**ORIGINAL ARTICLE**



# **Uni‑directional graph structure learning‑based multivariate time series anomaly detection with dynamic prior knowledge**

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## **Abstract**

In the Internet of Things (IoT) system, sensors generate a vast amount of multivariate time series data and transmit it to the data center for aggregation and analysis. However, due to equipment failure or attacks, the collected data may contain anomalies, which in turn afect the overall performance and reliability of IoT services. Therefore, an efective multivariate time series anomaly detection (MTSAD) method is a crucial issue to ensure the quality of service. Graph structure learning (GSL)-based methods become a promising technology in MTSAD, which learns an optimal graph structure joint with the anomaly detection task. However, most existing methods disregard the causal and dynamic relationships between sensors during the processing of IoT and assume that the data is devoid of any missing values. Therefore, we propose a uni-direction graph structure learning-based multivariate time-series anomaly detection with dynamic prior knowledge (DPGLAD), which learns the uni-directional relationships between sensors under the constraint of the dynamic prior graph and utilizes difusion convolutional recurrent neural networks (DCRNN) based on timestamp mask to extract temporal and spatial features. Extensive experiments show that our method has better detection performance and shorter training times than state-of-the-art techniques on four real-world datasets. Compared with the best GSL-based method GTA, DPGLAD achieves 4.16–7.29% more F1-score.

**Keywords** Multivariate time series · Anomaly detection · Graph structure learning · Graph neural network · Dynamic prior graph · Uni-directional graph structure

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# **1 Introduction**

In the Internet of Things (IoT) system, sensors generate large amounts of time series data [\[8\]](#page-15-0). Anomalies in the data may indicate device malfunctioning or system attacks. If the anomalies are not detected in time, they may result in economic losses [[9,](#page-15-1) [26](#page-16-0)]. Thus, anomaly detection plays an important role in IoT systems. In real applications, multivari-ate indicators.<sup>[1](#page-0-0)</sup> are collected to reflect the overall status of a system [[7,](#page-15-2) [16](#page-16-1)] A multivariate time series (MTS) example from an industrial IoT system is presented in Fig. [1](#page-1-0), which includes data from seven diferent sensors installed in a tap water treatment system. These sensors are Flow meter *FIT*101, level transmitter *LIT*101, motorized valve *MV*101, sump pump *P*101, backup sump pump *P*102, conductivity analyzer *AIT*201, and pH analyzer *AIT*202.

<span id="page-0-0"></span>Various indicators afliated with the same system interrelate with each other, making it so that a sudden shift in several indicators may not be indicative of system failure.

Aberdeen AB24 3FX, UK <sup>1</sup> Here, "indicator" refers to the time series of a particular variable.



<span id="page-1-0"></span>**Fig. 1** A multivariate time series example of an industrial IoT system that showcases both normal (represented by green) and abnormal (represented by red) values

As shown in Fig. [1,](#page-1-0) despite the occurrence of a sudden decline in *P*101, *P*102, and *AIT*201 during the green segment, the system remains in a healthy status. This is due to the consistent trend of these three indicators. In contrast, the red segment shows an inconsistent pattern in *MV*101 compared to all other indicators, indicating system malfunction. Therefore, in the realm of multivariate time series anomaly detection (MTSAD), it is crucial to discover the presence of potential dependencies among the indicators [\[8](#page-15-0)].

Recently, graph neural networks (GNNs) [[22](#page-16-2), [23](#page-16-3)], especially spatio-temporal graph neural networks have garnered signifcant attention due to their ability to model inter-indicator relationships with satisfactory results. However, most GNNs [\[6](#page-15-3), [28\]](#page-16-4) presuppose an explicit graph structure or treat the graph structure as a complete graph. In real-world settings, the graph structure may be unavailable, rendering the inter-dependencies between sensors unknown.

To handle unknown graph structure, MTSAD grounded in Graph Structure Learning (GSL) [[2,](#page-15-4) [3,](#page-15-5) [5\]](#page-15-6). It is a promising method that efectively acquires knowledge about the concealed graph structure in conjunction with the downstream GNNs task. Figure [2](#page-1-1) visually illustrates the typical GSL-based anomaly detection method process. The graph structure learner generates a graph structure. This graph structure is then fed into the detection model, leading to a joint update of parameters in both the detection model and the graph structure learner. In this way, the graph structure is iteratively refned. This iterative parameter update scheme can obtain a more optimal graph structure that aligns with the requirements of the downstream anomaly detection task.

Nonetheless, the graph structure learning-based anomaly detection method still confronts numerous challenges.

• **Most of the present graph structure learning-based MTSAD** [[3,](#page-15-5) [5\]](#page-15-6) **method only captures undirected** 



<span id="page-1-1"></span>**Fig. 2** A general framework of Graph Structure Learning-based anomaly detection

**dependencies, leaving uni-directional dependencies unaccounted for. The existing uni-directional graph structure** [\[2](#page-15-4)] **learning-based MTSAD method has considerable overhead.** Several anomaly detection based on graph structure learning calculate node similarity to construct an undirected graph. However, there is a special processing of IoT. The upstream status decides the downstream operation. The downstream sensor depends on the upstream sensor. The relationship between sensors is uni-directional. Although Graph Learning with Transformer for Anomaly detection (GTA) [[2](#page-15-4)] employs a fully parameterized graph learning method to obtain uni-directional graphs, the training time required is too lengthy and inefficient. Therefore, an efficient graph structure learning method is needed to extract the one-way dependence between sensors.

- **The static nature of the prior graph limits its ability to represent the dynamic relationship between sensors.** To improve the quality of learned graph structure, prior information is often provided by a prior graph. Existing methods utilize all raw data as input to obtain the *K* nearest neighbor (KNN) graph as prior knowledge, which is a static graph. However, the relationship between sensors changes over time. Using only a static prior graph can not adapt to varying data features and task requirements.
- **The existing methods are susceptible to data with missing values.** In current works, it is commonly assumed that training data is entirely normal and devoid of any missing values [[11](#page-16-5)]. However, in the real world, collected data often contain missing values, especially when dealing with large volumes of data.

To address the three challenges, we explore a uni-direction graph structure learning-based multivariate time series anomaly detection with dynamic prior knowledge (DPGLAD), which utilizes uni-directional graph structure learning to model relationships between sensors under the constraint of the dynamic prior graph, and difusion convolutional recurrent neural networks (DCRNN) based on timestamp mask to extract temporal and spatial features. Our major contributions can be summarized as follows:



<span id="page-2-2"></span>**Fig. 3 Left**: The frst two processes of Secure Water Treatment (SWAT) [[4](#page-15-8)] testbed. **Right**: The abstract relationships between sensors

- To mine one-way dependencies between sensors at a low cost, we utilize a lightweight uni-directional graph structure (UGL) learning method. UGL learns two embedding vectors for each sensor to represent the source node and destination node of the edge, respectively, instead of one embedding vector or one feature vector.
- To improve the quality of the learning graph, we propose a dynamic prior graph generation to obtain a dynamic prior graph changing over time instead of a static prior graph, which provides accurate prior information and adapts to varying data features and task requirements.
- To effectively handle data with missing values, we propose a timestamp mask-based difusion convolutional recurrent neural network (DCRNN) to actively mask some values and robustly predict the next value of the time series. The prediction error is exploited to detect anomalies.
- Extensive experiments conducted on four public and realworld datasets show that our method has better detection performance and shorter training times than state-ofthe-art techniques. Compared with the best GSL-based method GTA, DPGLAD achieves 4.16–7.29% more F1-score.

The subsequent sections of this paper are organized as follows. Section [2](#page-2-0) explains the background for our work. Section [3](#page-2-1) presents an overview of the related work. Section [4](#page-3-0) provides a presentation of the problem description and the preliminaries. Section [5](#page-4-0) provides a comprehensive explanation of DPGLAD, including both a general overview and a step-by-step guide. In Sect. [6,](#page-8-0) we conduct experiments to evaluate the performance and efficiency of the model. Finally, our work is concluded in Sect. [7.](#page-14-0)

# <span id="page-2-0"></span>**2 Background**

In this section, we take an example to display the one-way dependence between sensors. An illustration of the frst two processes in the Safe Water Treatment (SWAT) testbed is shown in the left of Fig. [3](#page-2-2). In process 1, the water level sensor (LIT101) in the tank has a causal effect on the pump control system (P101). When the water level in the tank drops below a certain threshold, it triggers the pump control system to activate and start pumping water for further treatment. Similarly, in process 2, the chemical dosing system (P201, P203, P205) is infuenced by the data from the water quality sensor (FIT201, AIT201). Once the water quality meets the required standards, the addition of chemicals will be ceased.

In this simplifed illustration, it is evident that the processes have a uni-directional infuence on each other, indicating the presence of a uni-directional relationship among the sensors. We can obtain a uni-directional graph for these sensors as shown in the right of Fig. [3](#page-2-2).

# <span id="page-2-1"></span>**3 Related work**

In this section, we review anomaly detection methods based on temporal feature, graph neural networks, and graph structure learning.

# **3.1 Temporal feature‑based anomaly detection methods**

The recurrent neural networks (RNNs) and their variants are prevalent in MTSAD due to their natural aptitude for handling time series data. LSTM-NDT [\[10\]](#page-15-7) utilizes Long Short-Term Memory (LSTM) to learn the temporal features and generate predictions. It collects the error between predicted and actual values to form an error vector, which is exponentially averaged and weighted to compute a threshold for anomaly detection. In addition, various combined models of recurrent neural networks and generative models are employed in MTSAD for reconstructing time series. For instance, Omnianomaly [\[20](#page-16-6)] employs a stochastic recurrent neural network to efectively capture and represent normal patterns, thereby facilitating the reconstruction of the observed data. DAGMM [[29\]](#page-16-7) trains both deep autoencoder and Gaussian mixture models to produce reconstruction errors for detecting anomalies. MAD-GAN [[12](#page-16-8)] employs LSTM to establish a Generative Adversarial Network (GAN) framework that efectively captures the temporal correlation of time series distributions, and identifes anomalies through discrimination and reconstruction processes. USAD [[1\]](#page-15-9) adversarially trains an encoder-decoder framework to achieve fast and efficient training. LSTM-VAE  $[17]$  $[17]$  $[17]$  maps multimodal observations and temporal dependencies' relations to the latent space and reconstructs the expected distribution. MSCRED [[25](#page-16-10)] combines convolutional layers, LSTM layers, and attention mechanisms to construct the Encoder, thus increasing the network's ftting capability.

Although RNNs have shown promising results in modeling the temporal dependence of time series data in the temporal dimension, they cannot directly capture the correlations between sensors.

### **3.2 Graph‑based anomaly detection methods**

The effectiveness of graph attention networks in predicting temporal dependencies and modeling correlations between sensors has been demonstrated in recent studies. For instance, MTAD-TF [[6](#page-15-3)] employs multi-scale convolution and graph attention networks to capture the feature in temporal patterns. MTAD-GAT [[28\]](#page-16-4) uses two parallel graph attention layers to model correlations between indicators. Arvalus and its variant D-Arvalus [[18](#page-16-11)] employs system deployment meta-information to construct a graph structure and introduces a new graph convolution (GC) technique to model correlations between indicators.

Although graph neural networks-based anomaly detection methods have shown promising results in modeling correlations between indicators, they still have some limitations. For instance, the Arvalus and its variant D-Arvalus [\[18\]](#page-16-11) assume that there is a known graph structure predefned by domain knowledge. This assumption limits their generality and makes them sensitive to graph predefnition [[27\]](#page-16-12). On the other hand, MTAD-TF [[6\]](#page-15-3) and MTAD-GAT [[28](#page-16-4)] treat the relationship between indicators as a complete graph, which increases computational overhead.

# **3.3 Graph structure learning‑based anomaly detection methods**

To handle multivariate time series without a comprehensive real graph structure, GSL-based anomaly detection methods emerged. For instance, GDN [[3\]](#page-15-5) constructs a KNN graph by the similarity between the learned node embedding vectors. The learned graph structure is then fed into a graph attention neural network to extract dependencies between indicators and predict future behavior, where the prediction error is used to calculate the anomaly score. Similarly, FuSAGNet [[5\]](#page-15-6) partitions sensors based on their functions within a particular process and recursively encodes a group of sensors in the same process to construct a KNN graph. GTA [[2\]](#page-15-4) considers the elements of the adjacency matrix as learnable parameters and automatically learns the graph structure using a Transformer-based architecture to model temporal dependencies.

The graph structure obtained by pair-wise similarity, as with the GDN [[3\]](#page-15-5) and FuSAGNet [[5\]](#page-15-6), is undirected, which can not refect the unidirectional dependencies between sensors. Although GTA [\[2](#page-15-4)] can obtain a uni-directional graph, the fully parametric learning method is complicated and has low training efficiency. Therefore, an efficient uni-directional graph structure learning method is necessary for MTSAD.

Compared with graph-based spatial and temporal learning, we use graph learning techniques rather than a predefned graph structure based on expert experience. Compared with previous temporal graph structural learning technique, we learn a uni-directional graph to model one-way relationships between sensors.

# <span id="page-3-0"></span>**4 Problem defnition and preliminaries**

### **4.1 Problem defnition**

Multivariate time series data comprises a substantial amount of regularly spaced sampling and uninterrupted observation points, characterized by *K* indicators and *N* timestamps, which can be denoted by  $X = (x_1, x_2, \dots, x_N)^T \in R^{K \times N}$ . The *i*-th indicator can be represented by  $x^i = (x^i_1, x^i_2, ..., x^i_N)$ . The *t*-th timestamp contains *K* values of indicators, which is denoted by  $x_t = (x_t^1, x_t^2, \dots, x_t^k)^T$ . Define the historical time series window of length  $\omega$  at time  $t$  as subsequence  $X_t = (\mathbf{x}_{t-\omega}, \mathbf{x}_{t-\omega+1}, \dots, \mathbf{x}_{t-1})^T \in R^{K \times \omega}$ . When  $\mathbf{x}_t$  is considered abnormal, the label  $y_t$  is set to 1.

Multivariate time series anomaly detection aims to identify whether the timestamp  $(x_t)$  is anomalous. According to the historical time series  $X_t$ , it predicts the value of timestamp *t*, and the diference between the prediction and the ground truth is taken as an anomaly score to identify the anomaly. The process is formulated as follows:

$$
\hat{x}_t = f(X_t) \tag{1}
$$

$$
s(t) = \varphi\big(x_t, \hat{x}_t\big) \tag{2}
$$

$$
\hat{y}_t = \begin{cases} 1, & \text{if } s(t) > T \\ 0, & \text{if } s(t) \le T \end{cases}
$$
\n(3)

where  $\hat{x}$ <sup>*t*</sup></sup> is the predicted value of timestamp *t*, *s*(*t*) is the anomaly score of timestamp *t*, and *T* is the threshold. When the anomaly score  $s_t$  exceeds the threshold  $T$ , an anomaly is considered to have occurred at timestamp *t*.

#### **4.2 Anti‑symmetric matrix**

A matrix *A* is said to be an *anti-symmetric matrix* if it satisfes the following conditions:

- *A* is a square matrix, meaning it has an equal number of rows and columns.
- For each element  $A_{i,j}$  in matrix  $A$ , it holds that  $A_{i,j} = -A_{j,i}$ , i.e.,  $A^T = -A$ .

The anti-symmetric matrix is exploited to implement unidirectional graph learning.

#### **4.3 Graph structure learning**

Given the time series  $X \in R^{K \times N}$ , the purpose of the graph structure learning is to obtain a graph  $G = (V, E)$  and its graph topology or adjacency matrix  $A \in \mathbb{R}^{K \times K}$ . The node *v* in the graph is a sensor that produces an indicator, and the hidden relationship between the sensors is considered the edge *E*. The adjacency matrix *A* stores the edge information in the graph, which refects the underlying dependencies among indicators. The elements in the adjacency matrix are composed of 0 and 1.  $A_{i,j}$  is 1, which represents an edge between node *i* and node *j*. On the contrary, there is no edge between node *i* and node *j*, when  $A_{i,j} = 0$  [\[15](#page-16-13), [21](#page-16-14), [30](#page-16-15)].

If a graph is directed, its adjacency matrix satisfes that if  $A_{i,j}$  equals 1, then  $A_{j,i}$  must be 0.

# <span id="page-4-0"></span>**5 Our proposed methodology**

This section provides a comprehensive explanation of our proposed approach. The notation used in this section is described in Table [1.](#page-4-1)

# **5.1 Overview**

Complex topological relationships often exist among monitored indicators in real-world scenarios, which can

<span id="page-4-1"></span>**Table 1** List of notations

Notation	Meaning Multivariate time series		
X			
$X_t$	historical time series window of length $\omega$ at time t		
$\sim$ $X_t$	The masked historical time series		
$\mathbf{x}^i$	The <i>i</i> -th indicator values		
$\boldsymbol{x}_t$	The indicator values at timestamp t		
$T_f()$	The masking transformation		
$\hat{x}$	The prediction		
K	The number of indicators		
N	The number of timestamps		
$y_t$	The label of timestamp t		
G	Graph		
$\overline{A}$	Adjacency matrix		
$\theta$	Prior adjacency matrix		
$V_i^{(t)}$	The feature vector of sensor $i$ at timestamp $t$		
$E_1$	The source embedding vector		
$E_{2}$	The destination embedding vector		
$Err_i(t)$	The prediction error at timestamp $t$ for sensor $i$		
s(t)	Anomlay scores		

be represented as a graph. In this graph, each indicator is regarded as a node, while the relationships between them are represented by edges connecting the nodes. Most previous methods [\[3,](#page-15-5) [5\]](#page-15-6) learn an undirected graph that cannot represent one-way dependencies between sensors. Although GTA [[2](#page-15-4)] uses a direct method to obtain a uni-directional graph, the GTA method is inefficient. Therefore, we propose a uni-directional Graph Structure Learning-based Multivariate Time Series Anomaly Detection with Dynamic Prior Knowledge. Figure [4](#page-5-0) illustrates the framework for our method. Essentially, our method comprises four key components:

- **Uni-directional graph structure learner:** To mine oneway dependencies between sensors at a low cost, we construct a uni-directional graph using the antisymmetric matrix with the ReLu function.
- **Dynamic prior graph generator:** To improve the quality of the learning graph, we utilize a dynamic prior graph to provide dynamic prior information for learning graph.
- **DCRNN predictor based on timestamp mask:** To efectively handle data with missing values, we utilize the timestamp masking mechanism to eases the impact of missing values in the raw data. The time series is masked and then fed into DCRNN with the uni-directional graph to predict future values for each sensor.
- **Anomaly score calculation:** After the predictor is trained, the prediction error is used to calculate the anomaly score.



<span id="page-5-0"></span>**Fig. 4** The DPGLAD framework comprises four main modules. The frst module, depicted in gold, models the inter-indicator relationships. The second module, depicted in cyan, is responsible for generating a dynamic prior graph that provides prior information to the

graph structure learner. The third module, shown in grey, utilizes a timestamp mask-based DCRNN predictor to generate accurate predictions of indicators. The last module, shown in lilac, perform anomaly score calculation. Loss functions are highlighted in red

#### **5.2 Uni‑directional graph structure learner**

Many of the current graph structure learning-based anomaly detection methods  $[3, 5]$  $[3, 5]$  $[3, 5]$  $[3, 5]$  depend on node similarity metrics to construct the graph structure. Consequently, the graph structure is undirected and the relationship between nodes is symmetrical. However, there are uni-directional relationships between nodes.

Our uni-directional graph structure learner is specially tailored to identify and extract one-way dependencies. It is implemented by a source node embedding vector and a target node embedding vector as follows:

$$
M_1 = \tanh\left(\alpha E_1 \beta_1\right) \tag{4}
$$

$$
M_2 = \tanh\left(\alpha E_2 \beta_2\right) \tag{5}
$$

<span id="page-5-1"></span>
$$
A = \text{ReLU}\left(\tanh\left(\alpha \left(M_1 M_2^T - M_2 M_1^T\right)\right)\right) \tag{6}
$$

where  $E_1$  and  $E_2$  represent the source and target node embedding vectors, respectively,  $\beta_1$ ,  $\beta_2$  are the model parameters, and the activation function's saturation rate is symbolized by  $\alpha$ .  $E_1$  and  $E_2$  are initialized as random, which are updated by the backpropagation of graph learning loss. Subtraction operation  $(M_1M_2^T - M_2M_1^T)$  in Eq. [\(6](#page-5-1)) can construct an antisymmetric matrix according to Eq. [\(7\)](#page-6-0). In an anti-symmetric matrix *A*, the value of  $A_{j,i}$  equals  $-A_{i,j}$ .

$$
\begin{pmatrix} 5 & 3 & 2 \ 7 & 1 & 3 \ 6 & 3 & 2 \end{pmatrix} \bullet \begin{pmatrix} 2 & 3 & 3 \ 4 & 6 & 7 \ 2 & 1 & 2 \end{pmatrix} = \begin{pmatrix} 26 & 35 & 40 \ 24 & 30 & 34 \ 28 & 38 & 43 \end{pmatrix}
$$
  
\n
$$
M_1 \bullet M_2^T \qquad M_1 \bullet M_2^T \qquad \bullet M_1^T \bullet M_2^T \qquad \bullet M_1^T \qquad \bullet M_2^T \bullet M_1^T
$$
  
\n
$$
\begin{pmatrix} 2 & 4 & 2 \ 3 & 6 & 1 \ 3 & 7 & 2 \end{pmatrix} \bullet \begin{pmatrix} 5 & 7 & 6 \ 3 & 1 & 3 \ 2 & 3 & 2 \end{pmatrix} = \begin{pmatrix} 26 & 24 & 28 \ 35 & 30 & 38 \ 40 & 34 & 43 \end{pmatrix} M_1 \bullet M_2^T - M_2 \bullet M_1^T
$$
  
\n
$$
M_2 \bullet M_1^T \qquad M_2 \bullet M_1^T
$$

<span id="page-6-1"></span>**Fig. 5** The process of constructing a uni-directional matrix

$$
(M_1M_2^T - M_2M_1^T)^T = (M_1M_2^T)^T - (M_2M_1^T)^T
$$
  
= (M\_2M\_1^T) - (M\_1M\_2^T)  
= -(M\_1M\_2^T - M\_2M\_1^T) (7)

Subsequently, the uni-directional adjacency matrix is obtained by setting the negative value  $A_{j,i}$  to 0 by the ReLU activation function. Figure [5](#page-6-1) gives a simple example to illuminate the construction of a uni-directional matrix. To construct a one-way graph, it is necessary to calculate the similarity weights for every pair of node embedding vectors, which incurs a computational cost of  $O(K^2)$ .

To reduce the computation cost, only the frst *k* large values are considered as neighbors, and the rest are set to 0 as follows:

for 
$$
i = 1, 2, ..., K
$$
:  
\n
$$
idx = \arg \text{topk}(A_{i,:})
$$
\n
$$
A_{i,j} = 1, \quad j \in idx
$$
\n(8)

where the index of the top-k largest values of a vector is returned by arg topk $(·)$ .

# **5.3 Dynamic prior graph generator**

To enhance the quality of the learning graph, the existing graph structure learning method provides prior knowledge in the format of a prior graph for graph learning. Currently prior graph generation methods typically utilize all raw data as input and transform them into a KNN graph as prior knowledge. This prior graph is a static graph and can only describe fxed relationships between indicators.

However, the relationships between indicators usually change over time. As shown in Fig. [6,](#page-6-2) the purple line and the blue line exhibit synchronous fluctuations from  $t_1$  to  $t_2$ , but they diverge and move in opposite directions after  $t_3$ . Therefore, it is necessary to capture the various and dynamic relationships between sensors. Specifcally, the dynamic prior graph generator comprises two essential components: the feature extractor and the KNN graph generator.



<span id="page-6-2"></span><span id="page-6-0"></span>**Fig. 6** The relationship between sensors changes over time

#### **5.3.1 Feature extractor**

To represent each sensor, we design a feature extractor that generates a feature vector for each sensor. The feature vector characterizes the diverse behaviors of diferent sensors. To capture the relationships changing over time, the input of the feature extractor at timestamp *t* is the subsequence  $X_t$  instead of the whole time series. The feature vector of the sensor *i* at timestamp *t* is obtained by applying two onedimensional convolutional layers and a fully connected layer [[19\]](#page-16-16) as follows:

$$
V_i^{(t)} = FC\left(\text{Conv}\left(\text{Conv}\left(x_i^{(t)}\right)\right)\right) \tag{9}
$$

where  $x_i^{(t)} = (x_{t-<sub>0</sub>}, x_{t-<sub>0</sub>+1}^i, ..., x_{t-1}^i)$  ∈  $R<sup>w</sup>$ , and  $V_i^{(t)}$  is the feature vector of sensor *i* at timestamp *t*. Conv stands for the one-dimensional convolutional layer and FC stands for the fully connected layer.

#### **5.3.2 KNN graph generator**

The KNN graph generator uses the features vector from the feature extractor to generate prior graphs. The initial step of the KNN graph generator is to compute the cosine similarity of two feature vectors as follows:

$$
\cos\left(V_i^{(t)}, V_j^{(t)}\right) = \frac{V_i^{(t)} \cdot V_j^{(t)}}{\left| \left| V_i^{(t)} \right| \right| \cdot \left| \left| V_j^{(t)} \right| \right|} \tag{10}
$$

where  $\|\cdot\|$  denotes magnitude. We choose the most similar *k* nodes for each node as follows:

$$
\theta_{i,j}^{(t)} = 1, j \in \text{topk}\left(\cos\left(V_i^{(t)}, V_j^{(t)}\right)\right) \tag{11}
$$



<span id="page-7-0"></span>**Fig. 7** A simple example of timestamp mask

where  $\theta_{i,j}^{(t)}$  denote the element located in the *i*-th row and *j*-th column of the prior graph and topk(⋅) selects the *k* node indices with the highest cosine similarities [\[3](#page-15-5)].

In this way, we can generate a list of prior graphs  $\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(\frac{N}{\text{stride}} - \omega + 1)},$  where *N* is the total length of the time series, the *stride* is the step size of the sliding window, and  $\omega$  is the size of the sliding window.

Although the obtained prior graph is undirected, it still provides efficient knowledge for uni-directional graph structure learning. In detail, the undirected edges in the prior graph represent the relationships between connected nodes, and the graph learner strives to determine the direction of these edges within the constraint of the prior graph. The prior graph  $\theta^{(t)}$ serves as the direction candidates for graph learning.

#### **5.4 DCRNN predictor based on timestamp mask**

To handle the missing value in prediction, we propose the timestamp mask-based DCRNN predictor. It combines a timestamp mask mechanism and a recurrent graph neural network to robustly make predictions of future values by actively masking some values. The masked subsequence  $X_t$  and the learned adjacency matrix *A* from the graph structure learner are utilized as input for the recurrent graph neural network to predict the following value of the subsequence.

#### **5.4.1 Timestamp masking**

For a given subsequence  $X_t \in R^{K \times \omega}$ , a masking vector  $m \in$  ${0, 1}^\omega$  is first sampled, where each element is drawn from a Bernoulli distribution with probability *p* independently [[24](#page-16-17)]. Then, we mask the subsequence  $X_t$  with  $m$ , resulting in the First, we mask the subsequence  $A_t$  with  $m$ , restriction of a masked subsequence denoted by  $X_t$ .

$$
\widetilde{X}_t = T_f(X_t, m) = \left[ \mathbf{x}^1 \odot m, ..., \mathbf{x}^K \odot m \right]^T
$$
\n(12)

where  $T_f$ () is the masking transformation, and  $x^i \in R^\omega$  is the transpose of the *i*-th row vector of  $X_t$ . Fig. [7](#page-7-0) gives a simple example of masking process. The input of the DCRNN pre- $\alpha$  and the adjacency matrix *A*.

#### **5.4.2 DCRNN predictor**

DCRNN [[13\]](#page-16-18) is designed for uni-directional graphs and can capture the temporal and spatial features simultaneously. DCRNN captures spatial features by difusion convolution and temporal features by Gated Recurrent Unit (GRU).

The difusion convolution can aggregate *L* hops neighbors features, which is defned as follows:

$$
W_Q \circ Y = \sum_{l=0}^{L} \left( w_{l,1}^Q \left( D_O^{-1} A \right)^l + w_{l,2}^Q \left( D_I^{-1} A^T \right)^l \right) Y \tag{13}
$$

where  $\circ$  represents diffusion convolution operation,  $D<sub>O</sub>$  and  $D_I$  are the out- and in-degree matrices,  $w_{l,1}^Q$  and  $w_{l,2}^Q$  denote the model parameters, and  $L$  is the diffusion degree.

GRU is designed to capture the temporal features. To compensate for the capability of capturing spatial features, DCRNN uses the difusion convolution operation to replace the linear multiplication in GRU, which is formulated as follows:

$$
R_{t} = \text{sigmoid}\left(W_{R} \circ \left[\tilde{x}_{t} || H_{(t-1)}\right] + b_{R}\right)
$$
\n(14)

$$
C_{t} = \tanh\left(W_{C} \circ \left[\tilde{x}_{t}|| (R_{t} \odot H_{(t-1)})\right] + b_{C}\right)
$$
\n(15)

$$
U_{t} = \text{sigmoid}\left(W_{U} \circ \left[\tilde{x}_{t} || H_{(t-1)}\right] + b_{U}\right) \tag{16}
$$

$$
H_{(t)} = U_t \odot H_{(t-1)} + (1 - U_t) \odot C_t \tag{17}
$$

where  $\tilde{x}_t$  and  $H_{(t)}$  are the input and output at timestamp *t*,  $\circ$  is the difusion convolution operation, || is the concatenation operation of two features,  $R_t$ ,  $C_t$ , and  $U_t$  are the update gate, reset gate and the candidate hidden state, respectively.

For the masked subsequence  $X_t$ , DCRNN utilizes an encoder and decoder architecture to predict the value of the next timestamp. Its process can be summarized as follows: In the encoder, the hidden feature  $H_{(.)}$  is updated from timestamp  $t - w$  to timestamp  $t - 1$ , where *w* denotes the length of the subsequence. This updating process accumulates the information from multiple historical timestamps, resulting in the total hidden feature  $H_{(t-1)}$  of the subsequence, as illustrated in Fig. [4.](#page-5-0) In the decoder, the total hidden feature  $H_{(t-1)}$  is decoded by a DCRNN layer to predict the value  $\hat{x}_t$  at timestamp *t*.

### **5.5 Loss function**

Generally, the mean absolute error is employed as the loss function  $loss_n$  for the prediction task.

$$
loss_p = \frac{1}{K} \sum_{i=1}^{K} |\hat{x}_t^i - x_t^i|
$$
 (18)

where  $\hat{x}$ <sup>*i*</sup></sup> and  $x$ <sup>*i*</sup> represent the predicted value and ground truth of the *i*-th indicator at timestamp *t*, respectively.

To improve the quality of the learning graph, we introduce a graph learning loss during model training to impose constraints on the learning graph. The graph learning loss loss<sub>a</sub> is expressed as the cross-entropy between the prior knowledge  $\theta^{(t)}$  and the learned graph structure *A* as follows:

$$
loss_g = \sum_{ij} -\theta_{i,j}^{(t)} \log A_{i,j} - \left(1 - \theta_{i,j}^{(t)}\right) \log \left(1 - A_{i,j}\right) \tag{19}
$$

To mitigate overfitting, an  $L<sub>2</sub>$  regularization term is incorporated into the loss function. The total loss function of the model is defned as follows:

$$
loss = loss_p + \lambda_1 loss_g + \lambda_2 ||w||_2^2
$$
 (20)

where the parameter  $\lambda_1$  and  $\lambda_2$  is the regularization magnitude. The prediction  $\cos loss_n$  makes the prediction as close as possible to the ground truth. Meanwhile, the graph learning loss  $loss<sub>e</sub>$  controls the learning direction of the graph learning to capture meaningful spacial dependencies. Regularization term prevents from overftting and enhances the model's generalization to unseen data.

#### **5.6 Anomaly score calculation**

We identify anomalies that deviate from normal behavior based on the ground truth and prediction values. As a result, the frst step is to calculate the individual anomaly score for each sensor. These scores are later combined to obtain the aggregative anomaly score for each timestamp. Whenever the aggregative anomaly score surpasses a predetermined threshold, it is regarded as an anomaly.

We compare the ground truth and the predicted value at timestamp *t* to calculate the prediction error  $Err<sub>i</sub>(t)$  for sensor *i* as follows:

$$
Err_i(t) = \left| x_i^i - \hat{x}_i^i \right| \tag{21}
$$

To ensure the consistency of metric scales among sensors with varying value ranges, a standard normalization is conducted on the prediction error as follows:

$$
s_i(t) = \frac{Err_i(t) - \mu_i}{\sigma_i} \tag{22}
$$

where  $\mu_i$  and  $\sigma_i$  are the mean and standard deviation of  $Err_i(t)$ , respectively.

Then, the aggregative anomaly score at timestamp *t* is determined by the highest anomaly score among all sensors as follows:

$$
s(t) = \max_{i} s_i(t) \tag{23}
$$

# **5.7 Threshold selection**

To determine the optimal threshold, a grid search technique is employed. The upper and lower bounds of the threshold are defned as the maximum and minimum values of *s*(*t*), respectively. An exhaustive search of all possible thresholds is conducted with a step size of 0.01. The threshold with the highest F1 score is selected as the optimal threshold. In addition, we use a point-adjust strategy for anomaly scores according to Ref. [[20\]](#page-16-6).

# <span id="page-8-0"></span>**6 Experiments and performance analysis**

In this section, we explain our experiments in detail and answer the following research questions:

- RQ1 (Detection Performance, Efficiency and Com**putation Complexity):** Does our method outperform the baseline method in terms of both performance and efficiency in anomaly detection? What is the computer complexity of the model?
- **RQ2 (Parameter Infuence):** How sensitive is DPGLAD with diferent parameters?
- **RQ3 (Graph Structure Learner Performance):** Does our proposed UGL outperform other graph learning methods in anomaly detection models in terms of performance and efficiency?
- **RQ4 (Ablation Studies):** How does each component of DPGLAD affect its performance, and is DPGLAD more efectively to handle input data with missing values?

#### **6.1 Datasets**

In our experiments, we utilize four public and real-world datasets. The statistics of all these datasets are presented in Table [2.](#page-9-0)

The Safe Water Treatment (SWAT) dataset $2$  originates from a water treatment testbed that is overseen by the Public Utilities Authority of Singapore. The data collection process spanned 11 days and is continuously operating for 24 h a day, during which network traffic and values from all 51 sensors and actuators are recorded.

The Water Distribution (WADI) dataset<sup>[3](#page-8-2)</sup> is a comprehensive water distribution system consisting of a

<span id="page-8-1"></span><sup>2</sup> [https://itrust.sutd.edu.sg/itrust-labs-home/itrust-labs\\_SWAT/.](https://itrust.sutd.edu.sg/itrust-labs-home/itrust-labs_SWAT/)

<span id="page-8-2"></span><sup>3</sup> [https://itrust.sutd.edu.sg/itrust-labs-home/itrust-labs\\_WADI/.](https://itrust.sutd.edu.sg/itrust-labs-home/itrust-labs_WADI/)

<span id="page-9-0"></span>**Table 2** Description of datasets

Dataset	<b>SWAT</b>	WADI	MSL	<b>SMAP</b>
Indicators	51	127	55	25
# of training	495000	762970	58317	135183
# of testing	450000	172800	73729	427617
Anomalies	11.97%	5.99%	10.72%	13.13%

multitude of pipelines. As an extension of the SWAT testbed, WADI presents a more thorough and lifelike representation of water treatment, storage, and distribution networks. The dataset encompasses a continuous period of 16 days, during which 14 days encompass regular operations, and the remaining 2 days cover attack scenarios. The testbed is equipped with 127 sensors and actuators.

The Mars Science Laboratory rover (MSL) is a dataset of sensor and actuator data from the Mars rover by NASA. This dataset comprises 55 distinct metrics for 27 unique entities.

The Soil Moisture Active Passive satellite (SMAP) is a dataset of soil samples and telemetry collected by NASA using the Mars rover. This dataset comprises 25 metrics for 55 entities.

To accommodate the extensive volume of raw data, a down-sampling process is implemented every 10 s for both the SWAT and WADI datasets. The median value is captured during this interval. Once an anomaly occurs within a 10-s window, it is marked as abnormal.

# **6.2 Evaluation metrics**

It is common to adopt F1-Score (F1), precision (Prec), and recall (Rec) as evaluation metrics of anomaly detection performance as shown in Eqs.  $(24)$  $(24)$ ,  $(25)$  $(25)$  and  $(26)$  $(26)$ :

$$
Prec = \frac{TP}{TP + FP}
$$
 (24)

$$
Rec = \frac{TP}{TP + FN}
$$
 (25)

$$
F1 = \frac{2 \times \text{Prec} \times \text{Rec}}{\text{Prec} + \text{Rec}}.
$$
 (26)

where TP, TN, FP, and FN are the numbers of true positives, true negatives, false positives, and false negatives.

Besides, the efficiency is evaluated by assessing the training time per epoch for model training.

# **6.3 Baselines**

We compare DPGLAD with twelve machine learning and deep learning methods, which are AE, IF, DAGMM, LSTM-NDT, LSTM-VAE, MAD-GAN, OmniAnomaly, USAD, MTAD-GAT, GDN, FuSAGNet, and GTA.

- AE: Autoencoder is utilized to reconstruct the input data, and the reconstruction error is used as the anomaly score.
- IF [[14\]](#page-16-19): The isolation forest method is a tree-based anomaly detection algorithm. It efectively identifes anomalous samples by gaining insight into the distribution of the input data.
- DAGMM [[29](#page-16-7)]: It simultaneously trains a deep autoencoding and Gaussian mixture model, with the objective of generating a low-dimensional representation and identifying anomalies based on reconstruction errors.
- LSTM-NDT [\[10\]](#page-15-7): It uses LSTM to achieve high prediction performance and provides a nonparametric, dynamic, and unsupervised anomaly thresholding method to detect anomalies.
- LSTM-VAE [[17](#page-16-9)]: It projects multimodal observation and temporal dependencies into a latent space and reconstructs the expected distribution through LSTMbased VAE.
- MAD-GAN [[12\]](#page-16-8): It exploits LSTM as the base model in the GAN framework to capture the temporal correlation of time series distributions.
- OmniAnomaly [\[20](#page-16-6)]: It is a prior-driven stochastic model for timestamp anomaly detection that directly returns the reconstruction probability.
- USAD [[1\]](#page-15-9): It adversarially trains an encoder-decoder framework to achieve rapid and efficient training.
- MTAD-GAT [[28\]](#page-16-4): It treats the relationship between indicators as a complete graph and utilizes graph attention neural networks for anomaly detection.
- <span id="page-9-1"></span>• GDN [\[3](#page-15-5)]: It uses pair-wise cosine similarity between nodes to construct graph structures and utilizes attentional GNNs to learn the dependencies between time series and predict behavior.
- <span id="page-9-3"></span><span id="page-9-2"></span>• FuSAGNet [[5\]](#page-15-6): It learns the graph structure through pair-wise cosine similarity between recursive sensor embeddings and obtains a sparse representation of the input data through a sparse autoencoder, which is fed into a graph attention network to predict future sensor behavior.
- GTA [[2](#page-15-4)]: It involves automatically learning a graph structure and utilizes Transformer-based architecture to model temporal dependency.

<span id="page-10-1"></span>**Table 3** Precision, recall and F1 score on SWAT and WADI



The highest and second-highest results are highlighted with boldface and italics, respectively



# **6.4 Settings**

<span id="page-10-0"></span>**Table 4** Experimental parameter setting

The parameters for our experiments are set as shown in Table [4](#page-10-0). All experiments were conducted using Python 3.8, PyTorch 1.10, and CUDA version 11.3, and were trained on a server equipped with an Intel(R) Xeon(R) Platinum 8255C CPU and NVIDIA RTX 3080 GPU.

# **6.5 RQ1. Detection performance, efficiency and computation complexity**

Firstly, We evaluate the performance of DPGLAD by comparing it with all other baseline methods. Secondly, we compare its training time with existing GSL-based anomaly detection methods  $[2, 3, 5]$  $[2, 3, 5]$  $[2, 3, 5]$  $[2, 3, 5]$  $[2, 3, 5]$  $[2, 3, 5]$  Finally, we calculate the number of parameters of the model and plot the ROC curve.

#### **6.5.1 Detection performance**

As shown in Table [3](#page-10-1), the DPGLAD signifcantly outperforms other baseline methods. DPGLAD uses spatial and temporal graph neural networks relative to traditional CNN and LSTM (IF, DAGMM, LSTM-NDT, LSTM-VAE, MAD-GAN, OmniAnomaly, USAD) to effectively extract the relationship between indicators. In comparison to the latest GSL-based anomaly detection methods, such as GDN [\[3](#page-15-5)], FuSAGNet  $[5]$  $[5]$  and GTA  $[2]$  $[2]$ , DPGLAD efficiently extracts one-way relationships between nodes and enhances learning graph quality by dynamic prior graphs. The ROC-AUC curve of DPGLAD is shown in Fig. [8.](#page-11-0) All AUC of four dataset are over 0.9.

The performance of all methods on the WADI dataset is comparatively lower than the other datasets. This can be attributed to the WADI dataset's longer length, larger number of indicators, and lower anomaly rates compared to the other datasets, as shown in Table [2](#page-9-0). However, DPGLAD outperforms the baseline method on the WADI dataset due to its utilization of dynamic prior graphs as prior knowledge for graph structure learning. Thus, DPGLAD is efective in high-dimensional time series and sample imbalance scenarios, making it suitable for practical applications.

The anomaly detection performance of FuSAGNet on the SMAP and MSL datasets is insufficient. The reason is that FuSAGNet is primarily designed for Cyber-Physical Systems (CPSs), where CPS sensors can be categorized into various specifc processes [\[5](#page-15-6)]. FuSAGNet, as a result, incorporates sensors in each process individually. In contrast, the sensors present in the SMAP and MSL datasets lack specifc processes. Besides, LSTM-NDT  $[10]$  $[10]$  is also insufficient on the WADI datasets. The reason is that LSTM-NDT uses a

$\frac{1}{2}$				
Method	<b>SWAT</b>	WADI	<b>SMAP</b>	MSL
<b>GDN</b>	11.13	42.4	0.67	0.57
FuSAGNet	44.23	75.29	1.57	1.14
<b>GTA</b>	107.38	154.33	8.46	4.17
Our	26.37	42.5	1.67	0.83

<span id="page-11-1"></span>**Table 5** Running time of each epoch(s)

<span id="page-11-2"></span>**Table 6** Computation time and the number of parameters of DPGLAD

<b>Dataset</b>	<b>Computation Time(s)</b>	<b>Parameters</b>	
<b>SWAT</b>	791.1	1586090	
<b>WADI</b>	1275	1627814	
<b>SMAP</b>	50.1	1269917	
MSL.	24.9	1270511	



<span id="page-11-0"></span>**Fig. 8** The ROC curve of the model

dynamic error threshold method to compute the threshold, which is difficult to obtain an appropriate threshold when the dataset has a low anomaly rate.

#### **6.5.2 Training time and computation complexity**

Our method, when compared to FuSAGNet [\[5](#page-15-6)] and GTA [\[2\]](#page-15-4), boasts a shorter training time across all datasets while remaining in close proximity to GDN as shown in Table [5.](#page-11-1) GDN's shorter training time can be attributed to its simplistic architecture, only using a graph attention network. Conversely, GTA uses the Transformer for prediction, leading to a signifcantly increased complexity. FuSAG-Net joint trains a sparse autoencoder and a graph attention network for reconstruction and prediction. Its performance is superior to GDN [[3\]](#page-15-5) and inferior to GTA [[2](#page-15-4)], while its training time is inferior to GDN [\[3](#page-15-5)] and superior to GTA [[2](#page-15-4)]. DPGLAD uses timestamp mask-based DCRNN for prediction, which greatly reduces the training time while ensuring the model's performance. To evaluate the computation complexity of DPGLAD, we also present the computation time and the number of parameters of DPGLAD, as shown in Table [6.](#page-11-2) The WADI dataset with 127 indicators has the largest nodes among all the datasets in the anomaly detection feld. The training time of DPGLAD is still less than that of GTA. Therefore, the scalability of DPGLAD on large datasets is also commendable.

#### **6.6 RQ2. Parameter infuence**

To demonstrate the stability of our method to diferent parameters, we analyze the impact of hyperparameters and regularization parameters.

#### **6.6.1 Window size**

In this experiment, we examine the impact of window sizes. The window size is set from 5 to 60. The results are presented in Fig. [9.](#page-11-3) Notably, our method demonstrates a stable performance with diferent window sizes across several datasets, including SWAT, SMAP, and MSL. However, the window size has an impact on the detection performance of the WADI dataset. The reason is that the WADI dataset has a large sampling number and a low anomaly rate. In particular, DPGLAD outperforms both GDN and FuSAGNet with their default window size  $\omega$ of 5. Moreover, the DPGLAD with a window size of 15 outperforms GTA with its default window size of 60. Thus, compared with GDN, FuSAGNet, and GTA, our method exhibits superior performance, higher F1 scores, and lower complexity, while requiring only short-term history data.



<span id="page-11-3"></span>**Fig. 9** The impact of window size



<span id="page-12-0"></span>Fig. 10 The effect of regularization parameters

#### **6.6.2 Regularization parameters**

In this experiment, we present the impact of the regularization parameters  $\lambda_1$  and  $\lambda_2$  on four datasets. We vary  $\lambda_1$ from 1 to 15, and  $\lambda_2$  from 0.0001 to 0.0005. As shown in Fig. [10,](#page-12-0) the optimal performance is achieved and the performance appears to be generally stable, when  $\lambda_1$  is set to 1.  $\lambda_2$  has little effect on the performance.

#### **6.7 RQ3. Graph structure learner performance**

To demonstrate the efectiveness of the uni-directional graph structure learner of DPGLAD, we compare UGL with two existing graph structure learner methods: The k-neighbour Method (KNM) and the Fully Parameterized Method (FPM). Besides, we modify the UGL with only one node embedding to generate an undirected graph for comparison, which is termed as Undirected Graph Method (UGM). Among the three comprised methods, KNM and UGM learn an undirected graph.

#### **6.7.1 k‑neighbour method**

This method produces an embedding vector for each sensor and subsequently evaluates the cosine similarity between sensors. Finally, the top *k* most similar sensors are selected to build the adjacency matrix. It is referred to as KNM and exploited by GDN [[3](#page-15-5)] and FuSAGNet [[5](#page-15-6)].

$$
\cos\left(E_i, E_j\right) = \frac{E_i \cdot E_j}{\left| |E_i| \right| \cdot \left| |E_j| \right|} \tag{27}
$$

$$
A_{i,j} = 1, j \in \text{topk}(\cos(E_i, E_j))
$$
\n<sup>(28)</sup>

where  $\|\cdot\|$  denotes magnitude,  $A_{i,j}$  denote the element located in the *i*-th row and *j*-th column of the adjacency matrix and topk(⋅) selects the *k* node indices with the highest cosine similarities [\[3\]](#page-15-5).

#### **6.7.2 Undirected graph method**

To demonstrate the validity of the uni-directional graph structure, we use one node embedding instead of two node embeddings to construct an undirected graph using pair-wise similarity. It is referred to as UGM.

$$
M_1 = \tanh(\alpha E_1 \beta_1) \tag{29}
$$

$$
A = \text{ReLU}(\tanh(\alpha(M_1M_1^T))
$$
\n(30)

for 
$$
i = 1, 2, ..., K
$$
:  
\n
$$
idx = \arg \text{topk}(A_{i,:})
$$
\n
$$
A_{i,j} = 1, \quad j \in idx
$$
\n(31)

where  $E_1$  represents the node embedding vectors,  $\beta_1$  are the model parameters, and the activation function's saturation rate is symbolized by  $\alpha$ . The index of the top  $k$  largest values of a vector is returned by arg topk $(\cdot)$ .  $M_1M_1^T$  is a symmetric matrix, which generates a symmetric adjacency matrix after tanh and ReLU functions.

#### **6.7.3 Fully parameterized method**

This method frst randomly initializes the probability matrix  $\pi_1 \in R^{K \times K}$ . The adjacency matrix is Gumbel-Softmax sampled from the  $\pi_1$ . It is referred to as FPM and exploited by GTA [[2\]](#page-15-4).

$$
g_i = -\log(-\log(u)), u \sim \text{Uniform}(0, 1) \tag{32}
$$

$$
z_1^{i,j} = \frac{\exp\left(\left(\log \pi_1^{i,j} + g_1^{i,j}\right)/\tau\right)}{\sum\limits_{v \in \{0,1\}} \exp\left(\left(\log \pi_v^{i,j} + g_v^{i,j}\right)/\tau\right)}
$$
(33)

where  $u$  is samples drawn from the Uniform $(0,1)$  distribution,  $g_v^{i,j}$  satisfy the gumbel distribution, and  $\pi_1^{i,j}$  is the value of row *i* and column *j* of the probability matrix  $\pi_1$ , which represents the probability that node *i* is connected to

<span id="page-13-1"></span>**Table 8** Running time of each epoch(s) with diferent graph structure learner

Method	<b>SWAT</b>	WADI	<b>SMAP</b>	MSL	
<b>KNM</b>	23.03	36.02	1.4	0.67	
UGM	25.02	34.3	1.53	0.73	
<b>FPM</b>	29.06	62.42	1.30	0.83	
UGL.	26.37	42.5	1.67	0.83	

node  $j$ .  $\tau$  is the temperature parameter. As the temperature  $\tau$  approaches 0,  $z_1^{i,j}$  is close to 0 or 1 and the Gumbel-Softmax distribution becomes identical to the class distribution. Finally,  $A_{i,j}$  in adjacency matrix is set to  $z_1^{i,j}$ , which is set to 1 with probability  $\pi_1^{i,j}$ .

Table [7](#page-13-0) and Table [8](#page-13-1) compare the anomaly detection performance and training time of three methods with our proposed UGL. Although the *K*-neighbour and UGM exhibit superior training time compared to the UGL, their anomaly detection performance is compromised due to their inability to capture the uni-directional relationships among sensors. Although the FPM produces a uni-directional graph, it has a longer training time than the UGL method and lower detection performance.

We conduct a case study, as depicted in Fig. [11](#page-14-1). On the left side of Fig. [11,](#page-14-1) we can observe a partial graph structure that is learned by DPGLAD. On the right side, we present predictions for the relevant sensors. In this case, sensor AIT-202 is compromised, resulting in changes in its value between timestamps 708 and 730. Due to the uni-directional correlation between sensors in the water treatment process, the attack on AIT-202 causes the dosing pump P-203 to shut down, which in turn affects the permeate conductivity analyzer AIT-503 at timestamp 800. As depicted in the right side of Fig. [11,](#page-14-1) DPGLAD accurately predicts the behavior of AIT-503 and successfully detects the attack by identifying the signifcant diference between the predictions and the ground truth of AIT-503 at timestamp 800. On the left side of Fig. [11](#page-14-1), the correlation among the three sensors involved in this case is correctly represented.

<span id="page-13-0"></span>



The highest and second-highest results are highlighted with boldface and italics, respectively



<span id="page-14-1"></span>**Fig. 11 Left**: Partial graph structure learned on SWAT dataset. **Right**: Understand the relationship between sensors with ground truth and prediction

# **6.8 RQ4. Ablation studies**

In this experiment, ablation studies are conducted to showcase the necessity of DPGLAD components in achieving optimal detection performance. We focus on the dynamic prior graph generator and timestamp masking.

For the dynamic prior graph, we consider the following two methods.

- NPGLAD stands for DPGLAD in the absence of the priory knowledge and the graph learning loss function.
- SPGLAD utilizes a static prior graph extracted from all row data to replace the dynamic prior graphs in the graph learning loss function.

As shown in Table [9,](#page-14-2) the dynamic prior graph is proven to be more fexible and provides better prior information for the learning graph compared to no prior graph and the static prior graph, resulting in a better detection efect.

We evaluate the effectiveness of timestamp masking (*TM*) on the raw datasets and the datasets with missing values. We consider the method without *TM*.

• DPGLAD without *TM* eliminates the timestamp masking component, in which the raw subsequence  $X_t$  is fed into the DCRNN.

To demonstrate the performance with missing value, we randomly delete the data from the raw data as missing dataset. The percentage of missing values ranges from 0.05 to 0.2. As shown in Fig. [12](#page-15-10), as the increase of percentage of missing values, the F1 scores of two methods decreases. However, DPGLAD always outperforms that without *TM* in all missing percentages. Therefore, the *TM* component is found to be efective in handling data containing missing values.

# <span id="page-14-0"></span>**7 Conclusion and future work**

In this paper, we propose a uni-directional graph structure learning-based multivariate time series anomaly detection method with dynamic prior knowledge. In this method, we implement a more efective uni-directional graph structure learning method to capture the one-way relationship between sensors and use dynamic prior graphs to improve the quality of the learning graph. Besides, we combine the learning graph and *TM*-based DCRNN predictor to efficiently predict the future behavior of sensors. Compared with the baseline

<span id="page-14-2"></span>**Table 9** Ablation Study of the Dynamic Prior Graph



The highest and second-highest results are highlighted with boldface and italics, respectively





<span id="page-15-10"></span>**Fig. 12** The impact of missing values

on four public datasets, our proposed method achieves the best performance with short-term data while reducing the training overhead. Modeling the interconnections among sensors from multiple perspectives and improving the scalability when dealing with large graphs are future work.

**Data availability** The datasets used are all public datasets, and the links to obtain the datasets are as follows. SWAT: [https://itrust.sutd.edu.sg/](https://itrust.sutd.edu.sg/itrust-labs-home/itrust-labs_SWAT/) [itrust-labs-home/itrust-labs\\_SWAT/,](https://itrust.sutd.edu.sg/itrust-labs-home/itrust-labs_SWAT/) WADI: [https://itrust.sutd.edu.sg/](https://itrust.sutd.edu.sg/itrust-labs-home/itrust-labs_WADI/) [itrust-labs-home/itrust-labs\\_WADI/](https://itrust.sutd.edu.sg/itrust-labs-home/itrust-labs_WADI/), MSL/SMAP: [https://s3-us-west-2.](https://s3-us-west-2.amazonaws.com/telemanom/data.zip) [amazonaws.com/telemanom/data.zip.](https://s3-us-west-2.amazonaws.com/telemanom/data.zip)

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