MTGFlow: Unsupervised Multivariate Time Series Anomaly Detection via Dynamic Graph and Entity-aware Normalizing Flow

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ABSTRACT
Multivariate time series anomaly detection has been extensively studied under the semi-supervised 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 on the 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 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 the real-world datasets are conducted, demonstrating that MTGFlow outperforms the state-of-the-art (SOTA) by 5.0% and 1.6% AUROC for SWaT and WADI datasets respectively. Also, through the anomaly scores contributed by individual entities, MTGFlow can provide explanation information for the detection results.

CCS CONCEPTS
- Computing methodologies → Anomaly detection; • Theory of computation → Unsupervised learning and clustering.

KEYWORDS
multivariate time series, anomaly detection, normalizing flow, graph structure learning

1 INTRODUCTION
Multivariate time series 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 multivariate time series exhibit unusual data behaviours 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 [2, 3, 5, 6, 25–28, 32]. They heavily rely on an assumption that the training dataset with all normal samples can be easily obtained.

However, this assumption may not always hold in real-world scenarios [9, 34, 35], 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 [33], so that the performance of those OCC based methods could be severely degraded. Therefore, it is rewarding to develop unsupervised multivariate time series 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 [12, 17, 31]. 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 parametrized probability distribution in DeepAR [24], while it is challenging to model a more complex data distribution. To improve model competence of density estimation, Rasul et al. [19] further exploits normalizing flow to model complex distribution for high-dimensional multivariate time series [19]. However, they neglect the interdependencies among constituent series which plays an equally important role for the accurate density estimation.

The most related work is GANF, which tackles the same multivariate time series anomaly detection task [5]. In their design, the static directed acyclic graph (DAG) is leveraged to model intractable dependence among multiple entities, and normalizing flow [7, 18] is employed to estimate an overall distribution for all entities together. Although GANF has achieved SOTA results previously, it still suffers from two drawbacks. First, in real-world applications, entities could have complex and evolving mutual dependence. For example, in a water treatment plant, when the measured motorized valve is on, water level will rise. While water level exceeds the necessity, the measured motorized valve will be closed. The actuator of the motorized valve and the water level sensor for the same water tank actually have strong coupling relations, which can not be simply characterized by a DAG structure. Meanwhile, due to different work conditions, the water level needs to rise for storing water or fall when draining water. Such relationships are not set in stone, and thus the static graph structure fails to have a comprehensive modeling capacity on this evolving feature. Second,
each entity may have different working mechanisms. This leads to the diverse sparse characteristics of the anomalies for different entities. GANF projects these various sparse characteristics into one 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 multivariate time series 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 [29] is plugged into our model because of 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. For this purpose, we assign each entity to a unique target distribution. As a consequence, diverse entity densities can be estimated independently, thereby mitigating the performance compromise of simultaneous estimation of multiple entities. However, this fine-grained density estimation of MTGFlow multiplies memory overhead as the number of entities increases. We share entity-specific model parameters to reduce model size. As a result, MTGFlow achieves more fine-grained density estimation without extra memory consumption, which further promotes the anomaly detection performance.

Finally, maximum likelihood estimation is used to train all parameters of MTGFlow in an end-to-end manner. Experiments are conducted on two real-world datasets SWaT and WADI to demonstrate the effectiveness of MTGFlow. MTGFlow makes progress over the SOTA, achieving 84.8% AUROC on SWaT and 91.9% AUROC on WADI, outperforming 5.0% and 1.6% than GANF, respectively. What’s more, MTGFlow can interpret a detected anomaly via the log likelihood factors that each entity contributes. Through the learned graph structure, various dependence among individual entities can be represented. We summarize our contributions as follows:

- We propose MTGFlow, an approach for unsupervised multivariate time series anomaly detection, with the ability of result explanation and the anomaly localization.
- We model complicated interdependencies among entities as the dynamic graph. Through the learned dynamic graph structure, various mutual relations like evolving and periodic interdependencies can be captured among the individual entities.
- Aiming at different sparse characteristics existed in the individual entities, entity-aware normalizing flow is introduced to produce entity-specific density estimation.
- MTGFlow outperforms SOTA method GANF on public datasets SWaT and WADI, outperforming 5.0% AUROC on SWaT, 1.6% AUROC on WADI.

2 RELATED WORK

2.1 Time Series Anomaly Detection

Anomaly detection for time series is a classical research topic, which has been extensively investigated under OCC setting. Temporal correlation is one of the most important feature of time series. Compared with the normal, anomalous time points and sequences often present unusual temporal correlations. To model the distribution of normal time series, DeepSVDD [21] maps training data into preset hypersphere, assuming that anomalous data lie outside this space during the test. EncDecAD [16] leverages LSTM [13] to extract sequence features, and designs the reconstruction task to detect anomalies. USAD [2] and DAEMON [3] use adversarial learning to promote reconstruction quality. Considering the much more complex temporal dependence of multivariate time series, Omni-Anomaly [26] constructs informative stochastic representations for a more robust performance. More recent works [32] and [28] utilize Transformer [29] for anomaly detection, leaning on the superiority modeling capacity of the self-attention mechanism for long-range relations. However, all these works are based on the assumption that training data are all normal. Existence of abnormal time series in the training dataset could severely degrade the performance of these OCC based detection methods. Therefore, instead of fitting distribution of normal training dataset, MTGFlow estimates density of unlabelled training dataset, and detects anomalies depending on their inherent low density characteristics.

2.2 Graph Structure Learning

Given a structured data, graph convolution networks (GCN) [15] and graph attention networks (GAT) [30] achieve great success in modeling their intrinsic patterns. In real scenarios, the graph structure is hardly to obtain in advance. Therefore, it is important to learn the underlying graph structure. GDN [6] 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 on the node itself. GANF [5] 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 connect graph via self-attention mechanism, so that a much more flexible relation among entities can be represented.

2.3 Normalizing Flow for Anomaly Detection

Normalizing flow is an important technology on density estimation and has been successfully utilized in image generation task [7, 18]. Recently, normalizing flow is also explored for anomaly detection based on the assumption that anomalies are in low density regions. DifferNet [20] and CFLOW-AD [11] leverage normalizing flow to estimate likelihoods of normal embeddings extracted by an encoder. They declare image defects when the embedding is far away from the dense region. The more relevant work GANF models relationships among constituent series via DAG, and uses graph-augmented flow model to estimate densities of multiple time series. GANF makes a breakthrough for unsupervised anomaly detection on multivariate time series. However, in GANF, DAG fails to model mutual dependence existing among entities, and different entities with diverse patterns are all mapped into one distribution. Instead, we construct a fully connected graph to model such intractable temporal dependence. Meanwhile, we use entity-aware normalizing flow to have a much more precise estimation of the density.
3 PRELIMINARY

In this section, we give a brief introduction of the self-attention mechanism and normalizing flow.

3.1 Self-Attention

Transformer [29] has achieved great success for natural language processing (NLP), which largely benefits from the superior modeling capacity of the self-attention mechanism. For an input sequence, \( X = (x_1, x_2, x_3, ..., x_N) \), where \( N \) is the sequence length, and \( D \) is the embedding dimension. Self-attention applies linear projections to get queries \( Q \in \mathbb{R}^{N \times D} \) and keys \( K \in \mathbb{R}^{N \times D} \) via learnable parameter matrices \( W^Q, W^K \). After projections, attention scores are derived by scaled dot product between \( Q \) and \( K \), and a Softmax function is utilized to normalize the scores to \((0,1)\).

\[
Q = XW^Q \quad \text{and} \quad K = XW^K
\]

\[
\text{Attention}_{\text{matrix}} = \text{Softmax} \left( \frac{QK^T}{\sqrt{D}} \right)
\]  

(1)

With such a design, the pairwise relationships can be flexibly modeled in the neural network architecture. The obtained Attention matrix is the quantification of these relations.

3.2 Normalizing Flow

Normalizing flow is an unsupervised density estimation approach to map 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 \( x \in \mathbb{R}^D \sim X \) and a target distribution sample \( z \in \mathbb{R}^D \sim Z \). Bijective invertible transformation \( F_\theta \) aims to achieve one-to-one mapping \( z = f_\theta(x) \) from \( X \) to \( Z \). According to the change of variable formula, we can get

\[
P_X(x) = P_Z(z) \left| \det \frac{\partial f_\theta}{\partial x^T} \right|
\]  

(2)

Benefiting from the invertibility of mapping functions and tractable jacobian determinants \( \left| \det \frac{\partial f_\theta}{\partial x^T} \right| \). The objective of flow models is to achieve \( z = z^* \), where \( z = f_\theta(x) \). Parameters \( \theta \) of \( f_\theta \) can be directly estimated by maximum log likelihood as follows

\[
\hat{\theta}^* = \arg \max_{\theta} \log(P_X(x))
\]

\[
= \arg \max_{\theta} \left( \log(P_Z(z) + \log(\left| \det \frac{\partial f_\theta}{\partial x^T} \right|)) \right).
\]  

(3)

Design of \( f_\theta \) is an important topic in flow models. The core is to improve the flow model transferability under the premise of the tractable jacobian determinants. Representative flow model like RealNVP [7] utilizes the affine coupling, while MAF [18] applies autoregressive functions.

Flow models are able to achieve more superior density estimation performance when additional conditions \( C \) are input [1]. This is because \( C \) can usually provide relevant priors to accurately characterize the source distribution, such as time and position encoding [29]. Such the flow model is called conditional normalizing flow, and its corresponding mapping is derived as \( z = f_\theta(x|C) \). Therefore, the training objective is rewritten as

\[
\hat{\theta}^* = \arg \max_{\theta} \left( \log(P_Z(f_\theta(x|C)) + \log(\left| \det \frac{\partial f_\theta}{\partial x^T} \right|)) \right).
\]  

(4)
4 METHOD

4.1 Data Preparation
Multivariate time series are defined as \( x = (x_1, x_2, ..., x_k) \) and \( x_i \in \mathcal{R}^L \), where \( K \) represents the number of entities, and \( L \) denotes the total number of observations. We use the z-score to normalize the time series from different entities.

\[
\bar{x}_i = \frac{x_i - \text{mean}(x_i)}{\text{std}(x_i)} \tag{5}
\]

where \( \text{mean}(x_i) \) and \( \text{std}(x_i) \) represent the mean and standard deviation of \( i \)th entity along the time dimension, respectively.

To preserve the temporal correlation of the original series, we use a sliding window with size \( T \) and stride size \( S \) to sample the normalized multivariate time series. \( T \) and \( S \) can be adjusted to obtain the training sample \( x^c \), where \( c \) is the sampling count. For better clarification, we notate the \( x^c:S:cS+T \) as \( x^c \).

4.2 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 estimations enable the superiority of capturing low density regions, and further promote the anomaly detection performance even if there is high anomaly contamination in 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 graph convolution operation with above 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 \( z \) and \( z \) are measured by log likelihoods. Finally, all modules of MTGFlow are jointly optimized through maximum likelihood estimation.

4.3 Graph Structure Learning via Self-attention
Since dependence among entities is mutual and evolve over time, we exploit self-attention to learn a dynamic graph structure. Entities in multivariate time series are regarded as graph nodes. Given window sequence \( x^c \), the query and key of node \( i \) are represented by vectors \( x_i^cW^Q \) and \( x_i^cW^K \), where \( W^Q \in \mathcal{R}^{T \times T} \) and \( W^K \in \mathcal{R}^{T \times T} \) are the query weights and the key weights. According to Eq. 1, the pairwise relationship \( e_{ij}^c \) at the \( t \)th sampling count between node \( i \) and node \( j \) is described as

\[
e_{ij}^c = \frac{(x_i^cW^Q)(x_j^cW^K)^T}{\sqrt{T}} \tag{6}
\]

Attention score \( a_{ij}^c \) is used to quantify the pairwise relation from node \( i \) to node \( j \), calculated by

\[
a_{ij}^c = \frac{\exp(e_{ij}^c)}{\sum_{j=1}^{n} \exp(e_{ij}^c)} \tag{7}
\]

Attention matrix combines attention scores of each node, thus including mutual dependence among entities. Naturally, we treat attention matrix as the adjacency matrix \( A^c \), which is represented by

\[
A^c = \begin{bmatrix}
a_{11}^c & \cdots & a_{1N}^c \\
\vdots & \ddots & \vdots \\
a_{N1}^c & \cdots & a_{NN}^c
\end{bmatrix} \tag{8}
\]

Since input time series are evolving over time, \( A^c \) also changes to capture the dynamic interdependencies.

4.4 Spatio-temporal Condition
To better estimate the density of multiple time series, the robust spatio-temporal condition information is important. As described in Sec. 4.3, 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 \( k \), \( x_k^c \) the time representation \( H_k^t \) at time \( t \in [cS : cS + T] \) is derived by

\[
H_k^t = \text{RNN}(x_k^c, H_k^{t-1}) \tag{9}
\]

where \( W_1, W_2 \) are the graph convolution weights and history information weights, respectively. \( W_3 \) is used to improve the expression ability of condition representations. The time encoding and spatio-temporal conditions of \( x_k^c \) are obtained as \( H_k^t = \text{Concat}(H_k^t, H_k^{S+T-1}) \) and \( C_k^c = \text{Concat}(C_k^c, C_k^{S+T-1}) \) respectively, where \( \text{Concat}(.) \) denotes the concatenation operation.

4.5 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 will be largely limited and the unique inherent property of each individual entity will be ignored. Therefore, we design the entity-aware normalizing flow \( z_k = f_k(x|C) \) to make more detailed density estimation, where \( x, C, k \) 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 above target distribution is the identity matrix \( I \) for the better convergence. Moreover, in order to generate different target distributions \( Z_k \), we independently draw mean vectors \( \mu_k \in \mathcal{R}^T \) from \( N(0, I) \). 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

\[
P_{X_k}(x_k) = P_{Z_k}(f_{\theta}^k(x_k|C)) \left| \det \frac{\partial f_{\theta}^k}{\partial x_k} \right| Z_k = N(\mu_k, I)
\]

where each element of \(\mu_k\) is the same, and is drawn from the \(N(0, 1)\).

In such 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

\[
P_{X_k}(x_k) = P_{Z_k}(f_{\theta}(x_k|C)) \left| \det \frac{\partial f_{\theta}}{\partial x_k^T} \right|
\]

4.6 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 spatiotemporal conditions are utilized to contribute to entity-aware normalizing flow accurately estimating density of time series. To avoid getting stuck in local optimum for each module of MTGFlow, we jointly optimize all modules for overall performance of MTGFlow. The whole parameters \(W^*\) are estimated via maximum log likelihood.

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

\[
\approx \arg \max_W \frac{1}{N} \sum_{c=1}^{N} \sum_{k=1}^{K} \log(P_{X_k}(x_k^c))
\]

\[
\approx \arg \max_W \frac{1}{NK} \sum_{c=1}^{N} \sum_{k=1}^{K} \left[ \log(P_{Z_k}(f_{\theta}^k(x_k^c|C_k^c))) \left| \det \frac{\partial f_{\theta}^k}{\partial x_k^c} \right| \right]
\]

\[
\approx \arg \max_W \frac{1}{NK} \sum_{c=1}^{N} \sum_{k=1}^{K} \left[ \frac{1}{2} \| x_k^c - \mu_k \|_2^2 + \log \left| \det \frac{\partial f_{\theta}^k}{\partial x_k^c} \right| + \text{const} \right]
\]

where \(N\) is the total number of windows, and \(\text{const}_{\text{is a constant, equal to}} -\frac{T}{2} \ast \log(2\pi)\).

4.7 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. Taking this advantage, we further extend the above procedure to anomaly detection application and the corresponding interpretation function.

4.7.1 Anomaly detection. Taking the window sequence \(x_k^C\) 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:

\[
S_c = -\frac{1}{K} \sum_{k=1}^{K} \log(P_{X_k}(x_k^C))
\]

A higher anomaly score represents that \(x_k^C\) locates in the lower density region, indicating a higher possibility to be abnormal. Since abnormal series exist in training set and validation set, we cannot directly set the threshold to label the anomaly, such as the maximum deviation in validation data [6]. 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 anomaly threshold.

\[
\text{Threshold} = Q_3 + 1.5 \ast (Q_3 - Q_1)
\]

where \(Q_1\) and \(Q_3\) are 25th percentile and the 75th percentile of \(S_c\).

4.7.2 Anomaly interpretation. Abnormal behaviors of any entity could lead to the overall abnormal behaviour of the whole window sequence. Naturally, we can get the entity anomaly score \(S_{ck}\) for entity \(k\) according to Eq. 13

\[
S_c = -\frac{1}{K} \sum_{k=1}^{K} \log(P_{X_k}(x_k^C)) = \sum_{k=1}^{K} S_{ck}
\]

However, we map time series of each entity into unique target distributions, and different ranges of \(S_{ck}\) are observed. This bias will bring each entity plays different weights in contributing to \(S_c\), which we do not hope. To circumvent the above unexpected bias, we design the entity-specific threshold for each entity. IQR is used to set the respective thresholds, considering different scales of \(S_{ck}\). Therefore, the threshold for \(S_{ck}\) is given by

\[
\text{Threshold}_{ck} = \lambda_k (Q_{ck}^3 + 1.5 \ast (Q_{ck}^3 - Q_{ck}^1))
\]

where \(Q_{ck}^1\) and \(Q_{ck}^3\) are 25th percentile and the 75th percentile of \(S_{ck}\) across all observations, respectively. And \(\lambda_k\) adjusts the \(\text{Threshold}_{ck}\) because normal observations of entities also fluctuate with different scales. Moreover, it is possible for an anomaly \(A_i\) to arise from a group of entities (a group anomaly) or just arise from a single anomaly (a point anomaly). To detect the type of the anomaly, we can list the possible causes \(P_i^k\) at \(A_i\):

\[
P_i^k = S_{ck} - \text{Threshold}_{ck} \quad \text{for} \quad i, k \in S_{ck} \quad > \text{Threshold}_{ck}
\]

where \(S_{ck}^i\) represents the \(S_{ck}\) at \(A_i\). It is assumed that the location at root cause suffers from larger deviation \(P_i^k\). Therefore, according to the distribution of \(P_i^k\), we can tell if a detected anomaly is a group anomaly or a point anomaly.

5 EXPERIMENT

5.1 Experiment Setup

5.1.1 Dataset. The commonly used public datasets for multivariate time series anomaly detection in OCC are SMAP (Soil Moisture Active Passive satellite) [14], MSL (Mars Science Laboratory rover) [14], SMD (Server Machine Dataset) [26], SWaT (Secure Water Treatment) [8] and WADI (Water Distribution). However, the collected time series in SMAP and MSL do not have the same time span and different servers that generate time sequence in SMD are independent. Thereby, it will be inappropriate to employ these three datasets for our comparisons. In the most related previous work GANF [5], SWaT and two private datasets is utilized. Following their setup, we use two public datasets SWaT and WADI in our experiments.

SWaT collects 51 sensor data from a real-world industrial water treatment plant, at the frequency of one second. The dataset provides ground truths of 41 attacks launched during 4 days. WADI collects 121 sensor and actuators data from WADI testbed, at the frequency of one second. The dataset provides ground truths of 15 attacks launched during 2 days. Since only normal time series are
Table 1: The settings of SWaT and WADI.

| Dataset | Entity | Training/Test set | Anomaly ratio (%) |
|---------|--------|-------------------|-------------------|
| SWaT    | 51     | 269951/89984      | 17.7/5.2          |
| WADI    | 123    | 103680/69121      | 6.4/4.6           |

provided in these two datasets for training in OCC setting, we split the original testing dataset by 60% for training, 20% for validation, and 20% for testing in SWaT. As for WADI, the training split contains 60% data, and the test split contains 40% data. The specific statistics are listed in Table 1.

5.1.2 Implementation details. For both datasets, we set the window size as 60 and the stride size as 10. Adam optimizer with learning rate 0.002 is utilized to update all parameters. 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, we use one flow block and set the batch size as 512. WADI has about twice as many entities as SWaT, 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.

5.1.3 Evaluation metric. Following the same setting as the previous works, MTGFlow aims to detect the window-level anomalies. And, the window label is annotated as abnormal when there exists an anomalous time point within the corresponding time duration. We evaluate the performance of MTGFlow on SWaT and WADI by the Area Under the Receiver Operating Characteristic curve (AUROC).

5.1.4 Baselines. We compare the SOTA semi-supervised and unsupervised density estimation methods.

- DeepSAD [22]. A semi-supervised method maps normal data into preset hypersphere, and additional anomaly labels are leveraged to improve the detection performance.
- DeepSVDD [21]. An OCC method, maps normal data into preset hypersphere, and anomaly data are assumed to be located outside the hypersphere.
- ALOCC [23]. An OCC method, reconstructs inputs via GAN, and declares anomalies according to the output of the discriminator.
- DROCC [10]. An OCC method, constructs robust representations for normal data. Anomalies will deviate the learned representations.
- USAD [2]. An OCC method, leverages autoencoder to reconstruct inputs. Anomaly data suffer poor reconstruction quality.
- DAGMM [35]. A density estimation approach, combines autoencoder and Gaussian Mixture Model (GMM), the samples with high energy are declared as anomalies.
- GANF [5]. The density estimation approach joints DAG and flow model, and data on low density regions are identified as anomalies.

5.2 Performance

As shown in Table 1, SWaT and WADI have the high and low anomaly ratio, respectively. We test MTGFlow in these two datasets to present the performance.
extracted. Profiting from these, MTGFlow accomplishes 84.8% AUROC, outperforming the above mentioned methods. Moreover, we study log likelihoods for anomalies ranging from 2016/1/2 11:07:00 to 11:57:00 in Fig. 3. It is clear that log likelihoods are high for the normal series but lower for labeled abnormal ones (highlight 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 $S_x$ for MTGFlow and GANF in Fig. 4. As displayed in Fig. 4, 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 anomaly score discrepancy corroborates MTGFlow superior anomaly detection performance.

5.2.2 Performance on WADI. In the low anomaly ratio scenario, MTGFlow also has a consistently good performance. We show the results in Table 2, where MTGFlow outperforms all other compared methods. However, compared with the substantial advancement in SWaT experiments, MTGFlow achieve a smaller superiority in WADI. From the ROC curves of Fig. 2b, it can be seen that when false positive ration (FPR) is lower than 0.2, there is no obvious difference in the ROC curves. We analyze this phenomenon from AUROC mechanism. When FPR is low, the corresponding anomaly threshold is high. That means time series are all judged to be normal expect for the most obvious anomalies. And coupled with the low anomaly rate, above mentioned drawback of OOC setting is easier to hide, which cannot reflect the true detection ability. Hence, this leads the similar true positive ratio when FPR is below 0.2. With FPR increasing (i.e the threshold is decreasing), more accurate boundary makes TPR of MTGFlow rise rapidly. Conversely, other methods suffer from the unclear boundary between abnormal and normal series and causes slow increase in TPR, thereby widening the anomaly detection performance gap with MTGFlow.

5.3 Ablation Study

5.3.1 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 without graph as MTGFlow/G, and MTGFlow only without entity-aware normalizing flow as MTGFlow/E. The results are presented in Table 3, where MTGFlow/(G, E) obtains the worst performance. It is attributed to the lack of relational modeling among entities and the indistinguishable density estimation. Applying graph structure learning in model pairwise relations, MTGFlow/E achieves better performance. Also, considering more fine-grained density estimation, MTGFlow/G achieves an improvement over MTGFlow/(G, E). Integrating these two modules, MTGFlow accomplishes the best performance, which demonstrates the effective design of MTGFlow.

5.3.2 Hyperparameter robustness. We conduct a comprehensive study for the choice of the hyperparameters, the results are shown in Table 4. Concretely, we conduct experiments with various sizes for the sliding window and three different numbers for the normalizing flow blocks in Table 4. In SWaT, when window size is small, such as 40, 60, and 80, the increase in the number of blocks does not necessarily improve anomaly detection performance. Larger model causes the overfitting to the normal distribution where the abnormal series present in areas of high density. When the window size is large (i.e., 80, 100, and 120), distribution to be estimated is more

| Table 2: Performance of AUROC(%) on SWaT and WADI. |
|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| Dataset       | DeepSVDD      | ALOCC         | DROCC         | DeepSAD       | USAD          | DAGMM         | GANF          | MTGFlow       |
| SWaT          | 66.8±2.0      | 77.1±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      | 83.3±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**  |

| Table 3: Module ablation study (AUROC%). |
|-----------------------------------------|
| Graph Entity-aware | 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 4: Ablation study of hyperparameters (AUROC%). |
|-----------------------------------------|
| Blocks | Window size | 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±2.0 | 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±0.8 | 91.7±0.7 |
| 100   | 89.6±1.1    | 90.9±0.8 | 91.8±0.6 |
| 120   | 88.6±1.4    | 91.0±0.6 | 91.5±0.9 |

Figure 5: Effect of anomaly contamination ratio.
high-dimensional so that model needs more capacity. Therefore, detection performance derives average gain with blocks increasing due to more accurate distribution modeling. The analysis can also be applied to WADI dataset. According to the experimental results, 60 for window size and 1 normalizing flow block, and 60 for window size and 2 normalizing flow blocks are the best parameters of MTGFlow on SWaT and WADI, achieving 84.8%, 91.9% AUROC anomaly detection performance, respectively.

5.3.3 Anomaly ratio analysis. To further investigate the influence of anomaly contamination rates, we vary training splits to adjust anomalous contamination rates. The training split increases from 60% to 80% with 5% stride, and the corresponding anomaly ratios are 17.7%, 16.7%, 15.7%, 14.6%, and 13.9%, respectively. The test split is 20%. We present an average result over five runs on SWaT in Fig. 5. Although anomaly contamination ratio of training dataset rises, anomaly detection performance of MTGFlow remains at a stable high level, ranging from 84.2% to 84.9%. The robustness to anomaly contamination again confirms the advantage of MTGFlow, using density estimation to detect an anomaly.

5.4 Result Analysis
In order to further investigate the effectiveness of MTGFlow, we analyze the obtained results from different aspects on SWaT.

5.4.1 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 is set for the adjacency matrix to show an intuitive learned graph structure in test split. In Fig. 6, 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. Graph structure at 2016/1/1 14:00:00 is centered on sensor P201, while the edges in the graph have completely changed and the center has shifted from P201 to AIT503 at 2016/1/2 7:00:00. This alteration of graph structure may result from changing in working condition of water treatment plant. Therefore, it is necessary to use a dynamic graph to model such changeable interdependencies. 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 main pairwise relations (thick arrow) at 2016/1/1 14:00:00 is similar as the relations at 2016/1/2 14:00:00, which both centered on P201. It indicates that the interdependencies on multiple sensors is periodic. We also find mutual interdependencies from learned graph structures, such as the edges between P201 and AIT201 at 2016/1/2 13:00:00 and 2016/1/2 14:00:00. Furthermore, we compare the normalized anomaly score distributions of MTGFlow and MTGFlow/G in Fig. 7 for further analysis of the effectiveness of dynamic graph structure on anomaly detection. Such a dynamic graph design can push anomaly scores of normal series to 0 and enlarge the margin between normal and abnormal series. We summarize the findings: (1) Dynamic interdependencies among multiple entities. (2) Consistent interdependencies among multiple entities. (3) Periodic interdependencies among multiple entities. (4) Mutual interdependencies among multiple entities.

5.4.2 Entity-specific density estimation. We further explore whether distributions of all entities are transformed into different target distributions to verify our entity-aware design. Since the window size is 60, the corresponding transformed distributions are also 60 dimensional distributions. Each single dimension of the multivariate Gaussian distribution is a Gaussian distribution. For a better visualization, we present the 0th dimension of the transformed distributions in Fig. 8. Nine distributions of different entities are displayed. It can be seen that these distributions have been projected as unique distributions. Moreover, these distributions are successfully converted to preset Gaussian distributions with different mean vectors. The one-to-one mapping models entity-specific distributions and captures their respective sparse characteristics of anomalies. Fig. 9 shows the normalized anomaly score distribution for normal and abnormal series. We observe that the margin between normal and abnormal samples in MTGFlow is larger than that in MTGFlow/E. This demonstrates that MTGFlow amplifies the discrepancy between normal and abnormal samples with the help of the entity-specific density estimation.

5.4.3 Distinct sparse characteristics. To demonstrate the sparse characteristics vary with different entities, we study changes of $S_{ck}$ along time on SWaT. As shown in Fig. 10, $S_{301}$ of AIT201, AIT502, P102, FIT502, 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 $A_5$, alongside the time sequence. It can be observed that AIT201 and AIT502 have obvious fluctuations at $A_4$, while P102 reacts to $A_2$. Also, $P_{403}$ is sensitive to $A_2$ and $A_4$. FIT502 is sensitive to $A_4$ and $A_5$, yet LIT310 is sensitive to $A_2$, $A_3$, $A_4$, and $A_5$. According to the above results, we validate that different entities present the discrepancy of sparse characteristic.

5.4.4 Anomaly interpretation. MTGFlow can also provide the explanation of the detected anomaly via the deviations of their respective $S_{ck}$, and tell it is a group anomaly or point anomaly. From Fig. 10, the blue lines are the corresponding thresholds set according to Eq. 16, which considers different scales of individual entities. The value exceeding the thresholds is labeled an abnormal behaviors. In order to further localize the declared anomaly, $P$ is obtained according to Eq. 17 for all the above mentioned anomalies in Fig. 11. For $A_1$, $P_{301}^1$ and $P_{403}^1$ are positive and close, so we tend to declare $A_1$ is a group anomaly occurring at P102 and P403. Aiming at $A_2$, we can observe $P_{301}^2$ is much higher than $P_{403}^2$ and $P_{502}^2$, in this case the root cause of $A_2$ is believed that P102 is attacked, and causes the unusual behaviors of P102 and LIT301. The same analysis can be applied to $A_3$, $A_4$, and $A_5$.

6 CONCLUSION
In this work, we proposed MTGFlow, an unsupervised anomaly detection approach for multivariate time series based on the dataset with absolute zero known labels. Extensive experiments on the real-world datasets demonstrate its superiority, even if there exists high anomaly contamination. MTGFlow achieves 84.8% AUROC on SWaT and 91.9% AUROC on WADI, outperforming SOTA anomaly detection performance, respectively.
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 existing among 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 apply our model to more flow models and further improve the practicality of our approach.
Figure 10: Variation of Log likelihoods for different entities on the whole testing dataset. Anomaly ground truths are presented as red boxes.

Figure 11: Visualization of the possible causes $P$. 

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