i_m) + f^{res}_m(x)$ where $f^{emb}$ is embedding model and $f^{res}$ is a residual model.

We leveraged DeepGB algorithm in [16] to combine gradient boosting with embeddings. In general, gradient boosting trains several simple models sequentially. The key idea of boosting is that each subsequent model trains only on the difference of the output and previous model to leverage each model’s strengths and minimize the regression error. Our approach is conducting gradient boosting to fit weak learners on residuals to improve the previous models. We propose a loop wherein, each iteration, we freeze the previous embedding, new embedding added to models, and the network grows. The last residual model can be solved by deep neural networks, SVM, or other approaches. Our approach can be summarized as $f^m = [e^m_1, \ldots, e^m_L, r^m]$.

where $e_i, i = 1, \cdots, L$ are embedding models to capture categorical data, and $r$ represents the residual model. As proved in [16], the weights of layers can be frozen to simplify the training and skip computing the residuals. The summary of our boosted embedding is presented in 1.

Algorithm 1: Boosted Embeddings Algorithm

Input : $X = ((t_n, y_n))_{n=1}^N$, $N$: number of samples
Output : $f^m$

1. $f^m = []$
2. $F_0 := y$
3. For $1 \leq l \leq L + 1$:
   // iteration over the embedding models
4.   $e_l, fit(t, F_{l-1})$;
   // fitting the selected embedding model
5.   $F_l = F_{l-1} - e_l, predict(t)$;
   // residual computation
6.   if $|F_l - F_{l-1}| < \epsilon$;
5.     break
7.   $f^m, append(e_l)$
8. return $f^m$

4 Experiment

We compare our approach, LaF-AD, with state-of-the-art anomaly detection techniques in the literature: 1) KNN [3], 2) Isolation Forest (I.F) [21], and 3) an LSTM based Autoencoder (AeLSTM) [24]. First, we evaluate this comparison on a synthetic dataset with injected anomalies (Section 4.1). Second, we conduct experiment on a public dataset with a benchmark anomaly detection data set (Section 4.2).

Implementation Detail: All algorithms are implemented in Python 3.7. Methods DeepGB, AeLSTM and LaF-AD are implemented using TensorFlow 2.4.0, while the remaining approaches, i.e., IF, and KNN are implemented using scikit-learn 0.24.1. Experiments are performed on MacBook Pro with 12-core CPUs, 16 GB RAM.

Experimental Protocol: We apply the Algorithm 1 as is, since the selected public datasets are provided as preprocessed. Further, we enlarge the feature space by creating a rolling window of size $W$ for each timestamp. For example, if $W = 24$, then each timestamp will have the previous 24 values as features. In our setting we employ 80% data for training and the remaining for validation 5 times.

Table 1 summarizes the default parameter settings for our experiment in this case study. We use the default optimal settings for I.F recommended in their original papers [23, 6].

For KNN, there is no specific recommended default parameter setting. Instead, their optimal parameters need to be tuned by evaluating out-of-sample errors via cross-validation during the
Table 1: Default parameter setting

| Algorithm | I.F | KNN |
|-----------|-----|-----|
| t         | 100 | -   |
| n         | 5   | -   |
| ψ         | 256 | -   |
| c         | 0.1 | -   |

t: the number of trees, ψ: sub-sampling size, k: the number of neighbors, κ: kernel function, f_{rbf}(x, y) = e^{-\|x-y\|^2/c}, ν: outliers fraction, c: contamination, n: #neighbors

training. It, however, is not feasible in our problem setting and many industrial applications as no labels are available during the time of training. A number of experiments has been conducted with randomly selected parameters for KNN, but we was not able to find any meaningful changes in performance. Hence, we use a default parameter setting for KNN given by scikit-learn package [25].

For AE-LSTM, numerous possible structures with different performances are possible. We started with the architecture in Malhotra et al. [24] and fine tuned to the most exemplary structure that gives one of the best AUC performances.

4.1 Simulating synthetic anomaly data

We now analyze the performance of the algorithm on a synthetic dataset with simulated noise and injected anomalies. The goal of this experiment is to build a relationship between the signal-to-noise ratio (SNR) of the data and our method’s performance in a controlled environment. The synthetic data is generated from the following structural time series model with additive components:

\[ y_t = x_t + z_t + \epsilon_t \]

Where \( x_t \) is a periodic signal, \( z_t \) is a noise component, and \( \epsilon_t \) are injected anomalies. More specifically:

\[ x_t = a \sin(2\pi f t + \phi) + b \]
\[ z_t = \phi_1 y_{t-1} + \phi_2 y_{t-2} + \theta_1 w_t + \theta_2 w_{t-2} \]
\[ = \text{ARMA}(2, 2), w_t \sim \text{WhiteNoise}(0, \sigma_w^2) \]

Where the parameters for \( x_t \) are:

\[ a = 10, b = 20, \phi = 0, f = 5/T, T = 240 \]

where \( T \) is the total number of time steps in a 5-day period at 30-minute increments. Similarly, \( z_t \) is determined by:

\[ \phi_1 = \frac{1}{2}, \phi_2 = -\frac{1}{2}, \theta_1 = \theta_2 = 2, \sigma_w^2 = 1 \]

(6)

And finally, anomalies are injected through a mixture distribution \( \epsilon_t \) which follows:

\[ \epsilon_t \overset{\text{iid}}{\sim} \begin{cases} \text{Poisson}(\lambda_1) & \text{with probability } \pi \\ c_{\text{min}} + \text{Poisson}(\lambda_2) & \text{with probability } 1 - \pi \end{cases} \]

(7)

With the \( \epsilon_t \)’s parameters set to the values:

\[ \pi = 0.999, \lambda_1 < \lambda_2, \lambda_1 = c_{\text{min}} = 10 \]

which are chosen to ensure a sparse (\( \mathbb{E}[\# \text{ of Anomalies}] = n/1000 \)) yet realistic amount of injected anomalies. To better simulate realistic patterns of life, we alternate between generating enough observations from \( y_t \) for a 5-day work week followed by two days of weekend behavior by setting \( x_t = z_t = c_{\text{weekend}} = 0 \). We proceed by setting \( n = 13, 497 \) and varying the window size and \( \lambda_2/\lambda_1 \) to analyze the performance of our algorithm. The results of this simulation experiment are summarized in Table [2]
Table 2: AUC Performance summary Simulation Experiment for $\lambda_2/\lambda_1 = 1$

| Dataset      | $W$  | LaF-AD | I.F | KNN | AeLSTM |
|--------------|------|--------|-----|-----|--------|
| Simulation 1 | 5points | 0.987  | 0.712 | 0.821 | 0.987   |
| Variance     | -    | 0.0012 | 0.0032 | 0.0021 | 0.0012 |

4.2 Case Study 2: Validation with Public Datasets

We now evaluate our methodology on a public data set taken from the Numenta Anomaly Benchmark (NAB) repository. Specifically, we investigate the dataset `nyc_taxi` which describes the total number of taxi passengers in New York City taken from the NYC Taxi and Limousine Commission. The data is count-type data with non-negative integer support. The dataset consists of 5 anomalies occurring at various holidays and severe weather events.

`taxis` contains timestamps measured at regular intervals and provides a univariate time series for experimentation. Since the data set has labels, this enables us to compute various accuracy metrics on the known anomaly timestamps. `taxis` is typical of most telemetry datasets seen in practice; where sample size is large relative to a sparse set of anomalies. A numerical summary of the data set is presented in Table 3 along with results in Table 4.

Table 3: Public Datasets

| Dataset  | Count | Start Date  | End Date  | Frequency | Number of Anomalies |
|----------|-------|-------------|-----------|-----------|---------------------|
| `nyc_taxi` | 10320 | 2014-07-01 | 2015-01-31 | 30 minutes | 5                   |

Table 4: AUC Performance summary for `taxis` dataset

| Dataset  | $W$  | LaF-AD | I.F | KNN | AeLSTM |
|----------|------|--------|-----|-----|--------|
| `taxis`  | 5points | 0.82  | 0.44 | 0.82 | 0.53   |
| Variance | -    | 0.0023 | 0.0041 | 0.0023 | 0.0042 |

In Table 4, the AUC results are summarized for other comparable baseline algorithms. The best performance is marked with bold font. As we observe, LaF-AD selects the best model compared to other baselines. We can conclude that lower model variance is the indicator of high AUC without knowing the labels.

The table shows the experiment result of LaF-AD with other baseline anomaly detection algorithms for different window sizes. For the experiment, we assume the label is not available before the deployment, hence it is unknown to us which baseline algorithm and window size offers the best or the worst performance. It can easily seen that our algorithm consistently can outperforms the best baseline algorithm for all window sizes. The average and standard deviation of AUC performance over window sizes for each algorithm are shown in the last two rows. It shows that our algorithm not only outperforms in the average AUC but also has the most stable performance (i.e., the smallest model variance learned by our algorithm).

5 Conclusion

Unsupervised anomaly detection methods are widely used in a variety of research areas. In this paper, we propose a novel label-free anomaly detection algorithm, LaF-AD, for time series data. Furthermore, we develop a model evaluation metric based on the variance that quantifies the sensitivity of anomaly probability by learning bootstrapped models. We derive a new performance bound for bootstrap prediction. Empirical evaluations on both synthetic and public benchmark datasets demonstrate that the proposed method outperforms state-of-the-art unsupervised anomaly detection models for univariate time series. Finally, this paper opens up several new directions for further...
research. Extensive evaluation of our method on other complex domains is an immediate direction. The current approach is designed and model with univariate time-series analysis, however extending it to multivariate time series is an open problem and interesting to us from a practical application standpoint.

References

[1] Aggarwal, Charu C. 2016. Outlier Analysis. 2nd edn. Springer Publishing Company.

[2] Ahmad, Subutai, Lavin, Alexander, Purdy, Scott, & Agha, Zuha. 2017. Unsupervised real-time anomaly detection for streaming data. *Neurocomputing, 262*, 134–147. Online Real-Time Learning Strategies for Data Streams.

[3] Angiulli, Fabrizio, & Pizzuti, Clara. 2002. Fast Outlier Detection in High Dimensional Spaces. Pages 15–26 of: Elomaa, Tapio, Mannila, Heikki, & Toivonen, Hannu (eds), *Principles of Data Mining and Knowledge Discovery, 6th European Conference, PKDD 2002, Helsinki, Finland, August 19-23, 2002, Proceedings*, vol. 2431. Springer.

[4] Braei, Mohammad, & Wagner, Sebastian. 2020. Anomaly detection in univariate time-series: A survey on the state-of-the-art. *arXiv preprint arXiv:2004.00433*.

[5] Breunig, Markus M, Kriegel, Hans-Peter, Ng, Raymond T, & Sander, Jörg. 2000a. LOF: identifying density-based local outliers. Pages 93–104 of: *Proceedings of the 2000 ACM SIGMOD international conference on Management of data*.

[6] Breunig, Markus M., Kriegel, Hans-Peter, Ng, Raymond T., & Sander, Jörg. 2000b. LOF: Identifying Density-based Local Outliers. In: *Proceedings of the 2000 ACM SIGMOD International Conference on Management of Data*. SIGMOD ’00.

[7] Cai, Yongjie, Tong, Hanghang, Fan, Wei, Ji, Ping, & He, Qing. 2015. Facets: Fast Comprehensive Mining of Coevolving High-Order Time Series. In: *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. New York, NY, USA: Association for Computing Machinery.

[8] Campos, Guilherme O, Zimek, Arthur, Sander, Jörg, Campello, Ricardo JGB, Micenková, Barbora, Schubert, Erich, Assent, Ira, & Houle, Michael E. 2016. On the evaluation of unsupervised outlier detection: measures, datasets, and an empirical study. *Data mining and knowledge discovery, 30*(4), 891–927.

[9] Chen, Jinghui, Sathe, Saket, Aggarwal, Charu, & Turaga, Deepak. 2017. Outlier detection with autoencoder ensembles. Pages 90–98 of: *Proceedings of the 2017 SIAM international conference on data mining*. SIAM.

[10] Cho, Kyunghyun, Van Merriënboer, Bart, Gulcehre, Caglar, Bahdanau, Dzmitry, Bougares, Fethi, Schwenk, Holger, & Bengio, Yoshua. 2014. Learning phrase representations using RNN encoder-decoder for statistical machine translation. *arXiv preprint arXiv:1406.1078*.

[11] Dempster, A. P., Laird, N. M., & Rubin, D. B. 1977. Maximum Likelihood from Incomplete Data via the EM Algorithm. *Journal of the Royal Statistical Society. Series B (Methodological).*

[12] Goernitz, Nico, Braun, Mikio, & Kloft, Marius. 2015. Hidden Markov Anomaly Detection. Pages 1833–1842 of: Bach, Francis, & Blei, David (eds), *Proceedings of the 32nd International Conference on Machine Learning*. Proceedings of Machine Learning Research, vol. 37. Lille, France: PMLR.

[13] Görnitz, Nico, Kloft, Marius, Rieck, Konrad, & Brefeld, Ulf. 2014. Toward Supervised Anomaly Detection. *CoRR*.

[14] Hariri, Sahand, Kind, Matias Carrasco, & Brunner, Robert J. 2021. Extended Isolation Forest. *IEEE Transactions on Knowledge and Data Engineering, 33*(Apr), 1479–1489.

[15] Hoffmann, Heiko. 2007. Kernel PCA for novelty detection. *Pattern recognition, 40*(3), 863–874.
[16] Karingula, Sankeerth Rao, Ramanan, Nandini, Tahsambi, Rasool, Amjadi, Mehrnaz, Jung, Deokwoo, Si, Ricky, Thimmisetty, Charanraj, & Coelho Jr, Claudionor Nunes. 2021. Boosted Embeddings for Time Series Forecasting. arXiv preprint arXiv:2104.04781.

[17] Kim, Byol, Xu, Chen, & Barber, Rina. 2020. Predictive inference is free with the jackknife+-after-bootstrap. Pages 4138–4149 of: Larochelle, H., Ranzato, M., Hadsell, R., Balcan, M. F., & Lin, H. (eds), Advances in Neural Information Processing Systems, vol. 33. Curran Associates, Inc.

[18] Kirschen, DS, Bell, KRW, Nedic, DP, Jayaweera, D, & Allan, RN. 2003. Computing the value of security. IEE Proceedings-Generation, Transmission and Distribution, 150(6), 673–678.

[19] Knorr, Edwin M, Ng, Raymond T, & Tucakov, Vladimir. 2000. Distance-based outliers: algorithms and applications. The VLDB Journal, 8(3), 237–253.

[20] Li, Junlei, McCann, James, Pollard, Nancy, & Faloutsos, Christos. 2009. DynaMMo: Mining and Summarization of Coevolving Sequences with Missing Values. In: Proceedings of 15th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD ’09).

[21] Liu, Fei Tony, Ting, Kai Ming, & Zhou, Zhi-Hua. 2008. Isolation forest. Pages 413–422 of: 2008 eighth ieee international conference on data mining. IEEE.

[22] Liu, Fei Tony, Ting, Kai Ming, & Zhou, Zhi-Hua. 2012a. Isolation-based anomaly detection. ACM Transactions on Knowledge Discovery from Data (TKDD), 6(1), 3.

[23] Liu, Fei Tony, Ting, Kai Ming, & Zhou, Zhi-Hua. 2012b. Isolation-Based Anomaly Detection. ACM Trans. Knowl. Discov. Data, 6(1).

[24] Malhotra, Pankaj, Ramakrishnan, Anusha, Anand, Gaurangi, Vig, Lovekesh, Agarwal, Puneet, & Shroff, Gautam. 2016. LSTM-based encoder-decoder for multi-sensor anomaly detection. arXiv preprint arXiv:1607.00148.

[25] Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., & Duchesnay, E. 2011. Scikit-learn: Machine Learning in Python. Journal of Machine Learning Research, 12, 2825–2830.

[26] Principi, Emanuele, Vesperini, Fabio, Squartini, Stefano, & Piazza, Francesco. 2017. Acoustic novelty detection with adversarial autoencoders. Pages 3324–3330 of: 2017 International Joint Conference on Neural Networks (IJCNN). IEEE.

[27] Ramaswamy, Sridhar, Rastogi, Rajeev, & Shim, Kyuseok. 2000. Efficient algorithms for mining outliers from large data sets. Pages 427–438 of: Proceedings of the 2000 ACM SIGMOD international conference on Management of data.

[28] Rousseeuw, Peter J, & Hubert, Mia. 2018. Anomaly detection by robust statistics. Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery, 8(2), e1236.

[29] Schölkopf, Bernhard, Platt, John C, Shawe-Taylor, John, Smola, Alex J, & Williamson, Robert C. 2001. Estimating the support of a high-dimensional distribution. Neural computation, 13(7), 1443–1471.

[30] Sindhwani, Vikas, Niyogi, Partha, & Belkin, Mikhail. 2005. Beyond the point cloud: from transductive to semi-supervised learning. Pages 824–831 of: Proceedings of the 22nd international conference on Machine learning.

[31] Singh, Ashish, & Chatterjee, Kakali. 2017. Cloud security issues and challenges: A survey. Journal of Network and Computer Applications, 79, 88–115.

[32] Song, Xiuyao, Wu, Mingxi, Jermaine, Christopher, & Ranka, Sanjay. 2007. Conditional Anomaly Detection. IEEE Transactions on Knowledge and Data Engineering, 19(5), 631–645.

[33] Vapnik, Vladimir N. 1999. An overview of statistical learning theory. IEEE transactions on neural networks, 10(5), 988–999.
[34] Wen, Long, Gao, Liang, & Li, Xinyu. 2017. A new deep transfer learning based on sparse auto-encoder for fault diagnosis. *IEEE Transactions on Systems, Man, and Cybernetics: Systems, 49*(1), 136–144.

[35] Xiong, Liang, Chen, Xi, & Schneider, Jeff. 2011. Direct Robust Matrix Factorization for Anomaly Detection. Pages 844–853 of: 2011 IEEE 11th International Conference on Data Mining.

[36] Xu, Zekun, Kakde, Deovrat, & Chaudhuri, Arin. 2019. Automatic Hyperparameter Tuning Method for Local Outlier Factor, with Applications to Anomaly Detection. 2019 IEEE International Conference on Big Data (Big Data), Dec.