# HFN:Heterogeneous Feature Network for Multivariate Time Series Anomaly Detection

Jun Zhan<sup>a,b,e</sup>, Chengkun Wu<sup>b,c,\*</sup>, Canqun Yang<sup>d</sup>, Qiucheng Miao<sup>b</sup>, Xiandong Ma<sup>f,\*\*</sup>

 <sup>a</sup>School of Intelligent Manufacturing, Hunan First Normal University, Changsha, 410205, China
 <sup>b</sup> College of Computer Science, National University of Defense Technology, Changsha, 410073, China
 <sup>c</sup>State Key Laboratory of High Performance Computing, Changsha, 410073, China <sup>d</sup>National SuperComputing Center in Tianjin, Tianjin, 300000, China
 <sup>e</sup>Key Laboratory of Industrial Equipment Intelligent Perception and Maintenance Technology in College of Hunan Province, Hunan First Normal University, Changsha, 411201, China
 <sup>f</sup>School of Engineering, Lancaster University, LA1 4YW, Lancaster, UK

## Abstract

As the key step of anomaly detection for multivariate time-series (MTS) data, learning the relations among different variables has been explored by many approaches. However, most of the existing approaches do not consider the heterogeneity between variables, that is, different types of variables (continuous numerical variables, discrete categorical variables or hybrid variables) may have different and distinctive edge distributions. In this paper, we propose a novel semi-supervised anomaly detection framework based on a heterogeneous feature network (HFN) for MTS. Specifically, we first combine the embedding similarity subgraph generated by sensor embedding and the feature value similarity subgraph generated by sensor values to construct a time-series heterogeneous graph, which fully utilizes the rich heterogeneous mutual information among variables. Then, a prediction model containing nodes and channel attentions is jointly optimized to obtain better time-series

Preprint submitted to Information Sciences

 $<sup>^{*}</sup>$ Corresponding author

<sup>\*\*</sup>Corresponding author

*Email addresses:* chengkun\_wu@nudt.edu.cn (Chengkun Wu), xiandong.ma@lancaster.ac.uk (Xiandong Ma)

representations. This approach fuses the state-of-the-art technologies of heterogeneous graph structure learning (HGSL) and representation learning. Experiments conducted on four sensor datasets from real-world applications demonstrate that our approach detects the anomalies more accurately than those baseline approaches, thus providing a basis for the rapid positioning of anomalies.

*Keywords:* Heterogeneous neural network; Anomaly detection; Multi-sensor data; Multivariate time series; Deep learning

## 1 1. Introduction

As information technology develops, an increasing number of industrial 2 systems are exposed to the internet, posing serious risks to their ability to 3 operate securely [1]. Continuous monitoring the operation data of the system 4 and precisely and effectively identifying potential attacks or the evolution of 5 the equipment condition by using this data is an effective technique to handle 6 these challenges [2]. For instance, an operation and maintenance personnel in a large power plant can quickly identify abnormal sensor behavior using the 8 precise intrusion detection systems, which are developed by massive amounts 9 of data collected by the supervisory control and data acquisition (SCADA) 10 system [3], providing them a possibility to prevent potential system failures 11 before irreversible damage. However, these monitoring data always have com-12 plicated structures, high dimensionality, and hard labeling, making manual 13 tasks difficult to handle. Therefore, it is vitally necessary to investigate the 14 semi-supervised or unsupervised time-series anomaly detection approach by 15 utilizing a sizable amount of complicated unlabeled data. 16

Recently, deep learning technique has been applied successfully in vari-17 ous anomaly detection problems [4, 5, 6]. For high-dimensional MTS analy-18 sis, the temporal relations between different timestamps are considered first 19 [7]. Because of their capability of capturing long-term dependency relations, 20 recurrent neural network [8] and temporal convolutional network [9] were 21 demonstrated to achieve better results on the time-series tasks involving sin-22 gle or multiple variables [10]. However, various sensors could be mutually 23 coupled. The capacity of these approaches to detect abnormalities may be 24 constrained by their modeling of solely temporal variables. Therefore, it is 25 crucial to take into account both the temporal features of different times-26 tamps and potential correlations among these variables [11, 12]. Combining 27

the sequential network and the convolution neural network (CNN) is an ef-28 fective way to achieve this. Cross-correlation among high-dimensional data 29 can be extracted by using the local perception capacity of the convolutional 30 kernel [13]. However, CNN is primarily used to handle Euclid-space data, 31 such as image [14]. There exist some limitations on the MTS with different 32 attributes. In such cases, the graph neural network (GNN) has been success-33 fully applied into the modelling of MTS due to its good structure modelling 34 capability between complex data; the most advanced results are achieved in 35 [11, 15].36

With regards to the latent feature modeling of time-series data, the vari-37 able attributes from the data are generally seen as homogeneous in the most 38 existing papers; that is, the data types are treated without distinction, such 39 as use of the variational autoencoders [16] and generative adversarial net-40 works [17]. These methods model complex distribution from large-scale high-41 dimensional datasets. After the training is finished by using the dataset from 42 normal conditions, the similar generative data are viewed as normality, while 43 the dissimilar data are viewed as anomalies. However, there are still fewer 44 works considering the heterogeneity of time-series data, although this kind 45 of data are abundant in practical situations. For instance, in a large-scale 46 water processing system [17], the information, such as flow, pressure and liq-47 uid level collected by the sensors in the intermediate process, is collected as 48 the numeric continuous values. However, the signals, such as valve state and 49 location collected by the sensors of the actuator, are generally the categor-50 ical discrete values. Inputting the mixed type of heterogeneous data into a 51 deep learning network may cause the useful information to be ignored and 52 therefore satisfied results cannot be obtained. The fundamental reason is 53 that there are totally different edge distributions between the variables with 54 different types [18, 19]. 55

To overcome the limitation of deep learning model in such circumstances, 56 we propose a heterogeneous feature learning network for MTS, and study its 57 abnormal detection capability with the extensive real-world datasets. The 58 overall framework can be divided into three stages: 1) Heterogeneous graph 59 structure learning (HGSL) stage for MTS. We fuse the sensor embedding 60 vector similarity matrix and the feature value similarity matrix of different 61 variable categories to model the heterogeneous structural information. More-62 over, we propose a category-based fixed-length approach to replace the widely 63 used meta-path [20] for extracting heterogeneous relation subgraphs. 2) Het-64 erogeneous representation learning stage for MTS. We embed different kinds 65

of variables into vectors for fusion. Distinct from the previous heterogeneous 66 graph attention network [21], we further expand the channel attention on the 67 basis of node attention and semantic attention, so as to achieve a joint opti-68 mization training of node embedding representation with different types. 3) 69 Abnormal detection and location stage. By analyzing the deviation between 70 the predicted and real values, we calculate a condition score for each sensor, 71 where the largest condition score is considered as the maximum abnormal 72 probability. 73

<sup>74</sup> The major contributions of the paper are summarized as follows:

We propose a novel HGSL approach for MTS, which learns heteroge neous graph structure information between sensor-embedding vectors and category-based feature value vectors simultaneously.

 We propose a heterogeneous feature network (HFN) and apply it to MTS anomaly detection. Our approach successfully learned the dynamic dependency among different variables and timestamps by utilizing two single-level attention mechanisms, namely attention-based node embedding and channel aggregation.

The extensive experiments indicate that HFN can detect the anomalies
 from real-world MTS datasets and is proved to outperform the most
 existing methods. Besides, we analyze the condition scores of MTS,
 demonstrating that the proposed method has the advantage of locating
 the anomalies.

The rest of this paper is structured as follows. Section 1 describes the related work of MTS anomaly detection. Section 2 presents the structure and working principle of HFN-based MTS anomaly detection framework in detail. Section 3 show the performance of proposed method on three realworld MTS datasets. Finally, the conclusion and future improvements are given in Section 4.

## 94 2. Related work

MTS anomaly detection has extensive application prospects in the fields of industry, financial business, and the Internet of Things. As the key research problem in this paper, we firstly review the related work for MTS anomaly detection, which can generally be categorized as unsupervised, supervised, and semi-supervised. We focus on studying data heterogeneity modeling of
MTS, especially heterogeneity representation learning from time-series data,
graph structure learning, and heterogeneous graph neural network.

# 102 2.1. MTS anomaly detection

MTS anomaly detection is typically regarded as an unsupervised learning 103 problem [22], and algorithms based on clustering [23], such as fuzzy c-means 104 [24], or spatiotemporal clustering [25], are frequently used. By grouping 105 time-series data into various clusters, these techniques can identify anoma-106 lies by calculating the similarity or distance between the observed value [26] 107 and the cluster center [27]. However, unsupervised detection methods usu-108 ally focus more on static data model development. In contrast, a supervised 109 abnormal detection algorithm has a higher detection accuracy. Under the 110 circumstance of high-quality labeling, the indicator accuracy can be approx-111 imate to 100% [28]. However, the supervised detection requires that the 112 training set contains correctly both labeled positive and negative samples, 113 which is often not easy. [29]. Fortunately, in the actual cases, we have a 114 chance to obtain a large quantity of data under the normal conditions [17], 115 making the semi-supervised abnormal detection attract wide attentions [30]. 116 In the latest work, Miryam et al. [31] proposes the methods to show the 117 great advantages and extensive application prospects of the semi-supervised 118 algorithm in MTS abnormal detection. 110

# <sup>120</sup> 2.2. Modeling for heterogeneous data

The data heterogeneity has been widely concerned such as in the music 121 recommendation system [32], academic network [33] and social platform [34]. 122 The heterogeneous learning method usually focuses on capturing and inte-123 grating couplings with multiple variable types at the same or different levels. 124 To learn the embedding representation of heterogeneous data, the matrix de-125 composition method is traditionally adopted [35, 36]. However, it is usually 126 very expensive and low-efficient in terms of the computation cost of decom-127 posing a large-scale matrix [37]. Moreover, the discretization of continuous 128 features [38] or continuous data [39] are also a typical method; however this 120 transformation may ignore the correlation between variables. To solve these 130 challenges, heterogeneous graph embedding or heterogeneous graph repre-131 sentation learning [40] has been widely studied. Its main goal is to map the 132 input data into low-dimensional space while simultaneously preserving the 133 heterogeneous structure and semantic characteristics of the data [41]. For 134

instance, for the tasks of text classification, Wang et al. [21] proposed a het-135 erogeneous graph attention network (HAN), which aggregates the features 136 of meta-path based neighbors through a hierarchical manner to generate the 137 embedding representation of nodes. Fu et al. [42] proposed a meta-path ag-138 gregated graph neural network (MAGNN) by designing multiple candidate 139 encoder functions to extract heterogeneous information from the meta-path. 140 Wang et al. [43] combined the heterogeneous graph neural network with com-141 parison learning, and proposed a self-supervised heterogeneous graph neural 142 network from both heterogeneous network and meta-path for learning node 143 embedding representation. In the social or citation network, in order to cap-144 ture the dynamic performances of heterogeneous redgraphs, Hu et al. [44] 145 proposed a heterogeneous graph transformer (HGT) by introducing a relative 146 temporal encoding technique for solving the problem where the dynamic re-147 sult dependence is difficult to capture. Yang et al. [45] proposed a dynamic 148 heterogeneous graph (DvHAN) utilizing structural heterogeneity and time 149 revolution to learn node embedding. In addition, contrastive self-supervised 150 learning has been widely employed to address the limitation of sparse la-151 bel information in the potential ability of heterogeneous graph neural net-152 work models for representation learning. For instance, the HGCL method 153 proposed by Chen et al. [46] effectively utilizes the structural information 154 of heterogeneous graphs to capture relationships between different types of 155 nodes. Zhu et al. [47] combine heterogeneous graph contrastive learning with 156 a structure-enhancement method, proposing the STENCIL method. This 157 approach introduces a novel multi-view contrastive aggregation objective to 158 adaptively distill information from each view. Furthermore, the method en-159 riches the local structural patterns of the underlying heterogeneous graph to 160 better explore true and challenging negative examples in graph contrastive 161 learning. Although the above methods have achieved significant success in 162 their respective application domains, leveraging the structure of heteroge-163 neous graphs to enhance data representation capabilities and demonstrating 164 outstanding performance through representation learning methods, their ap-165 plicability may be subject to domain specificity and might not necessarily be 166 suitable for other areas such as multivariate time series anomaly detection. 167

## 168 2.3. Graph structure learning

MTS usually exists in the form of tabular data [48], lacking of predefined graph structure required for graph neural network [15], which constitutes the challenge for the modelling [49]. Hence, it is extremely vital to learn the links

between edges and refine the graph from the existing time-series data [50]. 172 The existing methods can mainly be divided into three categories: metric-173 based approaches usually implemented by using kernel function [51, 52], co-174 sine similarity [53, 54] or inner product [55] to calculate the similarity between 175 nodes as edge weights. Neural networks-based approaches have generally uti-176 lized a complex deep neural network to model the edge weights of the given 177 node features and representations. For instance, Luo et al. [56] proposed 178 a multilayer perception-based graph structure optimization approach, where 179 the edge number of a sparse graph is punished through parameterized net-180 work for pruning the edges that are unrelated to the tasks. Zhao et al. [11] 181 proposed a graph structure learning approach with redan attention coeffi-182 cient, while Sun et al. [57] utilized a dot-product self-attention to model the 183 dynamic connection relations between the nodes. Direct learning approaches, 184 regarding adjacent matrix as a learnable parameter, make associative learn-185 ing together with the follow-up tasks for optimization. For instance, Gao et 186 al. [58] proposed the graph learning neural networks (GLNNs) utilizing spec-187 tral graph theory for graph learning. However, these approaches mostly aim 188 at learning isomorphic graph structure. To enable capture the heterogene-189 ity between the data efficiently, Zhao et al. [41] proposed a heterogeneous 190 graph learning approach utilizing the fusion of feature similarity sub-graph, 191 feature propagation graph and semantic graph, which successfully learns an 192 appropriate graph structure for a heterogeneous graph neural network. 193

### <sup>194</sup> 3. Proposed Frameworks

#### 195 3.1. Problem statement

Generally, we define heterogeneous MTS dataset as a time-series dataset 196 with L variables, N different types of sensors, and T length, which is ex-197 pressed as  $X = \{ \boldsymbol{x}_{1:T}^N \}$ , where  $N \in \{ type^1, \cdots, type^n \}$  denotes the set of data 198 types. Note that the variable number contained in the specified categories 199 may be larger than 1. For instance, for arbitrary data type  $type^n$ , all time se-200 ries at the moment t can be denoted as  $\boldsymbol{x}_t^{type^n} \in \{x_t^{type_i^n}, for \ i \in \{0, \cdots, d\}\},\$ 201 where d represents the number of time-series sequence in this category. In 202 this paper, we adopt the sliding window-based model training approach. At 203 the moment t, we sample a continuous subsequence with the length of  $\omega$  as 204 the model input, denoted as  $S^{N}(t) = [\boldsymbol{x}_{t-w+1}^{N}, \cdots, \boldsymbol{x}_{t}^{N}]$ . For the abnormal 205 detection task, our target is to predict the value of all sensors  $\boldsymbol{x}_{t+1}^N$  at the 206

moment t + 1 by utilizing the input subsequence  $S^{N}(t)$ , and obtain the pre-207 dicted value  $\hat{x}_{t+1}^N$ . The mean square error (MSE) between the predicted 208 value and practical value is used as loss to optimize the model. According 209 to the usual semi-supervised abnormal detection methods, in the training 210 stage, only the data collected from normal conditions are chosen. However, 211 in the testing stage, the deviation between the predicted value and practical 212 value is further used for calculating the condition scores of the data, while 213 the scores of the corresponding data over the threshold are judged as the 214 anomalies, otherwise normal. 215

Specially, we divide time-series data into three data types, that is  $N \in \{C, CD, D\}$ :

• Continuous numerical variables C, where the value of data are taken from continuous real number, such as  $x_t^{C_i} \in \mathbb{R}$ .

• Discrete categorical variables D, where the value of data are taken from a limited set of values, such as  $x_t^{D_i} \in \{0, 1, 2\}$ .

• Hybrid variables  $S_t^{CD}$  which contain both numerical and categorical variables where the values of the element are taken from the above two categories.

We construct a heterogeneous dynamic graph to model the above MTS. 225 Different time-series variables are viewed as the node in the graph, while their 226 connection relation is seen as the edge. This dynamic graph can be denoted as 227  $\mathbb{G}_{S^{N}(t)} = (\mathcal{V}, \mathcal{E})$ , where  $\mathcal{V}$  and  $\mathcal{E}$  represent node and edge set respectively. We 228 respectively extract categorical feature subgraph  $\mathbb{G}_{S^{D}(t)}$ , numerical feature 229 subgraph  $\mathbb{G}_{S^{C}(t)}$ , and categorical and numerical mixed subgraph  $\mathbb{G}_{S^{CD}(t)}$  for 230 learning heterogeneous information. For the arbitrary subgraph, its adjacent 231 matrix is  $A_N \in \mathbb{R}^{|\mathcal{V}_N| \times |\mathcal{V}_N|}$ , where  $\mathcal{V}_N$  represents the node set with the specific 232 type. If there exist connection relations between two arbitrary nodes in the 233 subgraph, the corresponding element of adjacent matrix is 1. Noted that the 234 final node embedding integrates the node embedding representations of three 235 different subgraphs. 236

#### 237 3.2. Model Architecture

Our HFN-based approach aims at learning the complex correlation between different types of time-series data carried by the defined dynamic graph



Figure 1: Architecture of HFN-based MTS anomaly detection framework.

above. For each node, the potential temporal correlation is allowed to beconsidered with a sliding window along the dataset.

Figure 1 shows the proposed HFN-based semi-supervised abnormal de-242 tection framework architecture. It can be seen that for a given MTS, we 243 firstly learn a heterogeneous dynamic graph representing the structural in-244 formation between different variables (as shown in Figure 2), decomposing 245 the time-series data into different graph structures. On this basis, the cat-246 egorical feature subgraph, the continuous numerical feature subgraph and 247 the hybrid subgraph are extracted and then inputted into the HFN network 248 based on graph attention function to learn the potential embedding repre-249 sentations of each sensor (as shown in Figure 3). Then we predict the future 250 values of each sensor based on these embedding representations. Finally, the 251 deviation between the predicted and practical values is used for measuring 252 and locating the anomalies. 253

## 254 3.3. Graph structure learning pipeline

To learn the complex heterogeneous potential features between different 255 types of sensors, a key process is how to map the variable correlation from 256 MTS into the adjacent matrix of the graph. In the previous studies, all 257 assumed that the constructed graph is the static isomorphic graph, thus re-258 sulting in the loss of some key information. For instance, the significance 259 of variables exists great difference at the operating condition of full-load 260 and partial-load of generating equipment [59]. Hence, as shown in Figure 2, 261 we learn the potential heterogeneous graph structure of MTS from the per-262 spectives of global semantic correlation and local feature correlation. For 263 the global semantic correlation, we introduce a learnable embedding vector 264



Figure 2: Structure learning of MTS heterogeneous dynamic graph.

for each variable, and denote it as  $e_i \in \mathbb{R}^{1 \times \omega'}$ . For  $i \in \{0, \dots, L\}$ , where 265  $\omega'$  represents the dimension of embedding vector. This vector can be learned 266 together with subsequent prediction network parameters. For the local fea-267 ture correlation, we calculate the potential structural information based on 268 the feature values of the variables. We adopt a special mapping network 269 to project different types of input feature vector  $S^{N}(t)$  into a public space. 270 Taking data type C as an example, the projected feature of the arbitrary 271 variable  $x^{C_i}$  is denoted as  $f^{C_i} \in \mathbb{R}^{1 \times \omega'}$ : 272

$$f^{C_i} = SELU\left(x^{C_i} \bullet \boldsymbol{W}^{\boldsymbol{C}} + \boldsymbol{b}^{\boldsymbol{C}}\right) \tag{1}$$

where  $x^{C_i} \in \mathbb{R}^{1 \times \omega}$  is the subset of all continuous numerical variables.  $\omega$  is the time length of input feature vector.  $W^C \in \mathbb{R}^{\omega \times \omega'}$  is learnable weight matrix, and  $b^C \in \mathbb{R}^{1 \times \omega'}$  is biasing. Similarly, we can calculate and obtain the projected feature representation  $f^{D_i}$  of the discrete categorical variables.

# 277 3.4. Similarity Graphs

The main task of graph structure learning is to learn an adjacent matrix representing the mutual connection between nodes in the graph. Therefore, we propose a learning approach based on aggregating cosine similarity. According to the embedding for the variables and the mapping of variable feature vectors, we obtain the global semantic embedding matrix

 $\boldsymbol{E} \in \{e_1, \cdots e_L\}$  and local feature vector representation matrix  $\boldsymbol{F}^{\boldsymbol{N}} \in \{f^{N_1}, \cdots, f^{N_L}\}$ . 283 Clearly, these obtained matrices from different perspectives contain differ-284 ent information. Specifically, we first calculate cosine similarity between the 285 elements in different matrixes to obtain their connection information. After 286 obtaining the node embedding (NE) similarity matrix  $M^{E_s} \in \mathbb{R}^{L \times L}$  and node 287 feature (NF) similarity matrix  $M^{F_s} \in \mathbb{R}^{L \times L}$ , we fuse them to obtain an aggre-288 gating similarity matrix, where the value represents the similarity between 289 the arbitrary two nodes i and j and can be calculated as follows: 290

$$M^{E_s}[i,j] = \frac{e_i \bullet e_j}{e_i \times e_j} \tag{2}$$

$$M^{F_s}[i,j] = \frac{f^{N_i} \bullet f^{N_j}}{f^{N_i} \times f^{N_j}}$$
(3)

$$M^{A_s} = M^{E_s} \circ \boldsymbol{W}^{E_s} + M^{F_s} \circ \boldsymbol{W}^{F_s}$$
(4)

where  $\circ$  denotes Hadamard product between two matrixes.  $\boldsymbol{W}^{E_s} \in \mathbb{R}^{L \times L}$ 291 and  $\boldsymbol{W}^{F_s} \in \mathbb{R}^{L \times L}$  are learnable weight matrixes, which weigh the importance 292 of different dimensions of the different similarity matrixes. In  $M^{A_s}$ , when 293 the correlation coefficient is larger than a certain threshold, we consider that 294 there exists a connected relation between nodes; otherwise, the connected 295 relation does not exist. To obtain the optimal threshold, we define a learn-296 able parameter  $\tau \in \mathbb{R}$  for automatic choice, and obtain the adjacent matrix of 297 aggregating similarity graph through learning, which is denoted as: 298

$$A_{ij} = \begin{cases} 1 & for \ M^{A_s}[i,j] \ge \tau \\ 0 & for \ M^{A_s}[i,j] < \tau \end{cases}$$
(5)

In the heterogeneous dynamic graph, two objects can be connected through 299 different semantic paths, which is called meta-path. However, the selec-300 tion of meta-path has a strong subjective meaning, which is difficult for 301 complex MTS. Therefore, we propose a classifying-based fixed-length sam-302 pled method to replace meta-path for extracting heterogeneous relation sub-303 graphs. Specifically, we divide the aggregating similarity graph into the cor-304 responding classifying subgraphs, including discrete feature subgraph (DFS) 305  $\mathbb{G}_{S^{D}(t)}$ , continuous feature subgraph (CFS)  $\mathbb{G}_{S^{C}(t)}$  and hybrid feature sub-306 graph (HFS)  $\mathbb{G}_{S^{CD}(t)}$  according to data types. We further make a random 307 mask operation for the neighboring matrix of the subgraph and obtain the 308

final neighboring matrix with different relations. The transformed heterogeneous graph structure is  $A' = \{A^D, A^C, A^{CD}\}$ . The random mask is conducive to exchange information between different similarity matrixes in the graph structure learning process, thus improving the accuracy of subsequent tasks and relieving the overfitting problem.

## 314 3.5. Graph representation learning for MTS

It can be seen from the learned heterogeneous graph structure that each 315 type of subgraph contains different semantic properties. Hence, to aggregate 316 the node information from different types, we introduce a graph attention-317 based node embedding network and an attention-based channel aggregating 318 network to construct the HFN for MTS. The structure is shown in Figure 3. 319 Specifically, the obtained three subgraphs  $A^D, A^C, A^{CD}$  learned by graph 320 structure learning are inputted into three independent graph attention net-321 works, to learn the importance of different types of nodes for the neighbors 322 in the subgraphs. Moreover, the important neighboring information is aggre-323 gated to generate a new node embedding. As shown in Figure 3, taking the 324 continuous numerical variable channel as an example, for the arbitrary node 325  $v_i^C$  and its neighboring node  $v_j^C$  in subgraph  $A^C$ , we perform self-attention in 326 the nodes. The attention coefficient representing their relation importance 327 can be calculated as: 328

$$\xi_{ij} = att \left( \boldsymbol{W} f^{C_i}, \boldsymbol{W} f^{C_j}; A^C \right)$$
(6)

where  $f^{C_i} \in \mathbb{R}^{1 \times \omega'}$  and  $f^{C_j} \in \mathbb{R}^{1 \times \omega'}$  are mapped node feature vectors,  $\boldsymbol{W} \in \mathbb{R}^{\omega'' \times \omega'}$  is shared weight matrix.  $\omega'$  and  $\omega''$  are the calculated node feature vector dimensions before and after the embedding. After obtaining the importance of subgraph-based node pairs, we normalize them via the SoftMax function and obtain weight coefficient  $\alpha_{ij}$ :

$$\alpha_{ij} = softmax\left(\sigma_{ij}\right) = \frac{exp\left(\delta\left(\overrightarrow{a}^{T}\left[\boldsymbol{W}f^{C_{i}}||\boldsymbol{W}f^{C_{j}}\right]\right)\right)}{\sum_{\eta \in \mathbf{N}_{i}^{C}}exp\left(\delta\left(\overrightarrow{a}^{T}\left[\boldsymbol{W}f^{C_{i}}||\boldsymbol{W}f^{C_{\eta}}\right]\right)\right)}$$
(7)

where  $\delta$  is the activation function, and LeakyReLU function is usually adopted [55].  $\overrightarrow{a} \in \mathbb{R}^{2\omega''}$  is the learnable weight vector, which denotes the information concatenation of the two nodes. Finally, the output of each node can be obtained through aggregating its neighboring nodes. Multihead attention mechanism is proven to be beneficial in the learning process



Figure 3: Heterogeneous feature network structure of MTS.

of stabilizing self-attention [60]. To be convenient for training, we perform an
average operation to aggregate the results handled by multi-head attention.
After the graph attention-based nodes embed into the network, the implicit
vector can be represented as:

$$\boldsymbol{h}_{i}^{'C} = \sigma \left( \frac{1}{H} \sum_{h=1}^{H} \sum_{j \in \mathbb{N}_{i}^{C}} \alpha_{ij}^{h} \boldsymbol{W}^{h} f^{C_{j}} \right)$$
(8)

where  $N_i^C$  is the set of nodes *i*'s neighbors in the continuous subgraph. *H* denotes the number of multi-head attention mechanism head. According to the same computation method, we can obtain the node implicit vectors of discrete subgraph and mixed subgraph represented by  $\boldsymbol{h}_i^{'D}$  and  $\boldsymbol{h}_i^{'CD}$ .

To address the node semantic importance of different types in the hetero-347 geneous graph, we put forward an attention-based multi-channel node em-348 bedding aggregating network. We can clearly see from Figure 3 that the node 349 implicit vectors  $\boldsymbol{h}^{'C}$  and  $\boldsymbol{h}^{'D}$  singly from a continuous channel and discrete 350 channel first are concatenated in feature dimension to obtain the global node 351 implicit vector  $\boldsymbol{h}^{''DC}$ . The main purpose is to achieve the joint embedding 352 representation learning of all nodes simultaneously. Then  $h''^{DC}$  and the node 353 implicit vector  $\boldsymbol{h}^{'CD}$  from the mixed channel are sent to the multi-channel 354 node embedding aggregating network for aggregating their heterogeneous 355

information. The aggregating network automatically learns the importance degree  $\beta$  of the embedding vectors between different channel node implicit vectors, which can be explained as the contribution of the node correlation due to the different types of variables. The final embedding vector is computed as follows:

$$\boldsymbol{h} = \beta \left( \boldsymbol{h}^{'C} || \boldsymbol{h}^{'D} \right) + (1 - \beta) \, \boldsymbol{h}^{'CD}$$
(9)

where  $\beta \in \mathbb{R}$  is a learnable parameter representing the importance degree of the embedding vectors between different channel node implicit vectors, and || is a concatenation operation.

### 364 3.6. Prediction-based anomaly detection pipeline

From the above node heterogeneous feature learning network, we obtain new embedding representations of all nodes. Finally, as shown in Figure 3, we input the embedding data fused with  $\boldsymbol{h}$  and embedding vector  $\boldsymbol{E}$  into the MLP layer to have the predicted value  $\hat{\boldsymbol{x}}_t^N$  of all sensors at the moment t:

$$\widehat{\boldsymbol{x}}_{t}^{N} = SeLU\left(f\left(\boldsymbol{h} \oplus \boldsymbol{E}\right)\right)$$
(10)

where  $f(\cdot)$  is multiple layers of MLP output layer. *SeLU* is activation function, and  $\oplus$  is addition operation.

At the training stage, we adopt MSE as the loss function of the model:

$$\mathcal{L}_{mse} = \frac{1}{L} \sum_{i}^{L} \left( \boldsymbol{x}_{t}^{N} - \widehat{\boldsymbol{x}}_{t}^{N} \right)^{2}$$
(11)

After the training is finished, we apply the network to perform real-time abnormal detection tasks. By comparing the predicted and original values of the input, we calculate the condition scores of each sample in time-series data. We define the difference between the original value and predicted value as the condition scores. To eliminate the effect of different variable dimensions, we normalize the condition scores. Finally, the condition score is computed as follows:

$$Score_{i} = \frac{\left| \boldsymbol{x}_{t}^{N_{i}} - \widehat{\boldsymbol{x}}_{t}^{N_{i}} \right| - IQR_{i}}{\mu_{i} + 1}$$
(12)

where  $IQR_i$  denotes an interquartile range of the predicted value of the *i*th variable,  $\mu_i$  is its median. To achieve the anomaly positioning, we take

the largest value of  $Score_i$  as the condition score of overall record data at 381 the moment t, as denoted by  $Score=max(Score_i)$ . Finally, if the Score is 382 larger than the threshold, this record is judged as an anomaly. However, 383 because the threshold selection refers to complicated domain knowledge and 384 the selection methods are various depending on the applications [61], this 385 paper will not further explore the selection method for the threshold. The 386 experiment in the subsequent section will report the optimal value of each 387 evaluating metric (see details in Section 3.3). 388

#### 389 3.7. Training

Following the application of the components introduced in the preceding 390 sections, predictions for multivariate time series can be acquired. The fun-391 damental concept of our approach centers on maximizing the utilization of 392 diverse sensor data types within the time series, enhancing prediction accu-393 racy, and identifying anomalies based on prediction errors. To accomplish 394 this, we collaboratively optimize a heterogeneous feature network across mul-395 tiple channels to update the parameters of the entire network. Throughout 396 the training process, the comprehensive forward propagation procedure is 397 delineated in Algorithm 1. 398

## Algorithm 1 HFN training procedure

**Input:** Heterogeneous multivariate time series training dataset  $S^N(t-1) = [\boldsymbol{x}_{t-w}^N, \cdots, \boldsymbol{x}_{t-1}^N]$ , Batch Size  $\mathcal{B}$ ,Number of Epochs  $\mathcal{E}$ 

**Output:** Predicted values  $\widehat{\boldsymbol{x}}_{t}^{N}$ 

- 1: for epoch=1: $\mathcal{E}$  do
- 2: Calculate the projected feature  $f^{C_i}$  and node embedding vector  $\boldsymbol{e}_i$ ;
- 3: Calculate similarity matrix  $M^{E_s}$ ,  $M^{F_s}$  and  $M^{A_s}$  with Eq. (2), Eq. (3) and Eq. (4);
- 4: Calculate adjacent matrix  $A_N$  with Eq. (5);
- 5: Extract subgraph features to obtain the node implicit vectors  $h_i^{'C}$ ,  $h_i^{'D}$  and  $h_i^{'CD}$  with Eq. (8);
- 6: Calculate the final embedding vector  $\boldsymbol{h}$  with Eq. (9);
- 7: Calculate the predicted value  $\widehat{\boldsymbol{x}}_{t}^{N}$  with Eq. (10);
- 8: Calculate the loss  $\mathcal{L}_{mse}$  with Eq. (11);
- 9: Update parameters.
- 10: **end for**

Table 1: Statistics of the datasets.

| Items                | $\mathbf{SWaT}$ | WADI        | WTD      |
|----------------------|-----------------|-------------|----------|
| Time series<br>(C/D) | 51 (25/26)      | 123~(68/55) | 37(31/6) |
| Training dataset     | 496800          | 784571      | 1000000  |
| Testing dataset      | 449919          | 172803      | 940000   |
| Anomaly Rate $(\%)$  | 11.97%          | 5.99%       | 20.64%   |
| Sampling Rate        | 1Hz             | 1Hz         | 1Hz      |

#### 399 4. Experiments

We employ extensive experiments on two open and one private real-world datasets to answer the following research questions: (1) Whether the proposed model is more optimal than the baseline models? (2) How each component of the model affects the model? (3) How the proposed approach detects anomalies? (4) How the detection results locate anomalies?

#### 405 4.1. Benchmark datasets

The selected three datasets contain two datasets (SWaT and WADI) based on water treatment simulator testbed and a real-world dataset from a large-scale wind farm (WTD). The statistical data of the datasets are given in Table 1:

Secure Water Treatment (SWaT) Dataset [62]. This dataset was 410 collected from a six-stage Secure Water Treatment (SWaT) testbed. SWaT 411 represents a scaled-down version of a real-world industrial water treatment 412 plant. It took 11 days for the data collection process, which ran with nor-413 mal operation mode during the first seven days, and constituted a training 414 dataset. During the later four days, the testbed was implemented by inter-415 mittent network and physical attacks, which constituted the labeled testing 416 The data were collected once every second, containing 51 timedataset. 417 series features, including 25 continuous features and 26 discrete categorical 418 features. We chose this dataset for case study, and the primary sensors or 419 actuators involved are shown in the Table 2 below. 420

421 Water Distribution (WADI) Dataset [63]. This dataset was collected 422 from a water distribution testbed (WADI). It took 16 days for the data

| No. | Name    | Type                | Description   |  |  |  |  |
|-----|---------|---------------------|---|--|--|--|--|
| 1   | FIT-401 | Sensor (continuous) | Flow transmitter to control the UV dechlorinator.               |  |  |  |  |
| 2   | UV-401  | Actuator (discrete) | Dechlorinator to remove the chlorine from water.                |  |  |  |  |
| 3   | FIT-504 | Sensor (continuous) | Flow meter, a RO re-circulation flow meter.                     |  |  |  |  |
| 4   | P-501   | Actuator (discrete) | Pump to pump the dechlorinated water to RO.                     |  |  |  |  |
| 5   | LIT-401 | Sensor (continuous) | Level transmitter to regulate the RO feed water tank level.     |  |  |  |  |
| 6   | LIT-101 | Sensor (continuous) | Level transmitter to regulate the raw<br>water tank level.      |  |  |  |  |
| 7   | FIT-601 | Sensor (continuous) | Flow meter a UF backwash flow meter.                            |  |  |  |  |
| 8   | AIT-504 | Sensor (continuous) | RO permeate conductivity analyzer<br>to measure the NaCl level. |  |  |  |  |
| 9   | AIT-201 | Sensor (continuous) | Conductivity analyzer to measure the NaCl level.                |  |  |  |  |

Table 2: Statistics of the datasets.

collection process. During the last two days, the attack was launched to the
testbed with different intentions and time intervals, and the duration of the
attack lasted between 1.5 to 30 minutes to acquire the abnormal operating
data. The data were collected once every second, containing 123 time-series
features, including 68 continuous features and 55 categorical features.

Wind Turbine Dataset (WTD). This dataset was collected from a 428 large-scale wind farm [64]. It lasted 1 to 2 years for the data collection 429 process. At the training stage, there are no abnormal operating data since 430 only the time-based maintenance process was arranged for the wind turbines, 431 while at the testing stage, the abnormal operating data were detected in the 432 repairing process. All data have been labeled by the experts. The data were 433 collected once every 10 minutes, containing 37 time-series features, including 434 31 continuous features and 6 categorical features. 435

It is noteworthy that in this paper, the time scales of the time series datasets are uniform, with all datasets adhering to a fixed time scale of 1 second. However, it is crucial to recognize that the time scale, or the sampling rate of the data, can impact the identification results in time series analysis. The uniformity in time scales across the datasets employed in the paper ensures the effective facilitation of direct comparisons between different methods.

## 443 4.2. Baseline models

We first compare the FHN model with the most advanced approaches including LSTM-VAE [65], USAD [66], MAD-GAN [17], graph network based MTAD-GAT [11] and GDN [54]. These approaches are extensively concerned with the cross-time and cross-sequence correlation of MTS. The approaches based on sequence reconstruction or prediction are used to learn the representations of the whole time series. Moreover, the anomalies are judged by the reconstructing or predicting errors.

Furthermore, we compare the proposed approach with those classic shal-451 low anomaly detection approaches, including PCA [67], Isolation Forest (IF) 452 [68] and LightGBM [69]. These shallow detection methods are regarded as 453 the relatively direct abnormal detection methods, which usually can directly 454 locate the outlier. Moreover, to complete the anomaly detection in tempo-455 rally related contexts has also attracted the interests of the researchers, such 456 as LSTM-NDT [1]. The idea underlying this method is to model the tem-457 poral features of the data, predict the corresponding values, and then judge 458

whether the anomalies occur by comparing the deviation between the realvalue and the predicted value.

In addition, we also conducted comparisons with the latest methods 461 based on transformer and spatiotemporal graph approaches. These include: 462 TranAD [70], an anomaly detection and diagnostic model based on deep 463 transformer networks. It employs attention-based sequence encoders for 464 rapid inference, possessing knowledge of broader temporal trends in the data; 465 FuSAGNet [71], which combines sparse autoencoder and graph neural net-466 work. The latter predicts future time series behavior from sparse latent 467 representations learned by the former, along with graph structures learned 468 through recurrent feature embedding; MAD-SGCN [72], which effectively 469 captures the spatiotemporal correlations of input sequences using long short-470 term memory networks (LSTMs) and spectral-based graph convolutional net-471 works (GCNs). 472

# 473 4.3. Evaluation

#### 474 4.3.1. Metrics

We select precision, recall and F1 as the evaluating metrics of the model, 475 where  $Precision = \frac{TP}{TP+FP}$ ,  $Recall = \frac{TP}{TP+FN}$ ,  $F1 = \frac{2 \times Precision \times Recall}{Precision+Recall}$ . TP, FP and FN refer to true positives, false positives, and false negatives, re-476 477 spectively. These metrics are required to be obtained with a certain thresh-478 old. Hence, due to the different threshold selection methods among different 479 tasks, there exist large differences in the metric values. Therefore, to avoid 480 introducing additional hyperparameters, we report the evaluation metrics 481 values when the optimal F1 value is obtained. The threshold value is deter-482 mined by traversing between the maximum and the minimum scores of the 483 testing dataset. 484

We calculate the condition scores that decide the abnormal degree of 485 the overall dataset based on eq. (12). Noted that in unsupervised anomaly 486 detection for MTS (USAD) [66] and temporal hierarchical one-class network 487 (THOC) [73], the authors applied a specific evaluation method, called point 488 adjust, making F1 value higher and close to 1. It has been proved that 489 the capability of the model may be highly evaluated [74]. Hence, for the 490 comparison, we apply the open-source code of USAD, and utilize the same 491 parameters of the model in this paper to calculate the performance metrics 492 without adjustment. 493

## 494 4.3.2. Setup

We use Pytorch to achieve the HFN and its variants. Moreover, the model is trained on a server with Intel(R) Xeon(R) Gold 5218R CPU @ 2.1GHz and NVIDIA GeForce RTX 3090 graphics cards. We select Adam optimizer to train the model. Meanwhile, we adopt early stopping to relieve overfitting. The maximum training epoch is set to be 100. If the loss is less than 0.0001 after 10 epochs, the training stops automatically and the optimal model is saved.

The proposed HFN method and the compared baseline models have 502 strived to maintain a similar level of complexity in parameter settings, en-503 suring a fair comparison. For classical anomaly detection models, including 504 PCA and Isolation Forest, we have maintained the parameter settings at a 505 relatively standard level. The 'contamination' parameter for PCA has been 506 set to 0.05. In Isolation Forest, we opted for 100 isolation trees, each trained 507 using all features. In LightGBM, the 'num boost round' parameter has 508 been set to 1000 to ensure the model has a sufficient number of epochs for 509 training. 510

Regarding deep learning models, in LSTM-NDT, we employed a 4-layer 511 LSTM network, with each layer having 128 hidden nodes. Similarly, in 512 LSTM-VAE, a 4-layer LSTM network was used with 128 nodes in each hid-513 den layer and a latent space dimension of 32. The parameter settings for the 514 DAGMM model align with those specified by the authors in the open-source 515 code, utilizing a Gaussian Mixture Model composed of four individual Gaus-516 sian models. For the USAD model, a window length of 15 and a latent space 517 dimension of 40 were set. In the MTAD-GAT model, a convolutional kernel 518 size of 7 was chosen, and the hidden dimensions for the temporal and spatial 519 graph attention networks were set to 150. The prediction and reconstruction 520 networks comprise a 4-layer GRU network. The GDN model has a hidden 521 layer dimension of 128, an output layer with 64 hidden nodes, and a graph 522 network with 4 layers. 523

Finally, for the proposed HFN method, we selected a structure with a hidden layer dimension of 64 and 4 layers in the graph network to ensure consistency with other deep learning models. This configuration aims to provide each model with similar capabilities in learning data representations, facilitating a more equitable evaluation of their performance in anomaly detection tasks.

Table 3: Precision, recall and F1 values of HFN and all baseline methods on different datasets.

| Model       | SWaT         |       |               | WADI         |       |               | WTD   |              |               |
|-------------|--------------|-------|---------------|--------------|-------|---------------|-------|--------------|---------------|
|             | Pre.         | Rec.  | $\mathbf{F1}$ | Pre.         | Rec.  | $\mathbf{F1}$ | Pre.  | Rec.         | $\mathbf{F1}$ |
| PCA         | 0.249        | 0.216 | 0.230         | 0.395        | 0.056 | 0.100         | 0.160 | 0.513        | 0.244         |
| IF          | 0.951        | 0.588 | 0.727         | 0.299        | 0.158 | 0.207         | 0.278 | <u>0.953</u> | 0.430         |
| LightGBM    | 0.783        | 0.666 | 0.719         | <u>0.989</u> | 0.153 | 0.270         | 0.237 | 0.602        | 0.340         |
| LSTM-NDT    | 0.982        | 0.688 | 0.809         | 0.758        | 0.328 | 0.457         | 0.365 | 0.736        | 0.497         |
| LSTM-VAE    | 0.962        | 0.599 | 0.740         | 0.878        | 0.145 | 0.250         | 0.165 | 0.550        | 0.254         |
| DAGMM       | 0.470        | 0.666 | 0.551         | 0.544        | 0.267 | 0.360         | 0.164 | 0.242        | 0.195         |
| OmniAnomaly | 0.983        | 0.650 | 0.782         | 0.995        | 0.130 | 0.230         | -     | -            | -             |
| USAD        | 0.985        | 0.661 | 0.792         | 0.995        | 0.132 | 0.233         | 0.157 | 0.417        | 0.228         |
| MAD-GAN     | 0.990        | 0.637 | 0.770         | 0.414        | 0.339 | 0.370         | -     | -            | -             |
| MTAD-GAT    | 0.991        | 0.633 | 0.772         | 0.988        | 0.153 | 0.265         | 0.128 | 0.397        | 0.193         |
| GDN         | <u>0.994</u> | 0.681 | 0.810         | 0.975        | 0.402 | 0.570         | 0.385 | 0.937        | 0.546         |
| TranAD      | 0.976        | 0.699 | 0.815         | 0.353        | 0.829 | 0.495         | 0.305 | 0.715        | 0.428         |
| FuSAGNet    | 0.988        | 0.726 | 0.837         | 0.830        | 0.479 | <u>0.607</u>  | -     | -            | -             |
| MAD-SGCN    | 0.986        | 0.690 | 0.823         | 0.564        | 0.399 | 0.552         | 0.416 | 0.688        | 0.518         |
| HFN         | 0.973        | 0.758 | 0.852         | 0.827        | 0.413 | 0.551         | 0.505 | 0.837        | 0.630         |

## 530 4.4. Experimental analysis

The optimal metric values are shown in bold in Table 3. For the datasets SWaT and WADI, we refer to the results in USAD [66] and graph deviation network (GDN) [54]. For WTD dataset, to guarantee the objectivity of the results, we only report the metrics from the obtained open code approaches.

# 535 4.4.1. Performance comparison of anomaly detection

To demonstrate the performance of the proposed model, we evaluated 536 the precision, recall, and F1 of all methods on the test set. We can ob-537 serve from Table 3 that HFN shows a good abnormal detection capability 538 with remarkable performance improvements on SWaT and WTD. The im-539 provement range of the proposed approach is 5% to 14%, as compared with 540 the optimal baseline models. The optimal baseline GDN outperforms our 541 approach in terms of F1; however, our approach has a more optimal re-542 call rate. It is acceptable in real scenarios because we hope to detect more 543 anomalies. In short, HFN outperforms the selected baselines in terms of 544 the overall performances, because it not only concerns with the traditional 545 spatial-temporal correlation, but also obtains its heterogeneous attributes 546 from different types of data, making the model more robust. Moreover, we 547 observe that prediction-based algorithms such as HFN, GDN and LSTM-548 NDT outperform the reconstruction-based algorithms such as LSTM-VAE 549 and USAD on these datasets, indicating that the prediction-based models 550 have an advantage in the streaming abnormal detection tasks with a single-551 timestamp value as the target. The temporal information is also very vital 552 in the tasks for MTS abnormal detection. The results of LSTM-NDT show 553 that HFN outperforms all baselines except GDN. The PCA result is dissat-554 isfactory, because it gives more attentions to the point anomalies without 555 spatial-temporal correlation being considered. 556

Specifically, among these abnormal detection approaches, GDN, MTAD-557 GAT and HFN adopt the graph attention network to capture the tem-558 poral and feature correlations. Therefore, these types of models achieve 559 good results on all datasets. GDN approach recodes multidimensional data 560 at each moment, and utilizes its strong structural learning capability of 561 graph attention network to learn coupling relations between different sensors. 562 However, it does not consider the heterogeneity of data. MTAD-GAT ap-563 proach also captures time-dimension information through an attention mech-564 anism. Although it considers the spatial-temporal correlation of MTS, it 565 requires a configuration of hyper-parameters for fusing the prediction-based 566

and reconstruction-based condition scores, leading to the evident differences 567 in results when this approach is applied to different datasets. Compared to 568 the recently introduced transformer-based TranAD, as well as the spatial-569 temporal graph networks FuSAGNet and MAD-SGCN, HFN continues to 570 exhibit superior performance on the SWaT and WTD datasets. However, 571 the most recent experimental outcomes suggest that FuSAGNet achieved the 572 top results on the WADI dataset. Nonetheless, our attempts to reproduce 573 this outcome using the authors' open-sourced code were unsuccessful. 574

Furthermore, although we processed different types of data separately, our optimization efforts were predominantly concentrated on enhancing the network structure without introducing a significant increase in complexity. Consequently, the processing time did not exhibit a substantial increase when handling the same amount of data.

## 580 4.4.2. Ablation experiment

We utilize SWaT and WADI datasets to study the necessity of five com-581 ponents of our approach, namely, node embedding similarity matrix (NE), 582 node feature similarity matrix (NF), discrete feature subgraph (DFS), contin-583 uous feature subgraph (CFS), and hybrid feature subgraph (HFS). As shown 584 in Figure 4, we successively exclude the corresponding component from the 585 experiments to observe its effect on the model performance. The key idea 586 of our approach is to learn the potential steady representations from het-587 erogeneous MTS. Hence, first, we exclude NE or NF to study whether the 588 heterogeneous information is learned. Second, we discuss the anomaly detec-580 tion performance when we only use HFS or DFS and CFS. Specifically: 590

- Excluding NF (expressed as "-NF") degrades the overall performance
   of the approach and has a great influence on WADI dataset. This
   indicates that NF is in favor of feature extraction with high-dimensional
   dataset for the model; however, NF is not the key factor to determine
   the model performance.
- Excluding NE (expressed as "-NE") degrades the performances clearly,
   which implies that NE has an evident advantage in the graph structure
   learning process.
- Excluding DFS and CFS (expressed as "-DFS" and "-CFS") degrades the model performance; however, the descend range of model performance is less than that of NE. This approach is actually degenerated



Figure 4: Effects of different HFN components on anomaly detection performance.

- to the processing of isomorphic graphs, leading to the loss of heterogeneous information.
- Excluding HFS (expressed as "-HFS") degrades the model performance; however, it is superior to the cases when DFS and CFS are totally excluded. This indicates that the interaction between different types of sensors in the hybrid subgraph plays a complementary role in extracting the follow-up HFN heterogeneous information.

To sum up, it is necessary to extract heterogeneous structure information in the MTS datasets. The heterogeneous information can present different weights in the model according to the attention mechanism, which helps to improve the abnormal detection performance.

613 4.4.3. Case study

## 614 (1) Anomaly detection analysis

Figure 5 shows the abnormal detection results on SWaT testing dataset, where Figure 5(a) represents the actual data anomalies on this dataset, including network and physical attacks directed at the Secure Water Treatment (SWaT) testbed within the continuous four days. The data are labeled as 1 if the system is attacked at a certain timestamp; otherwise, it is labeled as 0. Figure 5(b) represents the results of HFN anomaly detection, where



Figure 5: SWaT dataset anomaly detection results.

the orange shadow represents the detected anomalies, the blue curve repre-621 sents the condition scores calculated as described in Section 3.6, and the red 622 straight line represents the threshold when the optimal F1 is obtained on 623 the testing dataset. It can be seen from Figure 5(b) that, aside from a few 624 anomalies that are very difficult to distinguish possibly due to labeling errors, 625 our approach accurately identifies the most anomalies. According to the in-626 structions provided by SWAT dataset [62], we select an attack case to further 627 interpret the abnormal detection capability of HFN. As shown in Figure 5(a), 628 the attack starts from  $14:16:00\ 28/12/2015$  to  $14:28:00\ 28/12/2015$  against 629 FIT401, UV401 and P501, where FIT401 is the flow transmitter for mea-630 suring the flow of UV de-chlorinator, UV401 is de-chlorinator for removing 631 chlorine from water, and P501 is pump actuator for pumping the dechlori-632 nated water to reverse osmosis. During the attack, as shown in Figure 6, the 633 flow value (continuous value) of FIT401 is set twice to the value deviating 634 from the normal mode. Meanwhile, the actuators UV401 and P501 (discrete 635 value), which should be kept to an open state, are forcefully closed. 636

Figure 6 shows the curves of actual and predicted values of attack-related 637 sensors and actuators and the HFN anomaly detection results. In order to 638 reduce the influence of data dimensions and accelerate the convergence of 639 the model, we have standardized the values of the dataset by min-max nor-640 malization. It is worth noting that we used the same normalized parameters 641 for both the training dataset and the testing dataset, which is why the nor-642 malized data of the testing data shown in Figure 6 has negative values. This 643 was done to reduce the impact of testing data information leakage on the 644 model performance. In the real water treatment process, the unit of the flow 645 sensors values are gallons per minute (GPM), while the actuators have two 646 conditions: 0 means turn on and - 1 means turn off. 647

It can be seen from Figure 6(a), (c) and (d) that before the attack, the 648 predicted values of HFN are consistent with the actual values, where the 649 prediction for both continuous variables and discrete variables achieves good 650 results. In the attack process, the flow variation arises from the prediction 651 result of FIT401 and UV401 simultaneously. This is due to the interaction 652 among these variables in the actual water treatment system. A larger devia-653 tion between the predicted value and the actual value would provide a better 654 basis for abnormal detection. Note that although the experiment personnel 655 did not launch the attack on FIT504 sensor in the attack process, we can see 656 from Figure 6(b) and (d) that the value changes of FIT504 are still detected, 657 which is due to being abnormally closed caused by the attack on P501. We 658 can observe from the detection results in Figure 6(e) that the proposed ap-659 proach shows a good detection capability of such complex anomalies. These 660 anomalies have been resulted from attacks to different types of sensors, in-661 cluding continuity, discreteness and their correlation, which represent real 662 scenarios. 663

## 664 (2) Anomaly localization analysis

From the above analysis, we can see that our method can successfully 665 detect the occurrence of anomalies. However, we cannot assume that all 666 the variables in a real complicated system are of the same significance. In 667 other words, the variables associated with a particular system component 668 will be impacted to varying degrees of operation when that component is 660 attacked or behaves abnormally. Therefore, it is necessary to locate vari-670 ables that have been strongly impacted by the attack, thus helping system 671 maintenance personnel to rapidly find and solve the problems. We use the 672 prediction error of each time-series sensor to represent the condition score of 673 the sequence where the sensor with the maximum score times is considered 674



Figure 6: Abnormal detection case. The orange shadow represents the detected anomalies. The blue curve denotes the actual value of sensor or actuator. The orange dotted line represents the predicted value. The green and red curves in Fig. 6(e) represent condition score and the threshold of the optimal F1, respectively.



Figure 7: Maximum number of sensor scores in the abnormal dataset.

to have the possibility of the biggest anomalies. Figure 7 shows the number 675 of times when the condition scores are above the threshold for different sen-676 sors within the attack period in the case analysis. It can be known from the 677 figure that the sensors FIT504 and FIT401 have the maximum score times, 678 which is consistent with the attacks where the experiment personnel made to 679 the sensor FIT401 and pump actuator P501 during the tests. The turn-off 680 attacks on P501 caused a sharp drop in the FIT504 flow values, as shown in 681 Figure 6(d), since they are physically connected. On the contrary, we can 682 also speculate which component of the system has been attacked or abnormal 683 according to the maximum score times. In this case, during real operation 684 and maintenance, particular attention should be paid to and checks should 685 be made on the locations relating to FIT504, FIT401, and LIT401. 686

#### 687 4.5. Feasibility analysis

To further illustrate how the heterogeneous relation in time series is learned and takes effect on the abnormal detection, we explain it through the similarity matrix before and after the anomalies due to the attacks. Figure 8 and Figure 9 represent different similarity matrices before and after the attack on SWaT, respectively. Its similarity value range is [-1,1], and



Figure 8: Example of similarity subgraphs under normal conditions.



Figure 9: Example of similarity subgraphs under attack conditions.

the closer to 1, the stronger the similarity is. Overall, HFN aggregates the 693 similarities of sensor signals from different perspectives to represent its het-694 erogeneous information. Embedding similarity matrix learns the structural 695 information among different sensors globally from the training data. Hence, 696 similar features are shown in Figure 8(b) and Figure 9(b) under abnormal 697 and normal states. However, concerning the feature similarity, we can see 698 clearly that there exist significant differences in feature similarity between 690 Figure 8(a) and Figure 9(a) at different timestamps, because the data vary 700 with time. Ignoring this part of information always degrades the abnormal 701 detection performance. 702

Specifically, as shown in Figure 8(a), before the attacks on FIT401, UV401 703 and P501, the similarity values of FIT504 flow value and other continuous 704 variable sensor values are close to 1. However, after the attack, we can see 705 from Figure 9(a) that the similarity value varies to -0.75. The sudden change 706 indicates that the sensor anomalies occur, while there are slight variations in 707 the embedding similarity. After comparing the adjacent matrix before and 708 after the attack in Figure 8(d) and Figure 9(d), we can find that the changes 709 in feature similarity cause the changes in the connection relation to improve 710 the ability of the algorithm in capturing dynamic feature correlation. This 711 further demonstrates that HFN, by aggregating the global data learning-712

<sup>713</sup> based embedding similarity matrix and the feature similarity matrix at a
<sup>714</sup> specific timestamp, can better capture the normal and abnormal conditions
<sup>715</sup> in MTS.

#### 716 5. Conclusions

In this paper, we propose a novel heterogeneous feature network for MTS 717 anomaly detection. This approach is able to learn the complex heteroge-718 neous structural information and temporal information between MTS data. 719 Therefore, it is suitable for abnormal detection in real scenarios where the 720 dataset comprises continuous numerical variables and discrete categorical 721 variables simultaneously. The extensive experiments indicate that our ap-722 proach outperforms the baseline models by assessing two open datasets from 723 water treatment plants and a private dataset from a wind power plant. Par-724 ticularly noteworthy is its significant performance improvement on the SWaT 725 and WTD-V2 datasets, where the F1 score increased by 5% and 14%, respec-726 tively, compared to the best baseline. Furthermore, our approach demon-727 strates a good abnormal interpretability and can help operation and main-728 tenance personnel rapidly discover and locate the anomalies. 729

In the future, we will continue to explore various avenues to enhance 730 the proposed algorithm. We plan to extend its capabilities by incorporat-731 ing more real and complex heterogeneous datasets, encompassing combined 732 time series data and textual information. This expansion aims to boost the 733 accuracy and practicality of the approach. While our method excels in di-734 verse data handling, potential challenges in computational efficiency may 735 arise with larger datasets. Future efforts will be directed towards optimizing 736 the algorithm for improved scalability, especially in scenarios involving more 737 extensive network scales. Additionally, we aim to investigate the impact of 738 varying sampling intervals on our method across different datasets, thereby 739 broadening its applicability. 740

#### 741 Acknowledgement

The work is supported by National Natural Science Foundation of China
(62006236), NUDT Research Project (ZK20-10), National Key Research and
Development Program of China (2020YFA0709803), Hunan Provincial Natural Science Foundation (2020JJ5673), National Science Foundation of China

(U1811462), National Key R&D project by Ministry of Science and Technology of China (2018YFB1003203), and Autonomous Project of HPCL
(201901-11, 202101-15).

#### 749 **References**

- [1] K. Hundman, V. Constantinou, C. Laporte, I. Colwell, T. Soderstrom,
   Detecting spacecraft anomalies using lstms and nonparametric dynamic
   thresholding.
- [2] H. Zhou, K. Yu, X. Zhang, G. Wu, A. Yazidi, Contrastive autoencoder
   for anomaly detection in multivariate time series, Information Sciences
   610 (2022) 266–280.
- [3] J. Zhan, R. Wang, L. Yi, Y. Wang, Z. Xie, Health assessment methods for wind turbines based on power prediction and mahalanobis distance, International Journal of Pattern Recognition and Artificial Intelligence 33 (02) (2019) 1951001.
- [4] G. Pang, C. Shen, L. Cao, A. V. D. Hengel, Deep learning for anomaly
  detection: A review, ACM Computing Surveys (CSUR) 54 (2) (2021)
  1-38.
- [5] H. Mamdouh Farghaly, M. Y. Shams, T. Abd El-Hafeez, Hepatitis c
  virus prediction based on machine learning framework: a real-world case
  study in egypt, Knowledge and Information Systems 65 (6) (2023) 2595–
  2617.
- [6] P. D. Rosero-Montalvo, Z. István, P. Tözün, W. Hernandez, Hybrid anomaly detection model on trusted iot devices, IEEE Internet of Things Journal (2023).
- [7] P. Wu, J. Liu, Learning causal temporal relation and feature discrimination for anomaly detection, IEEE Transactions on Image Processing 30 (2021) 3513–3527.
- [8] B. Lindemann, B. Maschler, N. Sahlab, M. Weyrich, A survey on anomaly detection for technical systems using lstm networks, Computers in Industry 131 (2021) 103498.

- [9] J. Yang, L. Zhang, C. Chen, Y. Li, R. Li, G. Wang, S. Jiang, Z. Zeng,
  A hierarchical deep convolutional neural network and gated recurrent
  unit framework for structural damage detection, Information Sciences
  540 (2020) 117–130.
- [10] A. Blázquez-García, A. Conde, U. Mori, J. A. Lozano, A review on outlier/anomaly detection in time series data, ACM Computing Surveys (CSUR) 54 (3) (2021) 1–33.
- [11] H. Zhao, Y. Wang, J. Duan, C. Huang, Q. Zhang, Multivariate time series anomaly detection via graph attention network (2020) 841–850.
- [12] S. Du, T. Li, Y. Yang, S.-J. Horng, Multivariate time series forecasting
  via attention-based encoder-decoder framework, Neurocomputing 388
  (2020) 269–279.
- [13] T.-Y. Kim, S.-B. Cho, Predicting residential energy consumption using
   cnn-lstm neural networks, Energy 182 (2019) 72–81.
- <sup>790</sup> [14] K. He, X. Zhang, S. Ren, J. Sun, Deep residual learning for image <sup>791</sup> recognition (2016) 770–778.
- [15] Z. Wu, S. Pan, G. Long, J. Jiang, X. Chang, C. Zhang, Connecting the
  dots: Multivariate time series forecasting with graph neural networks
  753–763.
- [16] Y. Guo, W. Liao, Q. Wang, L. Yu, T. Ji, P. Li, Multidimensional time
   series anomaly detection: A gru-based gaussian mixture variational au toencoder approach 97–112.
- [17] D. Li, D. Chen, B. Jin, L. Shi, J. Goh, S.-K. Ng, Mad-gan: Multivari ate anomaly detection for time series data with generative adversarial
   networks (2019) 703–716.
- [18] V. Borisov, T. Leemann, K. Seßler, J. Haug, M. Pawelczyk, G. Kas neci, Deep neural networks and tabular data: A survey, arXiv preprint
   arXiv:2110.01889 (2021).
- [19] A. Nazabal, P. M. Olmos, Z. Ghahramani, I. Valera, Handling incomplete heterogeneous data using vaes, Pattern Recognition 107 (2020)
  107501.

- [20] Y. Sun, J. Han, X. Yan, P. S. Yu, T. Wu, Pathsim: Meta path-based topk similarity search in heterogeneous information networks, Proceedings
  of the VLDB Endowment 4 (11) (2011) 992–1003.
- <sup>810</sup> [21] X. Wang, H. Ji, C. Shi, B. Wang, Y. Ye, P. Cui, P. S. Yu, Heterogeneous graph attention network 2022–2032.
- [22] M. Lngkvist, L. Karlsson, A. Loutfi, A review of unsupervised feature
  learning and deep learning for time-series modeling, Pattern Recognition
  Letters 42 (2014) 11–24.
- [23] J. Li, H. Izakian, W. Pedrycz, I. Jamal, Clustering-based anomaly detection in multivariate time series data, Applied Soft Computing 100 (4)
  (2020) 106919.
- [24] J. Zhao, K. Liu, W. Wang, Y. Liu, Adaptive fuzzy clustering based anomaly data detection in energy system of steel industry, Information Sciences 259 (2014) 335–345.
- <sup>821</sup> [25] M. Jones, D. Nikovski, M. Imamura, T. Hirata, Anomaly detection in <sup>822</sup> real-valued multidimensional time series.
- [26] E. G. S. Nascimento, O. de Lira Tavares, A. F. De Souza, A clusterbased algorithm for anomaly detection in time series using mahalanobis
  distance 622.
- [27] G. Pu, L. Wang, J. Shen, F. Dong, A hybrid unsupervised clusteringbased anomaly detection method, Tsinghua Science and Technology
  26 (2) (2020) 146–153.
- [28] W. Jia, R. M. Shukla, S. Sengupta, Anomaly detection using supervised
  learning and multiple statistical methods (2019) 1291–1297.
- [29] N. Görnitz, M. Kloft, K. Rieck, U. Brefeld, Toward supervised anomaly
   detection, Journal of Artificial Intelligence Research 46 (2013) 235–262.
- [30] L. Ruff, R. A. Vandermeulen, N. Görnitz, A. Binder, E. Müller, K.R. Müller, M. Kloft, Deep semi-supervised anomaly detection, arXiv
  preprint arXiv:1906.02694 (2019).

- [31] M. E. Villa-Pérez, M. A. Alvarez-Carmona, O. Loyola-González, M. A.
  Medina-Pérez, J. C. Velazco-Rossell, K.-K. R. Choo, Semi-supervised anomaly detection algorithms: A comparative summary and future research directions, Knowledge-Based Systems 218 (2021) 106878.
- [32] R. Wang, X. Ma, C. Jiang, Y. Ye, Y. Zhang, Heterogeneous information network-based music recommendation system in mobile networks, Computer Communications 150 (2020) 429–437.
- [33] X. Liang, Y. Ma, G. Cheng, C. Fan, Y. Yang, Z. Liu, Meta-path-based
  heterogeneous graph neural networks in academic network, International
  Journal of Machine Learning and Cybernetics 13 (6) (2022) 1553–1569.
- <sup>846</sup> [34] X. Deng, F. Long, B. Li, D. Cao, Y. Pan, An influence model based on
  <sup>847</sup> heterogeneous online social network for influence maximization, IEEE
  <sup>848</sup> Transactions on Network Science and Engineering 7 (2) (2019) 737–749.
- [35] X. Chen, J. Yin, J. Qu, L. Huang, Mdhgi: matrix decomposition and
  heterogeneous graph inference for mirna-disease association prediction,
  PLoS computational biology 14 (8) (2018) e1006418.
- [36] Y. Sun, J. Gao, X. Hong, B. Mishra, B. Yin, Heterogeneous tensor decomposition for clustering via manifold optimization, IEEE transactions on pattern analysis and machine intelligence 38 (3) (2015) 476–489.
- <sup>855</sup> [37] Y. Liu, X. Luo, X. Yang, Semantics and structure based recommenda-<sup>856</sup> tion of similar legal cases 388–395.
- [38] C. Wang, C. H. Chi, Z. Wei, R. Wong, Coupled interdependent attribute
  analysis on mixed data (2015).
- <sup>859</sup> [39] S. Jian, L. Cao, G. Pang, L. Kai, G. Hang, Embedding-based representation of categorical data by hierarchical value coupling learning (2017).
- [40] H. Cai, V. W. Zheng, K. C.-C. Chang, A comprehensive survey of graph
  embedding: Problems, techniques, and applications, IEEE Transactions
  on Knowledge and Data Engineering 30 (9) (2018) 1616–1637.
- <sup>864</sup> [41] J. Zhao, X. Wang, C. Shi, B. Hu, G. Song, Y. Ye, Heterogeneous graph structure learning for graph neural networks 35 (5) (2021) 4697–4705.

- [42] X. Fu, J. Zhang, Z. Meng, I. King, Magnn: Metapath aggregated graph
   neural network for heterogeneous graph embedding 2331–2341.
- <sup>868</sup> [43] X. Wang, N. Liu, H. Han, C. Shi, Self-supervised heterogeneous graph <sup>869</sup> neural network with co-contrastive learning 1726–1736.
- <sup>870</sup> [44] Z. Hu, Y. Dong, K. Wang, Y. Sun, Heterogeneous graph transformer <sup>871</sup> 2704–2710.
- <sup>872</sup> [45] L. Yang, Z. Xiao, W. Jiang, Y. Wei, Y. Hu, H. Wang, Dynamic heterogeneous graph embedding using hierarchical attentions (2020) 425–432.
- <sup>874</sup> [46] M. Chen, C. Huang, L. Xia, W. Wei, Y. Xu, R. Luo, Heterogeneous graph contrastive learning for recommendation (2023) 544–552.
- <sup>876</sup> [47] Y. Zhu, Y. Xu, H. Cui, C. Yang, Q. Liu, S. Wu, Structure-enhanced <sup>877</sup> heterogeneous graph contrastive learning (2022) 82–90.
- [48] P. Bloomfield, Fourier analysis of time series: an introduction, John
  Wiley & Sons, 2004.
- [49] R. Shwartz-Ziv, A. Armon, Tabular data: Deep learning is not all you need, Information Fusion 81 (2022) 84–90.
- <sup>882</sup> [50] Y. Zhu, W. Xu, J. Zhang, Q. Liu, S. Wu, L. Wang, Deep graph
  <sup>883</sup> structure learning for robust representations: A survey, arXiv preprint
  <sup>884</sup> arXiv:2103.03036 (2021).
- <sup>885</sup> [51] R. Li, S. Wang, F. Zhu, J. Huang, Adaptive graph convolutional neural <sup>886</sup> networks 32.
- <sup>887</sup> [52] X. Wang, M. Zhu, D. Bo, P. Cui, C. Shi, J. Pei, Am-gcn: Adaptive <sup>888</sup> multi-channel graph convolutional networks 1243–1253.
- <sup>889</sup> [53] Y. Chen, L. Wu, M. Zaki, Iterative deep graph learning for graph neural networks: Better and robust node embeddings, Advances in Neural Information Processing Systems 33 (2020) 19314–19326.
- <sup>892</sup> [54] A. Deng;, B. Hooi., Graph neural network-based anomaly detection in <sup>893</sup> multivariate time series, aaai2021 (2021).

- <sup>894</sup> [55] D. Yu, R. Zhang, Z. Jiang, Y. Wu, Y. Yang, Graph-revised convolutional <sup>895</sup> network 378–393.
- <sup>896</sup> [56] D. Luo, W. Cheng, W. Yu, B. Zong, J. Ni, H. Chen, X. Zhang, Learning
  <sup>897</sup> to drop: Robust graph neural network via topological denoising 779–
  <sup>898</sup> 787.
- <sup>899</sup> [57] Q. Sun, J. Li, H. Peng, J. Wu, X. Fu, C. Ji, P. S. Yu, Graph structure learning with variational information bottleneck, arXiv preprint arXiv:2112.08903 (2021).
- <sup>902</sup> [58] X. Gao, W. Hu, Z. Guo, Exploring structure-adaptive graph learning
   <sup>903</sup> for robust semi-supervised classification 1–6.
- <sup>904</sup> [59] P. Kaewprapha, P. Prempaneerach, V. Singh, T. Tinikul, N. Intarangsi,
  <sup>905</sup> T. Kijkanjanarat, Predicting full load, partial load efficiency of a com<sup>906</sup> bined cycle power plant using machine learning methods 11–16.
- <sup>907</sup> [60] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez,
  <sup>908</sup> L. Kaiser, I. Polosukhin, Attention is all you need, arXiv (2017).
- [61] H. Ren, B. Xu, Y. Wang, C. Yi, C. Huang, X. Kou, T. Xing, M. Yang,
  J. Tong, Q. Zhang, Time-series anomaly detection service at microsoft
  3009–3017.
- <sup>912</sup> [62] J. Goh, S. Adepu, K. N. Junejo, A. Mathur, A dataset to support re-<sup>913</sup> search in the design of secure water treatment systems (2017) 88–99.
- <sup>914</sup> [63] C. M. Ahmed, V. R. Palleti, A. P. Mathur, Wadi: a water distribution <sup>915</sup> testbed for research in the design of secure cyber physical systems.
- <sup>916</sup> [64] J. Zhan, S. Wang, X. Ma, C. Wu, C. Yang, D. Zeng, S. Wang, Stgat<sup>917</sup> mad: Spatial-temporal graph attention network for multivariate time
  <sup>918</sup> series anomaly detection 3568–3572.
- <sup>919</sup> [65] D. Park, Y. Hoshi, C. C. Kemp, A multimodal anomaly detector
  <sup>920</sup> for robot-assisted feeding using an lstm-based variational autoencoder,
  <sup>921</sup> IEEE Robotics and Automation Letters PP (99) (2017).
- <sup>922</sup> [66] J. Audibert, P. Michiardi, F. Guyard, S. Marti, M. A. Zuluaga, Usad:
   <sup>923</sup> Unsupervised anomaly detection on multivariate time series 3395–3404.

- J. Camacho, A. Pérez-Villegas, P. García-Teodoro, G. Maciá-Fernández,
   Pca-based multivariate statistical network monitoring for anomaly de tection, Computers & Security 59 (2016) 118–137.
- 927 [68] T. L. Fei, M. T. Kai, Z. H. Zhou, Isolation forest.
- <sup>928</sup> [69] M. Qi, Lightgbm: A highly efficient gradient boosting decision tree.
- [70] S. Tuli, G. Casale, N. R. Jennings, Tranad: Deep transformer networks
  for anomaly detection in multivariate time series data, arXiv preprint
  arXiv:2201.07284 (2022).
- <sup>932</sup> [71] S. Han, S. S. Woo, Learning sparse latent graph representations for anomaly detection in multivariate time series (2022) 2977–2986.
- <sup>934</sup> [72] P. Qi, D. Li, S.-K. Ng, Mad-sgcn: Multivariate anomaly detection with <sup>935</sup> self-learning graph convolutional networks (2022) 1232–1244.
- [73] L. Shen, Z. Li, J. Kwok, Timeseries anomaly detection using temporal
   hierarchical one-class network, Advances in Neural Information Process ing Systems 33 (2020) 13016–13026.
- <sup>939</sup> [74] S. Kim, K. Choi, H. S. Choi, B. Lee, S. Yoon, Towards a rigorous eval<sup>940</sup> uation of time-series anomaly detection (2021).