Fault Diagnosis of Process Systems based on Graph Neural Network

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Abstract: The fault diagnosis methods for process systems are generally based on rules and experience, which struggle with complex and uncertain issues. Therefore, In this study, a fault diagnosis method for process systems using adaptive Graph Neural Networks (GNNs) is proposed. This method effectively utilizes the correlations and dynamic changing among sensors, constructing a graph structure that reflects the complex relationships between sensors. By employing the graph convolutional neural network as the model foundation, it effectively extracts the primary changing features of faults, thereby addressing the problem of multi-class fault diagnosis. Comparative experiments were conducted using the fault diagnosis task of a three-phase flow system. The proposed method outperforms traditional models in terms of accuracy, precision, recall, and F1 score, demonstrating its effectiveness in fault diagnosis of process industrial systems.

1 INTRODUCTION

Process systems are complex systems that include various devices and subsystems. These devices are interconnected during operation, and a failure in any one device can affect the performance of the entire system. Therefore, fault diagnosis of process systems is of utmost importance. Traditional fault diagnosis methods often only consider the performance of individual devices, neglecting the correlations between devices, which limits the accuracy and efficiency of fault diagnosis. In traditional control systems, all analysis and control strategy designs are based on the premise that the characteristics of the process system remain unchanged, and all sensors, actuators, and signal transmission channels are functioning normally. A fault in any unit of the system can affect the normal operation and safe production of the system. Faults or failures in any part of the process control system can pose threats to property and personnel safety, causing immeasurable losses and even potentially leading to major accidents (Ma et al., 2019).With the development of modern process systems towards greater complexity, the likelihood of system failures increases, along with the economic losses and potential harms caused by system failures, such as casualties, property damage, and environmental pollution. Therefore, timely understanding of the operating state of process systems, effective anomaly monitoring, and fault diagnosis to take appropriate control strategies in response to anomalies or faults are crucial for ensuring the quality and safe operation of process systems, reducing operating costs, and are of great significance for the production efficiency of process systems. Real-time monitoring of the operational state of process systems, especially for the detection, diagnosis, and elimination of faults, is necessary to ensure the reliability and safety of actual systems. This requires the establishment of a process monitoring system to monitor the operational state of the entire control system in real-time, detect changes in the system, and read fault information promptly to take effective preventive measures, ensuring the safety of process systems and preventing catastrophic accidents. Constructing a reliable and stable equipment process supervision system has become a priority in mechanical equipment manufacturing, effectively reducing maintenance costs while ensuring the safety of industrial machinery equipment. Currently, most industrial equipment detection systems rely on multiple sensor data for monitoring, such as aircraft engines, rotating machinery rolling bearings, multiphase flow separators, etc., while these

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monitoring systems usually store historical data for training. For complex industrial mechanical systems, multi-sensor data often have high-dimensional and complex interaction characteristics (Jiang and Yin, 2018), posing many challenges to traditional fault diagnosis and health monitoring systems, making supervised machine learning methods feasible.

Traditional fault diagnosis methods often focus on Statistical Process Control (Yu and Wang, 2005) (SPC) and model-based approaches (Wang and Wang, 2006, 2009). Nowadays, fault diagnosis in complex industrial systems is categorized into two main types: model-based and data-driven methods. Due to the complexity and high cost of modeling in industrial systems, model-based methods are severely limited in practical applications. In contrast, data-driven methods, aiming to extract relevant data features and identify fault types through statistical analysis or feature discrimination learning, have been widely applied and rapidly developed. Common fault diagnosis techniques include Support Vector Machines(Mahadevan and Shah, 2009), (SVM), Multilayer Perceptrons (MLP), Convolutional Neural Networks, and Graph Neural Networks. Gu (Gu et al., 2014) employed a method combining Principal Component Analysis (PCA) and Support Vector Machine (SVM) to extract and analyze the fault features of rolling bearings. However, real-world data often contain noise and may be excessively large, which can affect the effectiveness of this diagnostic method. Wang(Wang et al., 2005) and others conducted fault diagnosis on mixed circuits using Multilayer Perceptrons (MLPs) to solve complex classification problems. MLPs address the issue of non-linearity between features, but when facing process fault diagnosis, the prevalence of clear fault data scarcity can lead to overfitting or obtaining local optimum solutions. Additionally, there is a lack of model interpretability. Convolutional Neural Networks (CNNs) have also gradually become widely applied. Chen (Chen and Yu, 2020) used CNNs for feature learning and fault diagnosis in multivariable processes. However, small datasets cannot support the training of deep networks, and for signals transmitted by mechanical or semiconductor components, which are mostly converted into image signals for convolutional training, this approach fails to capture the correlations between multiple components.

To address these challenges, this article proposes a fault diagnosis method for process systems based on adaptive Graph Neural Networks (GNNs). Recently, GNNs have been widely applied in the field of deep learning with significant success. Gori (Gori et al., 2005) first introduced GNNs, designed to directly process graph structures, including directed/undirected graphs, cyclic graphs, and labeled graphs. Due to their ability to accurately represent real-world systems, GNN-based fault diagnosis methods have potential advantages in processing complex mechanical industrial data, especially in mining the topological structures and interactions between sensor data. Wu (Wu et al., 2020) proposed a scalable graph convolution that enables semi-supervised learning with graph-structured data through the combined action of GNNs and Convolutional Neural Networks.

The application of fault diagnosis of process system to graph neural network has gradually become a trend. It handles complex relationships, automatically learns fault features and works for large industrial systems; and performs end-to-end training; handles dynamic graphs and multimodal fusion, etc. for instance Li (Li et al., 2020) by comparing the disadvantages of other deep learning networks to show the relationship between mining signals, we propose a multiple receptive field graph convolutional network (MRF-GCN) based on the original model to effectively carry out data relationship mining. Yang(Yang et al., 2021) this paper proposes a method based on the space-time graph, SuperGraph, which can transform the graph classification task into classifying the nodes in SuperGraph. Zhang (Yu et al., 2021) A fast graph convolution network is proposed, using the method of wavelet decomposition to preprocess the original vibration signal of wind power gearbox to show the time-frequency characteristics in the form of graph, using the fast graph convolution kernel and specific pooling improvement to reduce the number of nodes and realize fast classification. Stewart E (Ding et al., 2020) The deep graph convolution network (DGCN) based on graph theory is applied to the fault diagnosis of roller bearings. This method uses the graph structure constructed to detect the failure of roller bearings of different types and severity of the same type. Kenning (Kenning et al., 2022) The directed graph convolutional neural network (DGCNN) is proposed, and a simple method to alleviate the inherent class imbalance in the graph is described. Zhang (Tong et al., 2021) This paper proposes a transmission line fault detection and classification method based on graph convolution neural network, and establishes a transient fault detection and classification framework based on the idea of prior knowledge. It is not difficult to see that the fusion of data information is crucial for industrial process fault diagnosis (Tang et al., 2021).

For the identification and classification of faults, we need to extend them to the graph level classification level. When constructing the graph level classification model, the corresponding graph topology for each fault to form graph level differentiation. At the same time, in order to retain the graph structure characteristics, it is necessary to effectively fuse the multi-sensor data information to ensure the accuracy and comprehensiveness of fault identification.

This paper aims to elaborate an innovative method for process system in mechanical industry. This method is based on the graph neural network, and its core advantage is that it can deeply mine the topology structure and mutual influence information in the multi-sensor data, so as to improve the detection and diagnosis accuracy of system faults. First, this paper transforms the one-dimensional time-domain sensor data into graph structure data, where the nodes represent the measurements of each sensor and the edges represent the intercorrelation between the sensors. After the adaptive node importance screening, a graph neural network model was constructed. Through the model, hidden information about the fault features and topology in multi-scale sensor data.

2 MODELING

2.1 Relevance and Centrality Filtering

Fault diagnosis in process systems is a complex issue involving many variables and potential problems. It often overlooks the linear or nonlinear relationships between devices. Graph Neural Networks (GNNs) address this by modeling the interactions between devices (variables) in the system, thereby offering a better solution.

There is graph G (V, E), V is a collection of nodes and E is used to represent the connection between nodes. In statistics, Pearson cross-relations (Dominic. Edelmann et al., 2021) (Pearson Correlation Coefficient) It can be used to reflect the degree of linear correlation between two random temporal variables. With this point, this paper tries to measure the correlation relationship between nodes and construct graph data. The Pearson's correlation coefficient is as follows:

$$r = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \bar{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}} \quad (1)$$

The larger the value is, the stronger the correlation between the two nodes is, which solves the linear relationship between the device variables.

r The Pearson correlation coefficient is used to calculate the linear relationship between nodes, and then the threshold Q is set to restrict, thus further obtaining a streamlined graph data structure, reducing the redundancy of data calculation, and enhancing the efficiency of data feature extraction.

$$r_{ij} = \begin{cases} 0 \cdots\cdots r < Q \\ 1 \cdots\cdots r \geq Q \end{cases} \quad (2)$$

When the Pearson correlation coefficient between any nodes in the graph structure is greater than or equal to the threshold value, it is concluded that the two nodes are mutually first-order neighbors, and otherwise, the connection relationship cannot be constructed.

For each node feature vector v_iThe eigenvector centrality of node i is obtained, and the eigenvector centrality score for all nodes is finally calculated and normalized. Through the variant sigmoid function, the final node importance vector is multiplied as the node weight value by the graph adjacency matrix from the initial calculation, to obtain the final graph structure matrix, thus forming M fault sample maps.

Eigenvector centrality involves finding the principal eigenvector of the adjacency matrix (i. e., the eigenvector associated with the maximum eigenvalue). Suppose that λ is the maximum eigenvalue of the adjacency matrix A, and x is the corresponding eigenvector. Then, x satisfies the following characteristic equation:

$$Ax = \lambda x \quad (3)$$

Each element x in the feature vector x_iDenotes the eigenvector centrality score of the corresponding nodes. Usually, we standardize x:

$$A_{i,j}' = A_{i,j} \times min(sigmoid(normalize(x_i), \beta), sigmoid(normalize(x_j), \beta)) \quad (4)$$

2.2 Dataset of Graph

The graph dataset consists of n small graphs, denoted as G = {G1, G2, G3, G4, …, Gn}, where each graph Gi = (Xi, Vi, Ei, Yi). Here,$X_i \in (n_i \times m)$ denote the input feature matrix of the nodes, with n_i being the number of nodes in the i-th graph (in this paper, aside from the normal state graph data and the sixth fault graph data which have 24 nodes, all other graph data consist of 23 nodes), and m being the number of features per node. V_i is the set of nodes, E_i represents the connections between nodes (including the adjacency matrix$A_i^k \in \Re^{n_i^k \times n_i^k}$), and Y_i denotes the

one-hot encoded value of the i-th graph. In the graph convolutional layer, the input matrix for the k-th layer is denoted $H_i^k \in \mathbb{R}^{n_i^k \times d_k}$, where (n_i^k, d_k) represents the number and dimension of node embeddings in the k-th hidden layer, with the adjacency matrix being denoted A_i^k. accordingly. Following each graph convolutional layer is a graph average pooling layer, which calculates the feature vector for each node to obtain a global representation, with the value on each dimension being the average of the features of all nodes on that dimension. After passing through k-layers of convolutional and pooling layers, the output enters a fully connected layer and an Activation Function ReLU to produce the final output. The scores for each category are calculated using a Softmax function to obtain the model's predicted labels, which are then compared with the true labels. At the same time, a loss function (such as the CrossEntropy Loss function) is used to measure the performance of this graph-level classification model, and gradient Backward is performed. This process iteratively trains the model for effectiveness and stability.

2.3 Graph Neural Network Based on the Weighted Graph under the Correlation

This section is mainly carried out on the improvement of graph data operation, so that the graph convolutional neural network model is easier to extract the feature structure and make more accurate prediction.

In the face of non-European data, according to the graph node information and the data model of the original connection correlation calculation to get the new graph adjacent matrix, the method, while retaining the key connection information of the original model missing connection due to noise or other reasons, and solve the interference of the artificial design figure structure, reduce manpower and reduce labor cost.

Table 1 for the graph convolutional neural network model input and output parameter dimensions, after the original data calculation correlation can get the graph connection under different fault mode, and for each sensor data change adaptive central screening to realize multiple weighted graph data set, improve the accuracy and stability of GCN (Graph Convolution Networks) in data-driven fault diagnosis.

Table 1: Input-output dimensions of each layer.

Layer Name	Input Data Dimension	Output Data Dimensions
Convolutional Layer	*M∗ N∗ F*	*M∗ N∗ F'*
Pooling Layer	*M∗ N∗ F'*	*M∗ N'∗ F''*
Full Connect Layer	*M ∗ N'∗ F''*	*M*(categories)*

3 EXPERIMENTS

This section presents the performance evaluation of fault diagnosis in mechanical industrial processes based on Graph Convolutional Neural Networks (GCN). The model structure of the method proposed in this paper is shown in Figure 1. Experiments are conducted using a three-phase separator dataset to demonstrate the following points: Compared to traditional fault diagnosis methods, the graph convolutional neural network approach is effective and stable in fault diagnosis of process industrial systems.

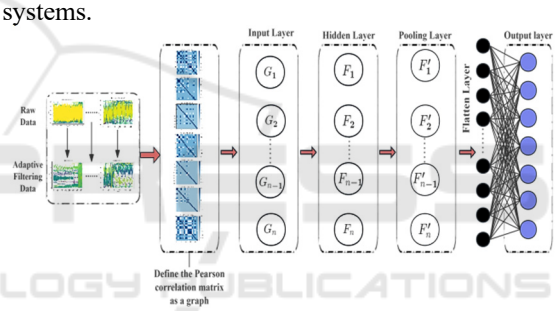


Figure 1: Model structure graph.

3.1 Introduction to the Dataset

The data set presented in this paper uses the Three-phase Flow Facility (TFF) data set of the University of Cranfield (Ruiz-Cárcel et al., 2015). The simulation encompasses the Three-phase flow process commonly encountered in sectors such as the oil and gas industry, involving three types of mixed inputs/outputs: gas, liquid, and solid particles, as illustrated in Figure 2. Within the TFF dataset, it is possible to introduce various types of faults into the system through specific manipulations, simulating issues that might occur in a real plant, such as blockages, operational errors, or unconventional operating conditions. In experiments, the dataset is collected under various operating conditions to ensure that fault detection is not limited to steady-state situations. The datasets can be used to evaluate and compare the performance of multivariate process monitoring techniques based on real experimental

data. The dataset includes normal states under steady-state working conditions and 6 types of simulated faults (all typical faults in actual operation), with each fault data transitioning from a normal state to a weak fault, to a severe fault, and back to a normal state, sampled at a frequency of 1Hz.

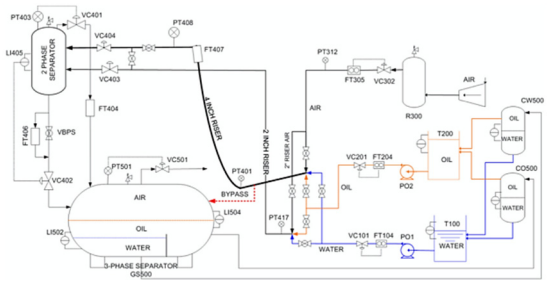


Figure 2: Architecture of the three-phase flow facility(Ruiz-Cárcel et al., 2015).

In this paper, normal data value in the fault data are removed, focusing only on the fault states, and normalization is applied to each sensor's data. Data normalization involves scaling input data to a common range, thereby eliminating the impact on model recognition caused by disparate ranges of feature parameters. The normalization process is represented as follows, constraining the input parameter values within the range [0,1].

$$x_n = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \tag{5}$$

During the process of creating sample graphs, every 20 data points are used to form a feature segment to construct the sample graph. Subsequently, the fault dataset and the normal dataset are randomly merged, with 70% of the combined dataset randomly selected as the training dataset and 30% as the test dataset. Table 2 displays the fault classification and the label values for each state. Figure 3 shows graph-level representations under different fault conditions, sequentially corresponding to the faults listed below. (a. Normal state; b. Airway blockage; c. Water pipe blockage; d. Top separator inlet blockage; e. Bypass valve open; f. Pressure surge; g. System operation anomaly (manual)).

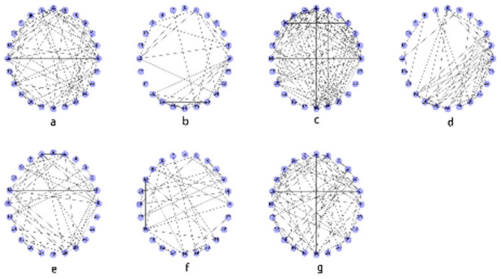


Figure 3: Display of each fault level diagram.

Table 2: Label parameters setting.

Label	Fault Type
0	Normal operation
1	Gas pipe blockage
2	Water pipe blockage
3	Top separator input is blocked
4	Bypass valve open
5	Pressure surge
6	Abnormal operation (artificial)

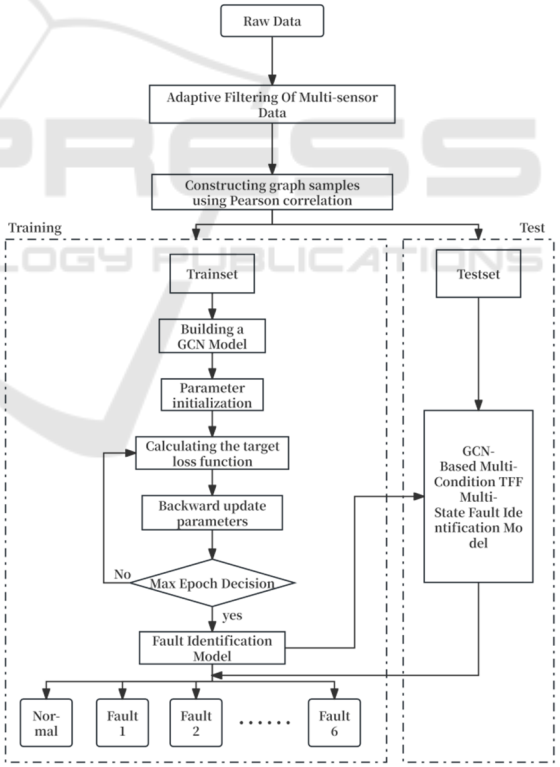


Figure 4: Experimental step.

3.2 Setup

The experimental procedure is illustrated in Figure 4. By utilizing different algorithms such as PCA+SVM, MLP, CNN, and GAT (Graph

Attention Networks) as benchmarks, the method presented in this paper is compared against them, evaluating the stability and effectiveness of fault diagnosis on the aforementioned dataset through various metrics.

This paper employs three metrics to evaluate data-driven classification models: Accuracy Estimation (Accuracy), Precision, Recall, and F1-score. Accuracy is the most common evaluation metric for classification problems, representing the probability of correct predictions for all test samples. Precision and Recall are often used together as indicators to assess the performance of classification models. Precision refers to the accuracy of the classification model in predicting positive samples correctly, that is, among the samples predicted as positive, how many are truly positive samples. Recall refers to the rate at which the classification model correctly identifies all true positive samples, indicating how many of the actual positive samples were correctly recognized. When precision is high, the model's analysis results are more reliable, but it may miss some true positive samples. On the other hand, when recall is high, the model can effectively identify all true positive samples, but it may mistakenly classify some negative samples as positive. The F1-score is the harmonic mean of precision and recall, incorporating the performance of both precision and recall, and is commonly used to evaluate the performance of binary classification models. The F1-score combines the model's precision and recall, providing a single numerical indicator to measure the model's overall performance. Its value generally ranges from 0 to 1, with higher values indicating better model performance.The F1-score includes three different scores: micro-F1, macro-F1, and weighted-F1. This paper uses the first two for calculating and evaluating the classification models. Micro-F1 calculates the F1 score by aggregating the global true positives (TP), false negatives (FN), and false positives (FP). First, the true positives (TP), false positives (FP), and false negatives (FN) values for all categories are summed up, and then these values are inserted into the F1 equation to obtain the micro-F1 score. Macro-F1 calculates the arithmetic mean of the F1 scores for each category. This method treats all fault categories equally without considering the importance of differences between categories.

The experiment comprises a total of 3281 sample sets, with each set consisting of 10 data points. The training and test sets account for 70% and 30% of the total number of samples, respectively, resulting in 2296 sets for the training set and 985 sets for the test set. Each experimental sample is represented by a matrix of size (10 × number of nodes) as the X input feature matrix. In this paper, except for the normal state and fault state with 6 nodes, which have 24 nodes each, all other fault states consist of 23 nodes.In model training, mini-batch training is employed with a BatchSize of 16, and the maximum training epoch is set to 100.The experimental method utilizes a cross-entropy loss function and employs the Adam optimizer along with model parameters, with the learning rate set at 0.0005. In the graph neural network model, two convolutional layers, one Dropout layer (rate = 0.5), and one fully connected layer are adopted, as shown in Table 3:

Table 3: Experimental model parameter setting.

Parameters/Settings	Value	Description	Remarks
Learning Rate	0.0005	Using the Adam optimizer	Search through the grid
Batch size	16		
Epoch	100		
Dropout Rate	0.5	After being applied to the convolution layer	Reduce overfitting
Hidden Layer Size	64		
GCN Layers	3		
Activation Function	ReLU		
Early Stop Strategy	yes	Based on the validation loss	Prevent overfitting

Moreover, the experimental method is implemented on the basis of PyTorch Geometric, and the experimental platform is a computer equipped with an NVIDIA RTX3070 and an Intel i7 10th generation CPU.

4 EXPERIMENTAL VALIDATION

This paper tests the performance of the model by inputting a randomly assigned test dataset into the model trained from the training set. A qualitative analysis of each model's fault identification classification performance is conducted visually

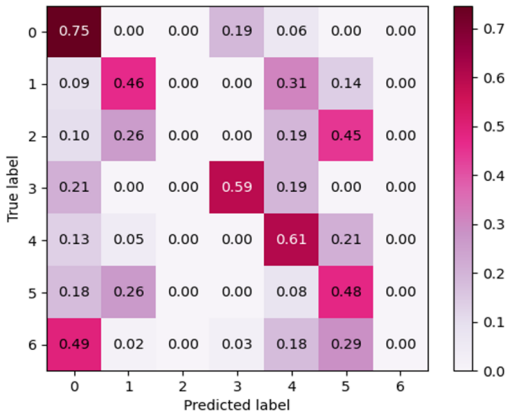
through confusion matrices, evaluating the recognition performance for each fault category. This analysis also identifies issues within the model in graph classification tasks. To reduce the impact of randomness in device computation during the experiment, the experiment was repeated multiple times. It was found that the results did not vary significantly, allowing the selection of one set of results for comparative analysis across different algorithms. This experimental method can quickly improve the model's classification accuracy during the computation process, and after multiple iterations, there is no significant fluctuation in the loss value, indicating the model's rapidity and stability. Table 4 assesses the performance of the experimental method from multiple perspectives by displaying the performance metrics of various algorithms.

It's not difficult to see from the accuracy metric that the model proposed in this paper significantly outperforms traditional fault diagnosis methods and existing popular methods, reaching up to 97% accuracy. This is a 9.2%, 9.4%, and 15% improvement over GAT, CNN, and MLP respectively, and a substantial 44% improvement compared to the traditional PCA+SVM method. In terms of precision, recall, and F1 score, the increase in these metrics further indicates a reduced probability of making incorrect predictions. Consequently, it can be intuitively judged that the model method proposed in this paper has improvements of 6%, 7.5%, and 9% over the CNN method, 25%, 14%, and 20% over the MLP method, and 5.8%, 6%, and 6% over the GAT model, respectively. From this comparative experiment, it can be concluded that the performance evaluation metrics of the proposed method are the highest. This also demonstrates that the method proposed in this paper is effective and robust when implementing dynamic process system fault diagnosis for different fault classification tasks.

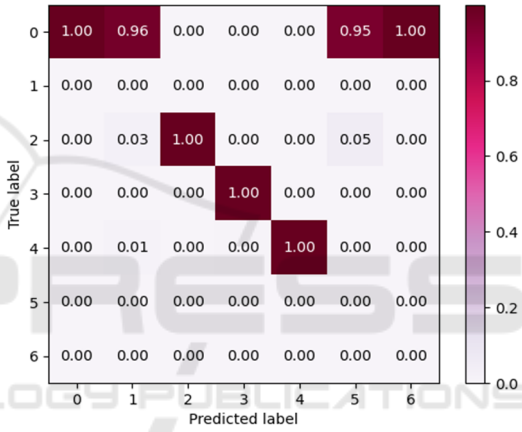
Table 4: Classify performance comparison of each model.

Model	Precision (%)	Accuracy (%)	Recall (%)	Micro F1	Macro F1
PCA+SVM	53.23	49.66	53.23	0.51	0.36
MLP	82.78	71.49	82.77	0.76	0.54
CNN	88.43	90.52	88.43	0.87	0.71
GAT	88.67	90.8	90.8	0.90	0.86
this paper	97.86	96.61	96.17	0.96	0.93

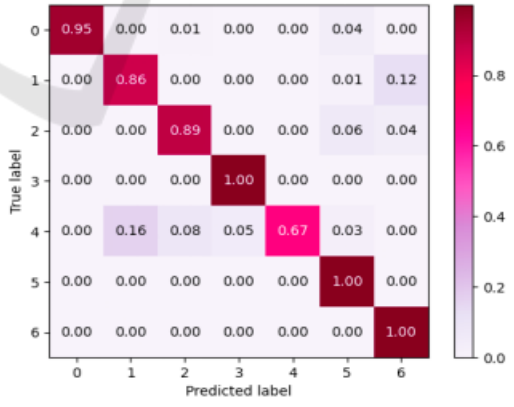
Figure 5 sequentially displays the confusion matrix diagrams for PCA+SVM, MLP, CNN, GAT, and the method mentioned in this paper:



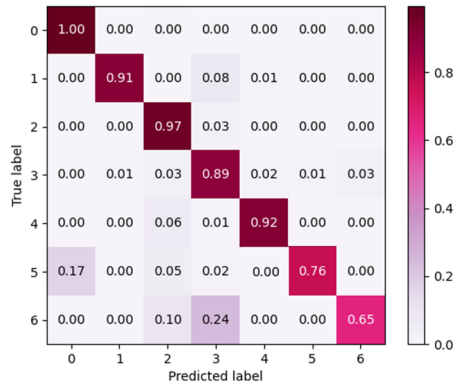
(a)PCA+SVM



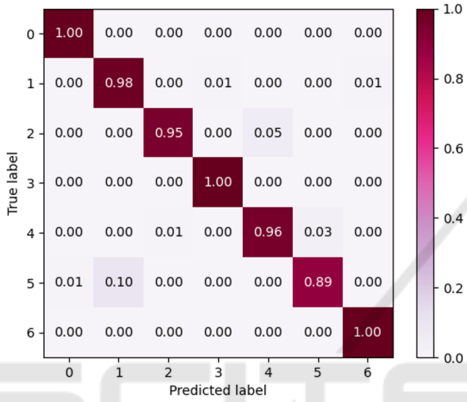
(b)MLP



(c)CNN



(d)GAT

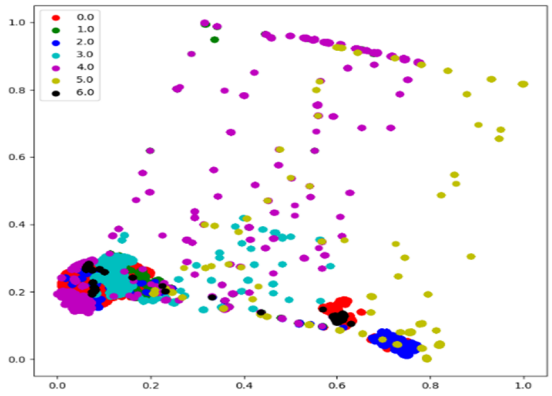


(e)Methods of this paper

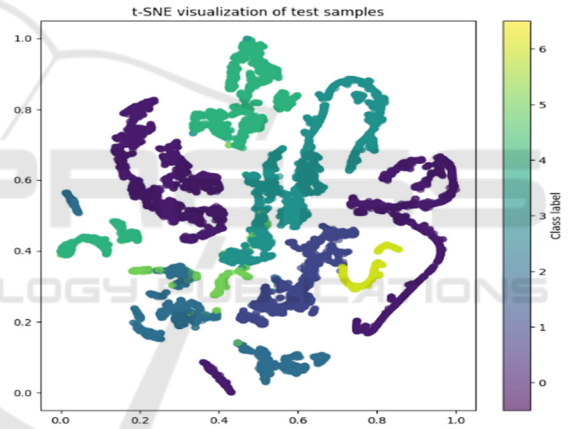
Figure 5: Confusion matrix diagram of each model.

In the confusion matrix, each column represents the predicted labels, and each row represents the true labels. The values on the main diagonal of each model's confusion matrix represent the percentage of samples correctly classified for each label during the testing phase, while the off-diagonal elements represent cases of misclassification.By comparing the main diagonals of the five models, it is more intuitively observed that PCA and MLP both exhibit cases where the misidentification rate is 100%. In the CNN model, the recognition rate for the fault of mistakenly opening the bypass valve is relatively low, and in the GAT model, the recognition rate for system faults under conditions of manual misoperation is low. The graph-structured optimized GCN model proposed in this paper demonstrates an accuracy rate of over 89% for the recognition of triphasic flow data compared to other models. This further proves the effectiveness and robustness of the graph neural network model under graph structure optimization for recognizing different fault categories. It has stronger generalization capabilities for fault recognition rates and can effectively extract fault features.

Furthermore, this paper utilizes the t-Distributed Stochastic Neighbor Embedding (t-SNE) method (Van Der Maaten and Hinton, 2008) to visualize the fault features learned by the model and the preprocessed original data in two-dimensional feature maps, as shown in Figures 6(a) and 6(b).



(a)Feature of Raw Data



(b)Features after model training

Figure 6: T-SNE Visualization in 2D.

It can be observed that the fault features after model learning exhibit better clustering performance and fault separation, effectively revealing the inherent structure and correlations within the data.

5 CONCLUSIONS

This paper proposes a fault diagnosis method for mechanical process industrial systems using a Graph Convolutional Neural Network (GCN) model, which, compared to traditional intelligent fault diagnosis methods that heavily rely on manual feature extraction, introduces a novel approach. The proposed method combines multi-dimensional time-

series data with improved graph data obtained through correlation calculations and original graph data, inputting them into the network model to extract features from different fault samples, thereby achieving fault type diagnosis. The experiments show a significant improvement in commonly used metrics such as Accuracy Estimation (Accuracy), Precision, Recall, and F1-score, as well as in the intuitive representation of confusion matrices and t-SNE visualizations, compared to traditional intelligent fault diagnosis methods. This demonstrates a certain superiority, enabling the model to fully capture and utilize the structural information in the data, thereby further enhancing the model's representational capability and prediction accuracy.

In future work, based on graph data under continuous time-series operating conditions, effective fault features can be extracted using weighted windows to enhance the timeliness of fault diagnosis by graph neural network models and to predict fault occurrence points in advance. Applying this to actual operations can effectively reduce maintenance costs and labor requirements.

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