Detecting Multivariate Time Series Anomalies with Zero Known Label

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Abstract
Multivariate time series anomaly detection has been extensively studied under the one-class classification setting, where a training dataset with all normal instances is required. However, preparing such a dataset is very laborious since each single data instance should be fully guaranteed to be normal. It is, therefore, desired to explore multivariate time series anomaly detection methods based on the dataset without any label knowledge. In this paper, we propose MTGFlow, an unsupervised anomaly detection approach for Multivariate Time series anomaly detection via dynamic Graph and entity-aware normalizing Flow, leaning only on a widely accepted hypothesis that abnormal instances exhibit sparse densities than the normal. However, the complex interdependencies among entities and the diverse inherent characteristics of each entity pose significant challenges to density estimation, let alone to detect anomalies based on the estimated possibility distribution. To tackle these problems, we propose to learn the mutual and dynamic relations among entities via a graph structure learning model, which helps to model the accurate distribution of multivariate time series. Moreover, taking account of distinct characteristics of the individual entities, an entity-aware normalizing flow is developed to describe each entity into a parameterized normal distribution, thereby producing fine-grained density estimation. Incorporating these two strategies, MTGFlow achieves superior anomaly detection performance. Experiments on five public datasets with seven baselines are conducted, MTGFlow outperforms the SOTA methods by up to 5.0 AUROC%.

Introduction
Multivariate time series (MTS) broadly exist in many important scenarios, such as production data produced by multiple devices in smart factories and monitoring data generated by various sensors in smart grids. Anomalies in MTS exhibit unusual data behaviors at a specific time step or during a time period. To identify these anomalies, previous methods mostly focus on training one-class classification (OCC) models from only normal data (Wu and Keogh 2021; Schölkopf et al. 1999; Su et al. 2019; Chen et al. 2021; Deng and Hooi 2021; Xu et al. 2021; Zhang et al. 2019). They heavily rely on an assumption that the training dataset with all normal samples can be easily obtained (Ruff et al. 2021).

However, this assumption may not always hold in real-world scenarios (Goodge et al. 2021; Zhang, Zhao, and Li 2019; Zong et al. 2018; Qiu et al. 2022), leading to noisy training datasets with the mixture of normal and abnormal data instances. Meanwhile, it is already verified that model training procedure is prone to overfitting noisy labels (Zhang et al. 2021), so that the performance of those OCC-based methods could be severely degraded (Wang et al. 2019; Huyan et al. 2021). Therefore, it is rewarding to develop unsupervised MTS anomaly detection methods based on the dataset with absolute zero known labels.

An effective unsupervised strategy is modeling the dataset into a distribution, relying only on a widely accepted hypothesis that abnormal instances exhibit sparse densities than the normal, i.e., the low-density regions consist of abnormal samples and the high-density regions are formed by the normal samples (Gupta et al. 2013; Pang, Cao, and Aggarwal 2021; Wang et al. 2020). Methods have been explored along side this strategy and the key challenge lies in the accurate density estimation of the distribution. Time series density is modeled as the parameterized probability distribution (Salinas et al. 2020; Rasul et al. 2021; Feng et al. 2022), while it is still challenging to model a more complex data distribution. To improve the model capacity of density estimation, Rasul et al. (Rasul et al. 2020) further exploits normalizing flow to model complex distribution for high-dimensional MTS (Rasul et al. 2020). However, they neglect the interdependencies among constituent series which also play an important role in accurate density estimation.

The most related work is GANF (Dai and Chen 2021), which tackles the same MTS anomaly detection task. In their design, the static directed acyclic graph (DAG) is leveraged to model intractable dependence among multiple entities, and normalizing flow (Dinh, Sohl-Dickstein, and Bengio 2016; Papamakarios, Pavlakou, and Murray 2017) is employed to estimate an overall distribution for all entities together. Although GANF has achieved state-of-the-art (SOTA) results previously, it still suffers from two drawbacks. First, rather than a static inter-relationship, in real-world applications, the mutual dependencies among entities could not only be complex but also evolving. This dynamic property cannot be simply characterized via a DAG struc-
ture. Second, entities usually have diverse working mechanisms, leading to diverse sparse characteristics when anomalies occurred. GANF projects all entities into the same distribution, resulting in a compromise for the density estimation of each individual time series. Thereby, the final anomaly detection performance could also be degraded.

In this paper, we propose MTGFlow, an unsupervised anomaly detection method for MTS anomaly detection, to tackle the above problems. First, considering the evolving relations among entities, we introduce a graph structure learning module to model these changeable interdependencies. To learn the dynamic structure, a self-attention module (Vaswani et al. 2017) is plugged into our model for its superior performance on quantifying pairwise interaction. Second, aiming at the diverse inherent characteristics existed among individual entities, we design an entity-aware normalizing flow to model the entity-specific density estimation. Thereby, each entity can be assigned to a unique target distribution and the diverse entity densities can be estimated independently. In addition, we also propose to control the model size by sharing entity-specific model parameters, which helps MTGFlow achieve fine-grained density estimation without much memory consumption.

We summarize our contributions as follows:

- We propose MTGFlow, a new SOTA method for unsupervised MTS anomaly detection. It essentially enables anomaly localization and interpretation.
- We model the complicated interdependencies among entities into the dynamic graph, which captures the complex and evolving mutual dependencies among entities. Also, entity-aware normalizing flow is introduced to produce entity-specific density estimation.
- Experiments on five datasets with seven baseline methods are conducted, outperforming the SOTA methods by up to 5.0 AUROC%.

Related Work

Time Series Anomaly Detection

Time series anomaly detection has been extensively investigated under OCC setting (Chalapathy and Chawla 2019; Hundman et al. 2018). Previous influential methods like DeepSVDD (Ruff et al. 2018), EncDecAD (Malhotra et al. 2016), OmniAnomaly (Su et al. 2019), USAD (Audibert et al. 2020) and DAEMON (Chen et al. 2021) firstly train a model with normally normal instances so that the abnormal instances would exhibit differently when they are fed into the model during testing. Along side this line, Anomaly Transformer (Xu et al. 2021) and TranAD (Tuli, Casale, and Jennings 2022) further investigate fine-grained representation learning procedure via techniques like self-attention (Vaswani et al. 2017), achieving good detection performance.

However, all these works are based on the assumption that a sufficient training dataset with all normal instances can be acquired, which is very hard for real-world applications since each instance should be manually checked carefully. In addition, once there exist abnormal instances in the training data, the performance of these OCC-based detection methods could be severely degraded (Wang et al. 2019; Huyen et al. 2021). Therefore, instead of fitting distribution of the normal training dataset, Dai and Chen propose GANF (Dai and Chen 2021) to detect MTS anomalies in an unsupervised manner. Inspired by them, we propose MTGFlow to facilitate the learning capacity and improve detection performance.

Graph Structure Learning

Graph convolution networks (GCN) (Kipf and Welling 2016) have achieved great success in modeling intrinsic structure patterns. However, such a graph structure is usually unknown in real-world scenarios so graph structure learning methods are in need (Velickovic et al. 2017). In the field of anomaly detection of MTS, some recent works attempt to explore this area. GDN (Deng and Hooi 2021) learns a directed graph via node embedding vectors. According to the cosine similarity of embedding vectors, top-K candidates of each node are considered to have interdependencies. GANF (Dai and Chen 2021) models relations among multiple sensors, using DAG, and learns the structure of the DAG through continuous optimization with a simplified constraint that facilitates backward propagation. Our work MTGFlow models the mutual complex dependence as a fully connected graph via the self-attention mechanism, so that a much more flexible relation among entities can be represented.

Normalizing Flow for Anomaly Detection

Normalizing flow is an important technology on density estimation and has been successfully utilized in image generation tasks (Dinh, Sohl-Dickstein, and Bengio 2016; Papamakarios, Pavlakou, and Murray 2017). Recently, it is also explored for anomaly detection based on the assumption that anomalies are in low-density regions, like DiﬀerNet (Rudolph, Wandt, and Rosenhahn 2021) and CFLOW-AD (Gudovskiy, Ishizaka, and Kozuka 2022), which leverage normalizing flow to estimate likelihoods of normal embeddings and declare image defects when the embedding is far away from the dense region. GANF is a great work that employs normalizing flow for unsupervised MTS anomaly detection. We follow this research line and facilitate model capacity through an entity-aware normalizing flow design.

Preliminary

In this section, we give a brief introduction of normalizing flow to better understand MTGFlow.

Normalizing Flow

Normalizing flow is an unsupervised density estimation approach to map the original distribution to an arbitrary target distribution by the stack of invertible affine transformations. When density estimation on original data distribution $X$ is intractable, an alternative option is to estimate $z$ density on target distribution $Z$. Specifically, suppose a source sample $x \in \mathcal{R}^D \sim X$ and a target distribution sample $z \in \mathcal{R}^D \sim Z$. Bijective invertible transformation $f_\theta$ aims to achieve one-to-one mapping $z = f_\theta(x)$ from $X$. 

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to $Z$. According to the change of variable formula, we can get $P_Z(z) = P_X(x) \left| \det \frac{\partial f}{\partial x} \right|$. Benefiting from the invertibility of mapping functions and tractable jacobian determinants $\left| \det \frac{\partial f}{\partial x} \right|$. The objective of flow models is to achieve $\hat{z} = z$, where $\hat{z} = f_0(x)$. Flow models are able to achieve more superior density estimation performance when additional conditions $C$ are input (Ardizzone et al. 2019). Such a flow model is called conditional normalizing flow, and its corresponding mapping is derived as $z = f_0(x|C)$. Parameters $\theta$ of $f_0$ are updated by maximum likelihood estimation (MLE): $\theta^* = \arg \max_\theta (\log(P_Z(f_0(x|C))) + \log(\left| \det \frac{\partial f}{\partial x} \right|))$.

**Method**

**Data Preparation**

MTS are defined as $x = (x_1, x_2, ..., x_K)$ and $x_i \in \mathbb{R}^L$, where $K$ represents the total number of entities, and $L$ denotes the total number of observations of each entity. We use the z-score to normalize the time series from different entities. $\bar{x}_i = \frac{x_i - \text{mean}(x_i)}{\text{std}(x_i)}$, where $\text{mean}(x_i)$ and $\text{std}(x_i)$ represent the mean and standard deviation of the $i$-th entity along the time dimension, respectively. To preserve temporal correlations of the original series, we use a sliding window with size $T$ and stride size $S$ to sample the normalized MTS. $T$ and $S$ can be adjusted to obtain the training sample $x^c$, where $c$ is the sampling count. $x^c$ is short for $x^{cS:cS+T}$.

**Overall Structure**

The core idea behind MTGFlow is to dynamically model mutual dependence so that fine-grained density estimation of the multivariate time series can be obtained. Such accurate estimation enables the superiority of capturing low-density regions, and further promotes the anomaly detection performance even if there is high anomaly contamination in the training dataset. Fig. 1 shows the overview of MTGFlow. In particular, we model the temporal variations of each entity, using RNN model. Meanwhile, a graph structure learning module is leveraged to model the dynamic interdependencies. Then, the derived time encoding, output of RNN, performs the graph convolution operation with the above corresponding learned graph structure. We regard above outputs as spatio-temporal conditions as they contain temporal and structural information. Next, the spatio-temporal conditions are input to help entity-aware normalizing flow achieve precise fine-grained density estimation. The deviations of $\hat{z}$ and $z$ are measured by log likelihoods. Finally, all modules of MTGFlow are jointly optimized through MLE.

**Graph Structure Learning via Self-attention**

Since dependence among entities is mutual and evolves over time, we exploit self-attention to learn a dynamic graph structure. Entities in multivariate time series are regarded as graph nodes. Given the window sequence $x^c$, the query and key of node $i$ are represented by vectors $x^c_i W_Q$ and $x^c_i W_K$, where $W_Q \in \mathbb{R}^{T \times T}$ and $W_K \in \mathbb{R}^{T \times T}$ are the query and key weights. The pairwise relationship $e_{ij}^c$ at the $c$-th sampling count between node $i$ and node $j$ is described as $e_{ij}^c = \frac{(x^c_i W_Q)(x^c_j W_K)^T}{\sqrt{T}}$. The attention score $a_{ij}^c$ is used to quantify the pairwise relation from node $i$ to node $j$, calculated by $a_{ij}^c = \frac{\exp(e_{ij}^c)}{\sum_{j=1}^N \exp(e_{ij}^c)}$. And the attention matrix consists of attention scores of each node, thus including mutual dependence among entities. Naturally, we treat the attention matrix as the adjacency matrix $A^c$ of the learned graph. Since input time series are evolving over time, $A^c$ also changes to capture the dynamic interdependencies.
**Spatio-temporal Condition**

To better estimate the density of multiple time series, the robust spatio-temporal condition information is important. As described above, underlying structure information is modeled as the dynamic graph. Besides spatio information, temporal correlations also play an important role to feature time series. Here, we follow the most prevalent idea, where RNN is utilized to capture the time correlations. For a window sequence of entity $k$, $x^e_k$, the time representation $H^t_k$ at time $t \in (cS : cS + T)$ is derived by $H^t_k = \text{RNN}(x^e_k, H^{t-1}_k)$, where RNN can be any sequence model such as LSTM (Hochreiter and Schmidhuber 1997) and GRU (Cho et al. 2014), and $H^t_k$ is the hidden state of RNN. To derive the spatio and temporal information $C^t_k$ of all entities at $t$, a graph convolution operation is performed through the learned graph $A^c$.

As mentioned in GANF, we also find that history information of the node itself helps enhance temporal relationships of time series. Hence, the spatio-temporal condition at $t$:

$$C^t = \text{ReLU}(A^c H^t W_1 + H^{t-1} W_2)W_3,$$

where $W_1$ and $W_2$ are graph convolution and history information weights, respectively. $W_3$ is used to improve the expression ability of condition representations. The spatio-temporal condition $C^t$ for window $c$ is the concatenation of $C^t$ along the time axis.

**Entity-aware Normalizing Flow**

Distributions of individual entities have discrepancies because of their different work mechanisms, and thus their respective anomalies will generate distinct sparse characteristics. If we map time series from all entities to the same distribution $N(0, I)$, as does in GANF, then the description capacity of the model will be largely limited and the unique inherent property of each entity will be ignored. Therefore, we design the entity-aware normalizing flow $z^c_k = f_\theta^k(x^c_k; C)$ to make more detailed density estimation, where $x^c_k$, $C$, $k$ are the input sequence, condition, and the $k$-th entity, respectively. Technically, for one entity, we assign the multivariate Gaussian distribution as the target distribution. The covariance matrix of the above target distribution is the identity matrix $I$ for better convergence. Moreover, in order to generate different target distributions $Z_k$, we independently draw mean vectors $\mu_k \in R^T$ from $N(0, I)$ (Izmailov et al. 2020). However, we find that such setting results in performance degradation. So, in our experiment, each element of $\mu_k$ is kept the same. Specifically, for the time series of the entity $k$, the density estimation is given by:

$$P_{X_k}(x_k) = P_{Z_k}(f_\theta^k(x_k; C)) \left| \frac{\partial f_\theta^k}{\partial x_k} \right|$$

where each element of $\mu_k$ is the same, and is drawn from the $N(0, 1)$. In such a case, model parameters will increase with the number of entities. To mitigate this problem, we share entity-aware normalizing flow parameters across all entities. So, the density estimation for $k$ reads:

$$P_{X_k}(x_k) = P_{Z_k}(f_\theta(x_k; C)) \left| \frac{\partial f_\theta}{\partial x_k} \right|$$

**Joint Optimization**

As described above, MTGFlow combines graph structure learning and RNN to capture the spatio and temporal dependence on multiple time series. Then, derived spatio-temporal conditions are utilized to contribute to entity-aware normalizing flow accurately estimating density of time series. To avoid getting stuck in the local optimum for each module of MTGFlow, we jointly optimize all modules for overall performance of MTGFlow. The whole parameters $W^*$ are estimated via MLE.

$$W^* = \arg \max_W \log(P_X(x))$$

$$\approx \arg \max_w \frac{1}{NK} \sum_{c=1}^N \sum_{k=1}^K \log(P_{Z_k}(f_\theta(x^c_k; C^t_k))) \left| \frac{\partial f_\theta}{\partial x^c_k} \right|$$

$$\approx \arg \max_w \frac{1}{NK} \sum_{c=1}^N \sum_{k=1}^K -\frac{1}{2} \|z^c_k - \mu_k\|^2 + \log \left| \frac{\partial f_\theta}{\partial x^c_k} \right|$$

where $N$ is the total number of windows.

**Anomaly Detection and Interpretation**

Based on the hypothesis that anomalies tend to be sparse on data distributions, low log likelihoods indicate that the observations are more likely to be anomalous.

**Anomaly Detection**

Taking the window sequence $x^c_k$ as the input, the density of all entities can be estimated. The mean of the negative log likelihoods of all entities serves as the anomaly score $S_c$, which is calculated by:

$$S_c = -\frac{1}{K} \sum_{k=1}^K \log(P_{X_k}(x^c_k))$$

A higher anomaly score represents that $x^c_k$ locates in the lower density region, indicating a higher possibility to be abnormal. Since abnormal series exist in the training set and validation set, we cannot directly set the threshold to label the anomaly, such as the maximum deviation in validation data (Deng and Hooi 2021). Therefore, to reduce the anomaly disturbance, we store $S_c$ of the whole training set, and the interquartile range (IQR) is used to set the threshold: $Threshold = Q_3 + 1.5 \times (Q_3 - Q_1)$, where $Q_1$ and $Q_3$ are 25-th and 75-th percentile of $S_c$.

**Anomaly Interpretation**

Abnormal behaviors of any entity could lead to the overall abnormal behavior of the whole window sequence. Naturally, we can get the entity anomaly score $S_{c,k}$ for entity $k$ according to Eq. (4).

$$S_{c,k} = -\frac{1}{K} \sum_{k=1}^K \log(P_{X_k}(x^c_k)) = \sum_{k=1}^K S_{c,k}$$

Since we map time series of each entity into unique target distributions, different ranges of $S_{c,k}$ are observed. This bias will assign each entity to different weights in terms of its contribution to $S_c$. To circumvent the above-unexpected bias, we design the entity-specific threshold for each entity. Considering different scales of $S_{c,k}$, IQR is used to set respective thresholds. Therefore, the threshold for $S_{c,k}$ is given as: $Threshold_{c,k} = \lambda_k (Q^1_{3} + 1.5 \times (Q^3_{2} - Q^1_{2}))$, where $Q^1_{2}$ and $Q^3_{2}$ are 25-th and 75-th percentile of $S_{c,k}$ across all observations, respectively. And $\lambda_k$ is used to adjust $Threshold_{c,k}$ because normal observations in different entities also fluctuate with different scales.
Experiment

Experiment Setup

Dataset The commonly used public datasets for MTS anomaly detection in OCC are MSL (Mars Science Laboratory rover) (Hundman et al. 2018), SMD (Server Machine Dataset) (Su et al. 2019), PSM (Pooled Server Metrics) (Abdulaal, Liu, and Lancewicki 2021), SWaT (Secure Water Treatment) (Goh et al. 2016) and WADI (Water Distribution) (Ahmed, Palleti, and Mathur 2017). The sensor data in SWaT and WADI is from water Treatment with 51 and 123 entities. MSL, SMD, and PSM are from Mars rover with 55 features, server metrics with 38 features, and server nodes at eBay with 25 features, respectively. Since only normal time series are provided in these datasets for training in OCC setting, we follow the dataset setting of GANF (Dai and Chen 2021) and split the original testing dataset by 60% for training, 20% for validation, and 20% for testing in SWaT. For other datasets, the training split contains 60% data, and the test split contains 40% data.

Implementation Details For all datasets, we set the window size as 60 and the stride size as 10. Adam optimizer with a learning rate 0.002 is utilized to update all parameters. One layer of LSTM is sufficient to extract time representations in our experiment. One self-attention layer with 0.2 dropout ratio is adopted to learn the graph structure. We use MAF as the normalizing flow model. For SWaT, one flow block and 512 batch size are employed. For other datasets, we arrange two flow blocks for it and set the batch size as 256. $\lambda$ is set as 0.8 for thresholds of all entities. The epoch is 40 for all experiments, which are performed in PyTorch-1.7.1 with a single NVIDIA RTX 3090 24GB GPU\(^1\).

Evaluation Metric As in previous works, MTGFlow aims to detect window-level anomalies, and labels are annotated as abnormal when there exists any anomalous time point. The performance is evaluated by the Area Under the Receiver Operating Characteristic curve (AUROC).

Baselines SOTA methods include semi-supervised methods DeepSAD (Ruff et al. 2019), OCC methods DeepSVDD (Ruff et al. 2018), ALOCC (Sabokrou et al. 2020), DROCC (Goyal et al. 2020), and USAD (Audibert et al. 2020) and unsupervised methods DAGMM (Zong et al. 2018) and GANF (Dai and Chen 2021).

Performance We list the AUROC metric results in Table 1. Note that the standard deviation of SMD is large because it comprises 28 sub-datasets, where we test the performance on each of them and average all the results. MTGFlow has superior performance over all the other seven baselines. Compared with MTGFlow, DeepSVDD and DROCC project all training samples into the hypersphere so that they cannot learn the accurate decision boundary distinguishing normal from abnormal samples. Adversarial learning used by ALOCC and USAD and semi-supervised learning strategy in DeepSAD leverage a more informative training procedure to mitigate the effect of high anomaly contamination. As for DAGMM, it is restricted to the distribution estimation ability of GMM for multiple entities. Although GANF obtains a better result, its detection performance is still limited by inadequate dependence modeling and indiscriminative density estimation. Due to a much more flexible modeling structure, MTGFlow outperforms the above baseline methods. Moreover, we study log likelihoods for anomalies ranging from 2016/1/2 11:07:00 to 11:37:00 in Fig. 2. It is clear that log likelihoods are high for the normal series but lower for labeled abnormal ones (highlighted in red). This variation of log likelihoods validates that MTGFlow can detect anomalies according to low density regions of modeled distribution. Meanwhile, to investigate anomaly discrimination ability of MTGFlow, we present the normalized $S_c$ for MTGFlow and GANF in Fig. 3. As it is displayed, for normal series, anomaly scores of MTGFlow are more centered at 0 than these of GANF, and the overlap areas of normal and abnormal scores are also smaller in MTGFlow, reducing the false positive ratio. This larger score discrepancy corroborates that MTGFlow has superior detection performance.

Ablation Study

Module Ablation Study To test the validity of each designed module, we give several ablation experiments. We denote MTGFlow without graph and entity-aware normalizing flow as MTGFlow/(G, E), MTGFlow only without graph as MTGFlow/G, and MTGFlow only without entity-aware normalizing flow as MTGFlow/E. Results are presented in

\(^1\)Code is available at github.com/zqhang/MTGFLOW.
Table 1: Anomaly detection performance of AUROC(%) on five public datasets.

| Dataset | DeepSVDD | ALOCC | DROCC | DeepSAD | USAD | DAGMM | GANF | MTGFlow |
|---------|----------|-------|-------|---------|------|-------|------|---------|
| SWaT    | 66.8±2.0 | 71.1±2.3 | 72.6±3.8 | 75.4±2.4 | 78.8±1.0 | 72.8±3.0 | 79.8±0.7 | 84.8±1.5 |
| WADI    | 83.5±1.6 | 83.5±1.8 | 75.6±1.6 | 85.4±2.7 | 86.1±0.9 | 77.2±0.9 | 90.3±1.0 | 91.9±1.1 |
| PSM     | 67.5±1.4 | 71.8±1.3 | 74.3±2.0 | 73.2±3.3 | 78.0±0.2 | 64.6±2.6 | 81.8±1.5 | 85.7±1.5 |
| MSL     | 60.8±0.4 | 60.3±0.9 | 53.4±1.6 | 61.6±0.6 | 57.0±0.1 | 56.5±2.6 | 64.5±1.9 | 67.2±1.7 |
| SMD     | 75.5±1.5 | 80.5±1.11 | 76.7±8.7 | 85.9±11.1 | 86.9±11.7 | 78.0±9.2 | 89.2±7.8 | 91.3±7.6 |

Table 2: Module ablation study (AUROC%).

|                                 | Graph | Entity | SwaT     | WADI     |
|---------------------------------|-------|--------|----------|----------|
| MTGFlow/(G, E)                  | ✗     | ✗      | 78.3±0.9 | 89.7±0.5 |
| MTGFlow/G                       | ✗     | ✓      | 82.4±1.0 | 91.3±0.4 |
| MTGFlow/E                       | ✓     | ✗      | 81.2±1.1 | 91.0±0.7 |
| MTGFlow                         | ✓     | ✓      | 84.8±1.5 | 91.9±1.1 |

Table 3: Ablation study of hyperparameters (AUROC%).

| Window size | Blocks | 1  | 2      | 3      |
|-------------|--------|----|--------|--------|
| SWaT        | 40     | 81.4±3.2 | 82.7±2.1 | 81.7±0.9 |
|             | 60     | 84.8±1.5 | 83.6±2.0 | 83.1±0.9 |
|             | 80     | 82.8±1.0 | 82.7±0.8 | 83.4±0.6 |
|             | 100    | 82.6±0.5 | 83.4±0.9 | 83.5±0.6 |
|             | 120    | 83.2±2.0 | 83.4±2.3 | 84.5±2.6 |
| WADI        | 40     | 90.8±1.3 | 91.7±1.2 | 91.7±1.3 |
|             | 60     | 89.2±1.9 | 91.9±1.1 | 91.5±0.8 |
|             | 80     | 89.8±2.0 | 90.7±2.8 | 91.7±0.7 |
|             | 100    | 89.6±1.1 | 90.3±1.8 | 91.3±1.6 |
|             | 120    | 88.6±1.4 | 91.0±1.6 | 91.3±1.9 |

Figure 4: Effect of anomaly contamination ratio.

Anomaly Ratio Analysis To further investigate the influence of anomaly contamination rates, we vary training splits to adjust anomalous contamination rates. For all the above-mentioned datasets, the training split increases from 60% to 80% with 5% stride. We present an average result over five runs in Fig. 4. Although the anomaly contamination ratio of training dataset rises, the anomaly detection performance of MTGFlow remains at a stable high level.

Result Analysis

In order to further investigate the effectiveness of MTGFlow, we give a detailed analysis based on SWaT dataset.

Dynamic Graph Structure Interdependencies among entities are not guaranteed to be immutable. In fact, pairwise relations evolve with time. Benefiting from self-attention, MTGFlow can model this characteristic into a dynamic graph structure. We treat the attention matrix as the graph adjacent matrix. An empirical threshold of 0.15 is set for the adjacency matrix to show an intuitive learned graph structure in the test split. In Fig. 5, the node size represents its node degrees, the arrow direction represents the learned directed dependence and the arrow width indicates the weight of the corresponding interdependencies. The graph structure at 2016/1/1 14:00:00 is centered on the sensor P[201], while the edges in the graph have completely changed and the center has shifted from P[201] to AIT[503] at 2016/1/2 7:00:00. This alteration of the graph structure may result from changing in working condition of water treatment plant. Besides, two similar graph structures can be found at 2016/1/2 13:00:00 and 2016/1/2 14:00:00. This suggests that the graph structure will be consistent if the interdependencies remain unchanged over a period of time, possibly due to repetitive work patterns of entities. In addition, the
Entity anomaly score $S_{ck}$

Figure 5: Dynamic graph structure in MTGFlow.

Figure 6: Transformed distributions of multiple entities.

Figure 7: Variation of log likelihoods for different entities on the whole testing dataset (anomalies are highlighted in red, and the blue line is the threshold according to $S_{ck}$).

Distinct Sparse Characteristics To demonstrate that the sparse characteristics vary with different entities, we study changes of $S_{ck}$ along time on SWaT. As shown in Fig. 7, $S_{ck}$ of AIT502, P102, FIT502, and LIT301 are presented. The highlighted regions denote marked anomalies. For a better illustration, we divide the anomalous regions as $A_1$, $A_2$, $A_3$, $A_4$, and $A_5$ along the timeline. We can observe that different entities react to different anomalies because of their different work mechanisms. Specifically, AIT502 has obvious fluctuations at $A_4$, while $P102$ reacts to $A_2$. In addition, FIT502 is sensitive to $A_4$ and $A_5$, yet LIT301 is sensitive to $A_2$, $A_3$, $A_4$, and $A_5$. Nevertheless, MTGFlow is still able to accurately distinguish and detect these anomalies.

Conclusion

In this work, we proposed MTGFlow, an unsupervised anomaly detection approach for MTS based on the dataset with absolute zero known label. Extensive experiments on real-world datasets demonstrate its superiority, even if there exists high anomaly contamination. The superior anomaly detection performance of MTGFlow is attributed to dynamic graph structure learning and entity-aware density estimation. In addition, we explore various interdependencies that exist between individual entities from the learned dynamic graph structure. And a detected anomaly can be understood and localized via entity anomaly scores. In the future, we plan to explore the performance of our method from more realistic scenarios (Wu and Keogh 2021), and further improve its practicality.
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