Weakly-supervised Deep Anomaly Detection with Pairwise Relation Learning

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Abstract
This paper studies a rarely explored but critical anomaly detection problem: weakly-supervised anomaly detection with limited labeled anomalies and a large unlabeled data set. This problem is very important because it (i) enables anomaly-informed modeling which helps identify anomalies of interests and address the notorious high false positives in unsupervised anomaly detection, and (ii) eliminates the reliance on large-scale and complete labeled anomaly data in fully-supervised settings. However, the problem is especially challenging since we have only limited labeled data for a single class, and moreover, the seen anomalies often cannot cover all types of anomalies (i.e., unseen anomalies). We address this problem by formulating the problem as a pairwise relation learning task. Particularly, our approach defines a two-stream ordinal regression network to learn the relation of randomly selected instance pairs, i.e., whether the instance pair contains labeled anomalies or just unlabeled data instances. The resulting model leverages both the labeled and unlabeled data to effectively augment the data and learn generalized representations of both normality and abnormality. Extensive empirical results show that our approach (i) significantly outperforms state-of-the-art competing methods in detecting both seen and unseen anomalies and (ii) is substantially more data-efficient.

Introduction
Anomaly detection aims at identifying exceptional data instances that have a significant deviation from the majority of data instances, which can offer important insights into broad applications, such as identifying fraudulent transactions or insider trading, detecting network intrusions, and early detection of diseases. Numerous anomaly detection methods have been introduced (Aggarwal 2017a; Chen et al. 2017; Schlegl et al. 2017; Zenati et al. 2018; Pang et al. 2018; Ruff et al. 2018), of which most are unsupervised methods. The popularity of the unsupervised methods is mainly due to that they avoid the prohibitive cost of labeling large-scale anomaly data. However, since they do not have any prior knowledge of the anomalies of interests, many anomalies they identify are data noises or uninteresting data instances, leading to high false positives or low detection recall.

To address this issue, we study a rarely explored but critical anomaly detection problem, i.e., weakly-supervised anomaly detection with a few (e.g., multiple to dozens) labeled anomalies and a large-scale unlabeled data set. The limited labeled anomalies can be leveraged as our prior knowledge of the anomalies to learn anomaly-informed detection models to reduce false positives (Aggarwal 2017b). Compared to fully-supervised anomaly detection techniques that require large-scale and complete labeled anomaly data, the weakly-supervised anomaly detection is much more practical, because although labeling large-scale anomaly data that covers all types of anomalies is too costly (if not impossible), a small set of labeled anomalies can often be made available with affordable/trivial cost in many real-world anomaly detection applications. These labeled anomalies may come from a deployed detection system, e.g., a few successfully detected network intrusion records, or they may be from end-users, such as a small number of fraudulent credit card transactions that are reported by bank clients.

However, this problem is especially challenging. This is because we have only limited labeled data for the anomaly class, and moreover, anomalies typically stem from unknown events. Therefore, the limited labeled anomalies often, if not always, cannot cover all types of anomalies. As a result, using these limited anomalies as supervision information is presented with significant challenges in generalizing detection models to detect seen and unseen anomalies (i.e., new types of anomalies that are unseen during training).

There have been a few early explorations in this research line using traditional methods (McGlohon et al. 2009; Tamosiunas et al. 2014; Zhang et al. 2018) or recently emerged deep anomaly detection methods (Pang et al. 2018), but they leverage the labeled anomalies as auxiliary data to enhance an existing anomaly measure or perform a classification-based anomaly detection. This leads to insufficient exploitation of the labeled data and/or poor generalization to unseen anomalies.

Additionally, note that well established semi-supervised anomaly detection (Noto et al. 2012; Görnitz et al. 2013)

1Deep anomaly detection methods refer to any methods that exploit deep learning techniques (Goodfellow et al. 2016) to learn feature representations or anomaly scores for anomaly detection.
A novel method, namely PRIOR, is instantiated from our generalizability to unseen anomalies than its contenders. The best contenders, and (iii) achieves substantially better precision-recall rates, (ii) obtains a substantially better data set and \( A = \{x_{N+1}, x_{N+2}, \ldots, x_{N+K}\} \) with \( K < N \) is a very small set of labeled anomalies that provide some prior knowledge of anomalies, our goal is to learn an anomaly scoring function \( \phi : A' \mapsto \mathbb{R} \) that assigns anomaly scores to data instances in a way that we have \( \phi(x_i) > \phi(x_j) \) if \( x_i \) is an anomaly and \( x_j \) is a normal data instance.

To obtain more labeled data and perform an end-to-end anomaly score learning, we formulate the problem as a pairwise relation learning task, of which we aim to assign substantially larger anomaly scores to the data instance pairs that contain at least one anomaly than the other instance pairs. This can be achieved by ordinal regression techniques (Gutiérrez et al. 2016). Specifically, let \( \mathcal{P} = \{ (x, x', y) \mid x, x' \in A' \text{ and } y \in \mathbb{N}\} \) be a set of unordered pairs of instances with artificial class labels, where each pair \( (x, x') \) belongs to one of the three different types of possible combinations: \{a, a\}, \{a, u\} and \{u, u\} (a \in A and \( u \in U \)) and \( y \in \mathbb{N}^+ \) is an ordinal class feature with decreasing value assignments to the respective \{a, a\}, \{a, u\} and \{u, u\} pairs, i.e., \( y_{\{a,a\}} > y_{\{a,u\}} > y_{\{u,u\}} \), then the learning of anomaly scores can be transformed as to learn a ternary ordinal regression function \( \phi : \mathcal{P} \mapsto \mathbb{R} \).

We then instantiate the formulation into the method PRIOR for deep anomaly detection. As shown in Figure 1, PRIOR consists of three modules: data augmentation, end-to-end anomaly score learner and ordinal regression. The data augmentation generates the labeled instance pair set \( \mathcal{P} \). The anomaly scoring \( \phi \) is a composition of a feature learner \( \psi \) and an anomaly score learner \( \eta \), which can be trained in an end-to-end manner with an ordinal regression loss function.

Table 1: Weakly- and Semi-supervised Approaches

| Approach          | Training Data                                      | Problem                                      |
|-------------------|---------------------------------------------------|----------------------------------------------|
| Semi-supervised   | Large normal data, large unlabeled data           | Learn patterns of labeled normal data        |
| Weakly-supervised | Limited (incomplete) anomaly data, large unlabeled data | Learn patterns of labeled anomalies that also generalize well to unseen anomalies |

This paper introduces a novel deep anomaly detection formulation and its instantiation, namely PRIOR knowledge-driven Ordinal Regression network (PRIOR), for the weakly-supervised setting. We formulate the problem as a pairwise relation learning task, of which a two-stream ordinal regression network is defined to learn the relation of instance pairs, i.e., to discriminate whether an instance pair contains the labeled anomalies or just unlabeled instances. Particularly, PRIOR first generates unordered pairs of instances from the small labeled anomaly set and a large unlabeled data set, and then augments the pairs with a synthetic ordinal class feature, in which larger scalar class labels are assigned to the instance pairs that contain at least one labeled anomaly than the other pairs. PRIOR further feeds these pair samples into the regression network to directly learn their anomaly scores. At the testing stage, PRIOR pairs test instances with the training instances and uses the regression network to infer their anomaly scores.

Unlike previous deep methods (Chen et al. 2017; Zong et al. 2016) that aim to improve existing anomaly measures with new feature representations, PRIOR uses the added ordinal feature to directly learn an anomaly measure, achieving more efficient use of the labeled data. PRIOR assigns large anomaly scores to instance pairs when they share similar characteristics to labeled anomalies or deviate from the interactions between unlabeled instance pairs. This helps identify both seen and unseen anomalies. Accordingly, this paper makes the following main contributions.

- We propose a novel formulation for inventing tailored data augmentation and ordinal regression to perform weakly-supervised deep anomaly detection via pairwise relation learning. This yields anomaly-informed detection models with good generalizability.
- A novel method, namely PRIOR, is instantiated from our formulation to directly learn anomaly scores, which optimizes the scores in an end-to-end fashion, achieving well-optimized anomaly scores and data-efficient learning.

Our empirical results on nine real-world data sets show that PRIOR (i) significantly outperforms four state-of-the-art contenders, e.g., at least 27% average improvement in precision-recall rates, (ii) obtains a substantially better data efficiency, e.g., it requires 50%–88% less labeled anomalies to perform comparably good to, or substantially better than, the best contenders, and (iii) achieves substantially better generalizability to unseen anomalies than its contenders.
Figure 1: PRIOR - Prior Knowledge-driven Two-stream Ordinal Regression Networks. It takes $C_{(a,n)}$, $C_{(a,u)}$, and $C_{(u,u)}$ instance pairs as inputs and learns to assign larger anomaly scores to the $C_{(a,n)}$ and $C_{(a,u)}$ instance pairs that contain at least one labeled anomaly than the $C_{(u,u)}$ pairs.

### End-to-end Anomaly Score Learner

An end-to-end anomaly score learner is then defined to take pairs of data instances as inputs and directly output the anomaly scores of the pairs. Let $Z \in \mathbb{R}^M$ be an intermediate representation space, we define a two-stream anomaly scoring network $\phi(\cdot, \Theta) : \mathcal{P} \rightarrow Z$ as a composition of a feature learner $\psi(\cdot; \Theta_r) : \mathcal{X} \rightarrow Z$ and an anomaly scoring function $\eta(\cdot, \Theta) : (Z, Z) \rightarrow \mathbb{R}$, where $\Theta = \{\Theta_r, \Theta_a\}$. Specifically, $\psi(\cdot; \Theta_r)$ is a neural feature learner with $H \in \mathbb{N}$ hidden layers and weight matrices $\Theta_r = \{W^1, W^2, \cdots, W^H\}$:

$$z = \psi(x; \Theta_r),$$

where $x \in \mathcal{X}$ and $z \in Z$. Different network structures can be used here, such as multilayer perceptrons for multidimensional data, convolutional networks for image data, or recurrent networks for sequence data (Goodfellow et al. 2016).

$\eta(\cdot, \Theta)$ is defined as an anomaly score learner which uses a linear neural unit in the output layer to compute the anomaly scores based on the intermediate representations:

$$\eta(z_i, z_j; \Theta_a) = \sum_{k=1}^{M} w_k^a z_{ik} + \sum_{l=1}^{M} w_0^a z_{ij} + w_2^a z_{2M+1},$$

where $z \in \mathcal{Z}$, $(z_i, z_j)$ is a concatenation operation of $z_i$ and $z_j$, and $\Theta_a = \{w^a\}$ ($w_2^a$ is the bias term). As shown in Figure 1 to reduce the optimization complexity, PRIOR uses a two-stream network with the shared weight parameters $\Theta_r$ to learn the representations $z_i$ and $z_j$.

Lastly $\phi((x_i, x_j); \Theta)$ can be formally represented as

$$\phi((x_i, x_j); \Theta) = \eta(\psi(x_i; \Theta_r), \psi(x_j; \Theta_r); \Theta_a),$$

which can be trained in an end-to-end fashion to directly map original data inputs to scalar anomaly scores.

Note that the concatenation results in an ordered pair $(z_i, z_j)$. This does not affect the unordered pairs from the $C_{(a,n)}$ and $C_{(a,u)}$ classes since the instances of these pairs come from the same data set (i.e., A or U), but it may produce inverse effects on our training with the $C_{(a,u)}$ pairs. We address this problem by transforming all unordered $C_{(a,u)}$ pairs into ordered pairs $C_{(a,u)}$ before training.

### Loss Functions for Ordinal Regression

PRIOR then feeds the ordinal class labels and the anomaly scores output by $\phi$ to optimize the scores using an ordinal regression objective, which aims to assign substantially larger anomaly scores than the current deep methods that focus on direct optimization of the anomaly scores, which is expected to have more data-efficient learning and optimized anomaly scores than the current deep methods that focus on optimizing feature representations in an unsupervised way.

Let $y$ be the ordinal label of an instance pair $\{x_i, x_j\}$, we define the loss as below to guide the optimization:

$$L(\phi((x_i, x_j); \Theta), y) = |y - \phi((x_i, x_j); \Theta)|,$$

The absolute loss is used to reduce the effect of potential noisy pairs due to the anomaly contamination in $U$. The three class labels $y_{(a,n)} = 8$, $y_{(a,u)} = 4$ and $y_{(u,u)} = 0$ are used by default to enforce large margins among the anomaly scores of the three types of instance pairs. PRIOR also works very well with other value assignments as long as they are reasonably large margins among the ordinal class labels.

Therefore, the overall objective function can be written as

$$\min_{\Theta} \frac{1}{|\mathcal{B}|} \sum_{(x_i, x_j, y) \in \mathcal{B}} |y - \phi((x_i, x_j); \Theta)| + \lambda R(\Theta),$$

where $\mathcal{B}$ is a sample batch from $\mathcal{P}$ and $R(\Theta)$ is a regularization term with the hyperparameter $\lambda$. These optimization settings are provided in the experiments section.
Anomaly Detection Using PRIOR

Training Stage Algorithm 1 presents the procedure of training PRIOR. Step 1 first extends the data $X$ into a set of instance pairs with ordinal class labels, $\mathcal{P}$. After an uniform Glorot weight initialization ([Glorot and Bengio 2010]) in Step 2, PRIOR performs stochastic gradient descent (SGD) based optimization to learn $\Theta$ in Steps 3-9 and obtains the optimized $\phi$ in Step 10. Particularly, stratified random sampling is used in Step 5 to ensure the sample balance of the three classes in $\mathcal{B}$. Step 6 performs the forward propagation of the network and computes the loss. Step 7 then uses the loss to perform gradient descent steps.

Algorithm 1 Training PRIOR

Input: $X \in \mathbb{R}^D$ with $X = \mathcal{U} \cup \mathcal{A}$ and $\emptyset = \mathcal{U} \cap \mathcal{A}$

Output: $\phi: (\mathcal{X}', \mathcal{X}) \mapsto \mathbb{R}$ - an anomaly score mapping

1: $\mathcal{P} \leftarrow$ Augment the training data with $\mathcal{U}$ and $\mathcal{A}$
2: Randomly initialize $\Theta$
3: for $i = 1$ to $n_{epochs}$ do
4: for $j = 1$ to $n_{batches}$ do
5: $\mathcal{B} \leftarrow$ Randomly sample $b$ data instance pairs from $\mathcal{P}$
6: $\text{loss} \leftarrow \frac{1}{b} \sum_{(x_i, x_j, y) \in \mathcal{B}} |y - \phi((x_i, x_j); \Theta)| + \lambda R(\Theta)$
7: Perform a gradient descent step w.r.t. the parameters in $\Theta$
8: end for
9: end for
10: return $\phi$

Testing Stage At the testing stage, given a test instance $x_k$, PRIOR first pairs it with data instances randomly sampled from $\mathcal{A}$ and $\mathcal{U}$, and then defines its anomaly score as

$$s_{x_k} = \frac{1}{2E} \left[ \sum_{i=1}^{E} \phi((a_i, x_k); \Theta^*) + \sum_{j=1}^{E} \phi((x_k, u_j); \Theta^*) \right]$$ (6)

where $\Theta^*$ are the parameters of a trained $\phi$, and $a_i$ and $u_j$ are randomly sampled from the respective $\mathcal{A}$ and $\mathcal{U}$. $s_{x_k}$ can be interpreted as an ensemble of the anomaly scores of a set of $x_k$-oriented pairs. Due to the loss in Eqn. (4), $s_{x_k}$ is optimized to be greater than $s_{x_k'}$ given $x_k$ is an anomaly and $x_k'$ is a normal instance. The ensemble scores are employed to achieve stable anomaly scoring. PRIOR can perform very stably as long as the ensemble size $E$ is sufficiently large due to the central limit theorem. $E = 30$ is used here.

Theoretical Foundation of PRIOR

Informative Data Augmentation

Augmenting $X$ to $\mathcal{P}$ substantially increases not only the total number of training samples but also the proportion of labeled anomaly data. Specifically, given $K$ labeled anomalies and $N$ unlabeled data instances, the labeled anomaly data accounts for $\frac{K}{N+K}$ only. After our data augmentation, the labeled anomaly data (i.e., the instance pairs that contain at least one labeled anomaly) accounts for $\binom{K}{2} + \binom{K}{1} \binom{N}{1}$, where $\binom{K}{2}$ and $\binom{N}{1}$ denote the number of the $C_{(a,a)}$ and $C_{(a,u)}$ pairs, respectively. After some transformations, we can see that the augmented labeled anomaly data remarkably extends the original proportion by a factor of about $2K$.

More importantly, since PRIOR uses a two-stream network in its representation learner $\psi(:, \Theta_r)$, it still performs feature learning in the original $X$ data space, but with substantially more labeled anomaly data, which helps learn more expressive intermediate feature representations.

Optimizing Anomaly Scores with Regression

This section shows that the anomaly scores defined in Eqn. (6) is well optimized via the regression to ensure anomalies having substantially larger anomaly scores than normal data instances. Specifically, given a test instance $x_k$, the first term $\phi((a_i, x_k); \Theta^*)$ in Eqn. (6) is equivalent to distinguishing the $C_{(a,a)}$ pairs from the $C_{(a,u)}$ pairs. Thus, the term enforces $x_k$ to have an anomaly score close to $y_{(a,a)}$ if $x_k$ is an anomaly, and likewise, close to $y_{(a,u)}$ if $x_k$ is a normal instance. Since $y_{(a,a)} > y_{(a,u)}$, this term can well guarantee that $x_k$ has a larger anomaly score when $x_k$ is an anomaly than when $x_k$ is normal. Similarly, the second term $\phi((x_k, u_j); \Theta^*)$ is equivalent to distinguishing the $C_{(a,u)}$ pairs from the $C_{(u,u)}$ pairs, fulfills the same guarantee as the first term. An average aggregation of these two terms is used to achieve statistically stable scoring results.

Also, this ternary ordinal regression empowers PRIOR to learn the abstractions of not only the anomalous behaviors but also the normal behaviors, so PRIOR is expected to assign large anomaly scores to unseen anomalies as long as they clearly deviate from the normality abstraction.

The above analysis assumes $u \in \mathcal{U}$ is mostly a normal instance because of the rarity of anomalies in real-world applications, and we found empirically that the SGD-based optimization could work very well with this assumption.

Experiments

Data Sets

As shown in Table 2, nine widely-used publicly available real-world data sets are used which are from diverse domains, e.g., intrusion detection, fraud detection, and disease detection ([Moustafa and Slay 2015] [Liu et al. 2012] [Pang et al. 2018] [Randhawa et al. 2018]). Specifically, the donors data is taken from KDD Cup 2014 for predicting excitement of donation projects, with exceptionally exciting projects used as anomalies (6% of all data instances). The census data is extracted from the US census bureau database, in which we aim to detect the rare high-income person (6%). fraud is for fraudulent credit card transaction detection, with fraudulent transactions (0.2%) as anomalies. celeba contains more than 200K celebrity images, each with

2donors and fraud are publicly available at https://www.kaggle.com/, w7a and news20 are available at https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/, backdoor is available at https://www.unsw.adfa.edu.au/unswnsw-canberra-cyber/cybersecurity/ADFA-NB15-Datasets/, celeba is at http://mmlab.ie.cuhk.edu.hk/projects/CelebA.html and the other data sets are accessible at https://archive.ics.uci.edu/ml/datasets/.
40 attribute annotations. We use the bald attribute as our detection target, in which the scarce bald celebrities (3%) are treated as anomalies and the other 39 attributes form the feature space. The backdoor data is for network attack detection with the backdoor attacks as anomalies (2.4%) against the ‘normal’ class, which is derived from a widely-used intrusion detection data set called UNSW-NB15 [Moustafa and Slay 2015]. w7a is a web page classification data set, with the minority classes (3%) as anomalies. campaign is a data set of bank marketing campaigns, with rarely successful campaigning records (11.3%) as anomalies. news20 is one of the most popular text classification corpora, which is converted into anomaly detection data via random downsampling of the minority class (5%) based on [Liu et al. 2012]. thyroid is for disease detection, in which the anomalies are the hypothyroid patients (7.4%).

Four of these data sets contain real anomalies, including donors, fraud, backdoor and thyroid. The other five data sets contain semantically real anomalies, i.e., they are rare and very different from the majority of data instances. This provides a good testbed for anomaly detection evaluation.

Competing Methods and Parameter Settings
PRIOR is compared with four methods, including REPEN [Pang et al. 2018], adaptive Deep SVDD (DSVDD) [Ruff et al. 2018], prototypical networks (denoted as FSNet) [Snell et al. 2017], and iForest [Liu et al. 2012], which are chosen because they are the respective state-of-the-art in four relevant areas: weakly-supervised deep anomaly detection, feature learning for anomaly detection, classification-based approach, and unsupervised anomaly detection. The original DSVDD cannot make use of the labeled anomalies. We adapted it based on [Tax and Duin 2004] to enforce a large margin between the one-class center and the labeled anomalies while minimizing the center-oriented hypersphere. This adaptation enhances DSVDD by over 30% accuracy.

Since our experiments focus on unordered multidimensional data, multilayer perceptron networks are used. Similar to the findings in REPEN [Pang et al. 2018], we empirically found that all deep methods perform best using an architecture with one hidden layer than using deeper architectures. This may be due to the limit of the available labeled data. Following REPEN, one hidden layer with 20 neural units is used in all deep methods. The ReLu activation function \( g(a) = \max(0, a) \) is used. An \( \ell_2 \)-norm regularizer with the hyperparameter setting \( \lambda = 0.01 \) is applied to avoid overfitting. The RMSprop optimizer with the learning rate 0.001 is used. All deep detectors are trained using 50 epochs, with 20 batches per epoch. The batch size is probed in \( [8, 16, 32, 64, 128, 256, 512] \). The best fits, 512 in PRIOR and DSVDD, 256 in REPEN and FSNet, are used by default.

Performance Evaluation Metrics
Two popular and complementary metrics, the Area Under Receiver Operating Characteristic Curve (AUC-ROC) and Area Under Precision-Recall Curve (AUC-PR) [Boyd et al. 2013], are used. AUC-ROC summarizes the ROC curve of true positives against false positives, which often presents an overoptimistic view of the detection performance due to the class-imbalance nature of anomaly detection data; whereas AUC-PR is a summarization of the curve of precision and recall w.r.t. the anomalies, which focuses on the performance on the anomaly class only and is often more practical. Larger AUC-ROC (AUC-PR) indicates better performance.

The reported AUC-ROC and AUC-PR are averaged results over 10 independent runs. The paired Wilcoxon signed rank [Woolson 2007] is used to examine the significance of the performance of PRIOR against its competing methods.

Default Experiment Settings
To replicate the real-life scenarios where a few labeled anomalies together with large unlabeled data are available, the anomalies and normal instances are first splitted into two subsets, with 80% data as training data and the other 20% data as test set. We then combine some randomly selected anomalies with normal training data to produce an anomaly-contaminated unlabeled data set \( U \). We further randomly sample a few anomalies from the anomaly class to form the prior knowledge, i.e., the labeled anomaly set \( \mathcal{A} \).

Under this setting we evaluate the performance of PRIOR w.r.t. its effectiveness in real-world data, data efficiency, robustness, and generalizability to unseen anomalies.

Effectiveness in Real-world Data Sets

**Experiment Settings**
We first evaluate the effectiveness of PRIOR in a wide range of real-world data. A consistent setting, 2% anomaly contamination and \( |A| = 30 \) labeled anomalies, is used across all data sets to gain insights into the performance in different real-life applications.

**Results**
The AUC-ROC and AUC-PR results on the nine real-world data sets are shown in Table 2. PRIOR obtains the best performance on eight data sets in both metrics, with comparably better performance on the data set where it ranks in second. On average, PRIOR performs substantially better than REPEN (9%), DSVDD (3%), FSNet (21%) and iForest (33%) in terms of AUC-ROC; more impressively, it achieves more substantial improvement in AUC-PR, i.e., 108% w.r.t. REPEN, 27% w.r.t. DSVDD, 111% w.r.t. FSNet, and 304% w.r.t. iForest. All of the improvement are significant at the 95% or 99% confidence level. It is often very challenging to achieve large AUC-PR due to the rareness of anomalies. Such impressive AUC-PR improvement shows the superior capability of PRIOR in reducing false positives.

This is very encouraging when considering the labeled anomalies account for only 0.005%-0.6% of training data and 0.08%-6% of the anomaly class (see \( f_1 \) and \( f_2 \) in Table 2).

The superiority of PRIOR is mainly due to its regression-based end-to-end anomaly score learning, which leverages the augmented instance pairs to efficiently learn the abstraction of both normality and abnormality, achieving more accurate anomaly scores than its counterparts that focus on feature learning. It is interesting that on census PRIOR outperforms DSVDD in AUC-PR but it underperforms in AUC-ROC, which may because the ternary ordinal regression allows PRIOR to emphasize more on detecting anomalies while DSVDD focuses on modeling the normal class only.
Data Efficiency

Experiment Settings This section examines the data efficiency by inspecting the performance w.r.t. different number of labeled anomalies, ranging from 5 to 120, with the contamination level fixed to 2%.

Results The AUC-PR results for the data efficiency test are shown in Figure 2. Similar results can also be observed in AUC-ROC. The unsupervised method iForest is insensitive to the labeled data and used as the baseline. The performance of all deep methods generally increases with increasing labeled data. However, the increased anomalies do not always help due to the heterogeneous anomalous behaviors taken by different anomalies. PRIOR is more stable and has better generalizability in such cases.

![Figure 2: AUC-PR w.r.t. the Number of Labeled Anomalies](image)

PRIOR is most data-efficient, which obtains the best average AUC-PR w.r.t. different number of labeled anomalies. Impressively, PRIOR can use 88% less labeled anomalies but achieves much better AUC-PR than the best contender DSVD on w7a, news20 and thyroid; and it requires 50% less labeled data to obtain considerably better performance to the best contender FSNet on donors. This difference is mainly due to the direct optimization of anomaly scores in PRIOR against the indirect optimization in its counterparts.

Compared to the unsupervised iForest, even when a very few (e.g., 5) labeled anomalies are used, the improvement of the weakly-supervised methods is very substantial on nearly all data sets, e.g., the average improvement of PRIOR using 5 labeled anomalies is more than 410%. This shows the superpower of the synthesis of deep models and few labeled anomalies. In campaign that may have very intricate anomalies, the deep methods need slightly more labeled anomalies to achieve the similar improvement.

Robustness w.r.t. Anomaly Contamination

Experiment Settings We examine the robustness w.r.t. different anomaly contamination levels, {0%, 2%, 5%, 10%, 20%}, with the number of labeled anomalies fixed to 30.

Results The AUC-PR results for the robustness are presented in Figure 3. PRIOR achieves the best robustness w.r.t. different contamination levels. Similar to the results based on 2% contaminated data in Table 2, PRIOR also significantly outperforms all four contenders by a large margin in the other contamination levels. Particularly, the substantial improvement of PRIOR persists consistently in different contamination levels on campaign, w7a, news20 and thyroid; PRIOR performs comparably well to the best competing method in the other data sets. The demonstrated robustness of PRIOR benefits from its efficiency of leveraging the limited labeled anomalies, i.e., its greater data efficiency helps defy the noisiness of the contaminated instances.

![Figure 3: AUC-PR w.r.t. Various Contamination Levels (%)](image)
Effectiveness of Detecting Unseen Anomalies

Experiment Settings

Although the above results, especially on campaign, w7a, news20 and thyroid, show impressive generalizability of PRIOR, this section explicitly evaluates its generalizability to unseen anomalies. The experiment is performed on the UNSW-NB15 data, from which our backdoor data set is derived. UNSW-NB15 is chosen because it contains various different types of real anomalies, including eight other network attacks such as DoS, worms, reconnaissance and shellcode [Moustafa and Slay 2015] besides backdoor attacks. Detection models are trained on the training data of the backdoor data. They are then evaluated on the test data of backdoor but replacing the backdoor attacks with randomly selected unseen anomalies from the eight types of new network attacks. We vary the number of the added unseen anomalies from 64 up to 1,024 and guarantee all the eight types of attacks are evenly presented in each test set.

Results

In terms of both AUC-ROC and AUC-PR, PRIOR performs consistently and substantially better than all the competing methods in identifying the unseen anomalies across all cases. As discussed in our theoretical analysis, in addition to the patterns of labeled anomalies, PRIOR also learns the abstractions of normal instances due to the ternary ordinal regression in its pairwise relation learning. Therefore, even if the unseen anomalies demonstrate different abnormal behaviors from the seen anomalies, PRIOR would assign large anomaly scores to them when they are different from the normal instances. This is the main driving force underlying the superior performance of PRIOR here.

Note that since the normal instances remain the same in all the test sets with only the anomalies changed, AUC-ROC is relatively stable on the five different test sets. However, on the right panel, increasing the number of anomalies enlarges the anomaly proportion, making it easier to obtain better detection recall, and thus, better AUC-PR performance.

Deep Anomaly Detection

Traditional anomaly detection approaches are often ineffective in high-dimensional or non-linear separable data due to the curse of dimensionality and the deficiency in capturing the non-linear relations [Aggarwal 2017a]. Deep anomaly detection has shown promising results in handling those complex data, of which most methods learn representations separately from anomaly measures [Hawkins et al. 2002; Chen et al. 2017; Schlegl et al. 2017; Zenati et al. 2018]. Very recent methods [Zong et al. 2018; Pang et al. 2018; Ruff et al. 2018] unify representation learning and anomaly detection methods to learn more optimal features for specific anomaly detectors. However, all of these methods have an optimization objective focusing on feature representations, so the anomaly scores output by the downstream anomaly measures are optimized in an indirect manner. By contrast, PRIOR performs an end-to-end learning of anomaly scores, which fulfills a direct optimization of anomaly scores.

We had a concurrent work DevNet [Pang et al. 2019] addressing a similar problem, but employs a completely different approach to this study. Here we formulate the problem as a pairwise relation learning task and address the problem using deep ternary ordinal regression without any assumption on data distribution, whereas DevNet assumes the anomaly scores of data instances follow a Gaussian distribution and leverages this prior to learn the anomaly scores by fitting to a Z-Score-based distribution. In terms of empirical performance, DevNet and PRIOR perform comparably well on the shared eight data sets.

Weakly- and Semi-supervised Anomaly Detection

Many studies have been introduced to leverage labeled normal instances to learn patterns of the normal class, which are commonly referred to as semi-supervised anomaly detection methods [Noto et al. 2012; Gornitz et al. 2013; Ienco et al. 2017]. The semi-supervised setting is relevant to our problem because of the availability of both labeled and unlabeled data, but they are two fundamentally different tasks due to the difference in training data and the problem nature. Specifically, we have only a few labeled anomaly data rather than large-scale labeled normal data; and the anomalies are often from different distributions or manifolds, so having only limited labeled abnormal data hardly cover all types of anomalies. Therefore, instead of modeling the labeled normal data, our problem requires to learn patterns of labeled anomalies that also generalize well to unseen anomalies. A few studies [McGlohon et al. 2009; Tamosy et al. 2014; Zhang et al. 2018; Pang et al. 2018] show that these limited labeled anomalies can be leveraged to substantially improve the detection accuracy. However, these studies exploit the labeled anomalies to enhance anomaly scoring via label propagation [McGlohon et al. 2009; Tamosy et al. 2014], representation learning [Pang et al. 2018] or classification models [Zhang et al. 2018], failing to sufficiently utilize the labeled data and/or detect unseen anomalies.
This research line is also relevant to few-shot classification [Fei-Fei et al. 2006] and positive and unlabeled data (PU) learning (Li and Liu 2003) because of the availability of the limited labeled positive instances (anomalies), but they are very different in that these two areas implicitly assume that the few labeled instances share the same intrinsic class structure as the other instances within the same class (e.g., the anomaly class), whereas the few labeled anomalies and the unseen/unknown anomalies may have diverse class structures. This presents significant challenges to the techniques of both areas.

Conclusions
This paper introduces a novel formulation and its instantiation to devise ordinal regression networks for weakly-supervised deep anomaly detection. Our approach achieves significant improvement over four state-of-the-art competing methods in terms of the effectiveness in real-world data, data efficiency, robustness, and generalizability to unseen anomalies. This in turn justifies the effectiveness of the synthesis of the pairing-based data augmentation and the ordinal regression-based anomaly score learning approaches.

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