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Artificial Intelligence-Based Prediction of Marine Microbial Biogeochemical Activity Using Multi-Omics Data

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Abstract. Marine microorganisms play a crucial role in global biogeochemical cycles, and accurately predicting their biogeochemical activities is essential for understanding changes in marine ecosystems. Addressing the challenges of high dimensionality, strong heterogeneity, and complex nonlinear relationships in multi-omics data, this paper proposes a deep learning prediction framework based on multi-omics fusion: AE-GAT-AFNet. This method first utilizes an autoencoder (AE) to perform feature compression and representation learning on high-dimensional multi-omics data, reducing redundant information and enhancing feature representation capabilities. Then, a microbial relationship graph is constructed, and a graph attention network (GAT) is used to model the potential structural relationships among microbial communities. Based on this, an attention fusion mechanism (AF) is introduced to adaptively weight and integrate different omics modalities, and the final prediction task is completed using a multilayer perceptron (MLP). Experimental results show that the proposed method outperforms several baseline models in both prediction accuracy and stability. Further ablation experiments validate the effectiveness of each key module in the model. The results show that this method can effectively integrate multi-omics information and capture the structural characteristics of microbial communities, providing a feasible intelligent analysis framework for predicting marine microbial biogeochemical activities.

Keywords: Multi-Omics Integration; Graph Attention Network (GAT); Marine Microbial Communities; Biogeochemical Activity Prediction.

1. Introduction

As global climate change becomes increasingly severe, the ocean plays a crucial role in regulating Earth's biogeochemical cycles (BGC) [1-2]. Marine microorganisms, as the most fundamental and active component of marine ecosystems, play essential roles in key biogeochemical processes such as carbon cycling, nitrogen cycling [3], and organic matter decomposition. For example, marine microorganisms participate in carbon fixation through photosynthesis and chemosynthesis, and regulate the transformation and recycling of nutrients in marine environments through various metabolic pathways [4-5]. Therefore, accurately characterizing the structure and functional activities of marine microbial communities, and further predicting the variation trends of their biogeochemical processes, is of significant scientific importance for understanding marine ecosystem stability and assessing global climate change.

In recent years, with the rapid development of high-throughput sequencing (HTS) and multi-omics analysis technologies, marine microbial research has entered a data-intensive stage [6-7]. Multiple omics data sources, including metagenomics (MG), transcriptomics (TR), metabolomics (MB), and environmental monitoring data (ENV), provide abundant information for exploring microbial community structures and functional mechanisms [8-9]. Complex interactions and hierarchical relationships often exist among different omics layers [10]. Using a single data source or simple feature concatenation strategies often fails to comprehensively capture the intrinsic dynamic characteristics of marine microbial systems.

With the advancement of artificial intelligence, deep learning (DL) methods have demonstrated significant advantages in modeling complex biological data. In recent years, many studies have attempted to analyze and predict microbial community structures using machine learning (ML) and

deep learning techniques. Although these methods have improved prediction performance to some extent, existing approaches still exhibit certain limitations. Most studies perform only simple fusion of multi-omics data, often ignoring the heterogeneity and relative importance among different data modalities. Moreover, marine microorganisms commonly exhibit complex ecological relationships such as symbiosis, competition, and metabolic dependency, which traditional models struggle to represent effectively. Consequently, how to integrate multi-omics data while simultaneously modeling the relational structure among microbial communities remains an important challenge in current research.

To address these challenges, this paper proposes a deep learning-based multi-omics fusion prediction framework for the intelligent prediction of marine microbial biogeochemical activities. Specifically, the proposed method first employs an AutoEncoder (AE) to learn low-dimensional feature representations from different omics datasets, thereby reducing noise and redundancy in high-dimensional data. Subsequently, a microbial interaction network is constructed, and Graph Attention Networks (GAT) are utilized to model the potential relationships among microorganisms, enabling the extraction of key interaction patterns within microbial communities. On this basis, an attention-based fusion mechanism, namely Attention Fusion (AF), is introduced to adaptively integrate features from multiple omics modalities. Finally, a Multilayer Perceptron (MLP) is adopted as the prediction head to estimate biogeochemical activity indicators. Experimental results demonstrate that the proposed framework achieves superior performance and stability in biogeochemical activity prediction tasks. The main contributions of this work are threefold. First, a deep learning-based multi-omics fusion framework is proposed to effectively integrate heterogeneous marine microbial datasets. Second, complex microbial interaction structures are modeled using Graph Attention Networks (GAT), enhancing the representation capability of community relationships. Third, the attention fusion mechanism improves the complementarity among multiple omics modalities, thereby significantly improving the prediction accuracy of biogeochemical activities.

2. Related work

With the rapid development of high-throughput sequencing technology, multi-omics data integration has gradually become an important research direction for revealing the mechanisms of complex biological systems [11]. Early studies mainly relied on statistical methods to analyze the correlations between different omics datasets or to perform dimensionality reduction to uncover potential biological patterns. However, these methods often suffer from insufficient representational capabilities when dealing with high-dimensional, heterogeneous, and highly nonlinear multi-omics data. DL methods have gained increasing attention in multi-omics integration research. AE,DNN, and multimodal learning models have been used to extract features and integrate information from different omics sources, significantly improving predictive performance [12]. However, most existing methods typically employ simple feature splicing or early fusion strategies, directly combining different omics features as input to the predictive model. These methods often ignore the differences in importance between different data modalities and the potential structural relationships within biological systems, thus limiting the model's ability to effectively represent complex biological processes.

Meanwhile, graph neural networks (GNNs) have demonstrated powerful capabilities in modeling relational data and have been increasingly applied to bioinformatics and ecosystem analysis. Biological systems inherently possess network structures, such as gene regulatory networks (GRNs), protein-protein interaction networks (PPIs), and microbial co-occurrence networks (MCNs). These structural relationships play a crucial role in understanding biological functions. However, such models can have limitations when dealing with heterogeneous neighbor contributions. GAT introduce an attention mechanism that assigns adaptive weights to neighboring nodes, enabling models to more flexibly capture complex relationships. In microbial community studies, various interactions often exist among microorganisms, including symbiosis, competition, and metabolic dependence. GAT can more effectively model these potential associations. Therefore, combining GNN with multi-omics

data fusion methods offers a promising approach for constructing microbial community structure models and predicting their biogeochemical activities.

3. Methodology

3.1. Problem Definition and Multi-omics Data Representation

The biogeochemical activities of marine microbial communities are influenced by a variety of factors. With the development of multi-omics technologies, different types of omics data can characterize the structure and functional features of microbial communities from multiple perspectives. However, different omics data vary significantly in terms of data dimensions, distribution formats, and information representation capabilities. Therefore, it is necessary to establish a unified data representation method to facilitate feature learning and fusion in subsequent models.

Assume that the marine microbial multi-omics dataset contains N samples, and each sample consists of K different omics modalities. The i-th sample can be represented as

$$X_i = \{X_i^{(1)}, X_i^{(2)}, ..., X_i^{(K)}\} \tag{1}$$

where $X_i(k) X_i^{(k)}$ denotes the feature matrix of the k-th omics modality, such as metagenomic features, transcriptomic features, or environmental variables. Since the dimensionality of different omics data may vary significantly, separate feature encoding procedures are required for each modality.

In practical applications, each sample is also associated with a target variable representing the biogeochemical activity indicator of the microbial community, such as carbon cycling activity, nitrogen cycling rate, or other ecological functional indices. Therefore, the prediction task can be formulated as a mapping from the multi-omics feature space to the target variable space, expressed as

$$yi = f(Xi) \tag{2}$$

where f(.)represents the predictive model to be learned and y_i denotes the biogeochemical activity label corresponding to the i-th sample.

To effectively utilize information from multiple omics sources, this study first performs independent representation learning for each omics modality and maps them into a unified low-dimensional feature space. For the k-th omics dataset, the feature representation can be defined as

$$z_i^{(k)} = \phi_k(X_i^{(k)}) \tag{3}$$

where $\phi_k(\cdot)$ denotes the encoding function for the k-th omics modality and $z_i^{(k)}$ represents the corresponding low-dimensional embedding.

After the encoding process, each sample can be represented by a set of multi-omics feature embeddings

$$Z_i = \{z_i^{(1)}, z_i^{(2)}, ..., z_i^{(K)}\} \tag{4}$$

Based on these learned multi-omics representations, the model can further explore the latent relationships among microbial communities and the complementary information across different omics modalities.

3.2. Multi-omics feature learning based on autoencoders

In the previous section, a unified representation of marine microbial multi-omics data was defined. However, multi-omics datasets are typically characterized by high dimensionality, noise, and redundant information. Directly feeding raw features into predictive models may not only increase computational complexity but also reduce the generalization capability of the model. Therefore, it is necessary to perform effective feature compression and representation learning before conducting multi-omics fusion modeling.

To address this issue, this study adopts an AE to learn low-dimensional representations for different omics datasets [12-13]. It is an unsupervised neural network model that consists of two main components: an encoder and a decoder. The encoder maps the input data into a low-dimensional latent space, while the decoder reconstructs the original input from the latent representation. Through this process, the model learns compact feature representations that capture the intrinsic structure of the data.

For the k-th omics dataset $X^{(k)}$ the encoder first transforms the input into a latent representation, which can be formulated as

$$h^{(k)} = \sigma(W_e^{(k)} X^{(k)} + b_e^{(k)}) \tag{5}$$

where $W_e^{(k)}$ $W_e^{(k)}$represents the encoder weight matrix, $b_e^{(k)}$denotes the bias vector, and $\sigma(\cdot)$denotes the nonlinear activation function. The resulting vector $h^{(k)}$ $h^{(k)}$represents the latent feature embedding of the corresponding omics dataset.

After obtaining the latent representation, the decoder attempts to reconstruct the original input data from the latent space. The decoding process can be expressed as

$$\hat{X}^{(k)} = \sigma(W_d^{(k)} h^{(k)} + b_d^{(k)}) \tag{6}$$

where $W_d^{(k)}$ and $b_d^{(k)}$ represent the decoder weight matrix and bias vector, respectively, and $\hat{X}^{(k)}$denotes the reconstructed data.

To ensure that the latent representation preserves the important information from the original data, the AE is trained by minimizing the difference between the input data and the reconstructed data. In this study, the Mean Squared Error (MSE) is adopted as the reconstruction loss function, which can be written as

$$L_{AE} = \frac{1}{N} \sum_{i=1}^{N} || X_i^{(k)} - \hat{X}_i^{(k)} ||^2 \tag{7}$$

where Nrepresents the number of samples, $X_i^{(k)}$denotes the original feature vector of the i-th sample, and $\hat{X}_i^{(k)}$represents the reconstructed feature vector. Through the above training process, the AE is able to learn compact and discriminative feature representations for each omics dataset. Consequently, the high-dimensional input data can be transformed into low-dimensional latent embeddings, which can be expressed as

$$z^{(k)} = Encoder_k(X^{(k)}) \tag{8}$$

After processing by the autoencoder, the high-dimensional features of different omics data are transformed into a unified latent representation space. This not only reduces the data dimensionality and noise impact, but also provides a more compact and effective feature representation for subsequent graph structure modeling and multi-omics fusion.

3.3. Microbial Relationship Modeling Based on GAT

After obtaining the low-dimensional feature representations of multi-omics data, the model further needs to capture the latent structural relationships among microbial communities. Marine microbial ecosystems naturally exhibit complex network structures, where different microorganisms may interact through symbiosis, competition, and metabolic dependency. These interactions play an important role in determining microbial community functions and biogeochemical activities. Therefore, relying solely on independent sample features for prediction may fail to fully exploit the structural information embedded in microbial communities.

To address this issue, this study constructs a microbial interaction graph based on the learned feature representations and employs GAT to model the relationships among microorganisms. The microbial interaction graph can be defined as

$$\mathrm{G} = (\mathrm{V},\mathrm{E}) \tag{9}$$

where Vrepresents the set of nodes and Erepresents the set of edges describing relationships between nodes. In this graph, each node corresponds to a microbial entity or sample feature representation, while edges represent interactions or similarities between microorganisms.

In the graph structure, the feature representation of each node is denoted as h_i. The Graph Attention Network updates node representations by aggregating information from neighboring nodes with adaptive attention weights. The propagation process of GAT can be expressed as

$$h_{i'} = \sigma\left(\sum_{j \in N(i)} \alpha_{ij} W h_j \right) \tag{10}$$

where $N(i)$denotes the set of neighboring nodes of node i, Wrepresents a learnable weight matrix, $\sigma(\cdot)$denotes a nonlinear activation function, and h_i'represents the updated node representation.

Unlike traditional GCN, Graph Attention Networks introduce an attention mechanism to assign different importance weights to neighboring nodes. The attention coefficient between node $i$and its neighbor node $j$is calculated as

$$\alpha_{ij} = \frac{\exp(LeakyReLU(a^T [Wh_i \,||\, Wh_j]))}{\sum_{k \in N(i)} \exp(LeakyReLU(a^T [Wh_i \,||\, Wh_k]))} \tag{11}$$

where $a$represents a learnable attention parameter vector. Through the above propagation process, the model can adaptively learn the strength of relationships between microorganisms and aggregate important information from neighboring nodes. Consequently, the updated node representations can be obtained as

$$\mathrm{H} = \mathrm{GAT}(\mathrm{Z}) \tag{12}$$

where Zrepresents the multi-omics latent feature representations obtained in the previous section.

3.4. Attention-Based Multi-Omics Fusion and Prediction

After modeling microbial structural relationships using GAT, the learned node representations still originate from different omics modalities. Since each omics dataset provides complementary information about the microbial community, effectively integrating these heterogeneous features is crucial for improving predictive performance. However, simple splicing strategies often treat all modalities equally, ignoring their relative importance. In reality, different omics sources may contribute differently to the prediction of biogeochemical activities. Therefore, an adaptive fusion

mechanism is needed to dynamically determine the contribution of each modality.

To address this issue, this study introduces an AF mechanism to integrate multi-omics features. Assume that the representation learned from the k-th omics modality after feature learning and graph modeling is denoted as $z^{(k)}$. The model first computes an attention score for each modality to measure its relative importance. The attention weight for the k-th modality can be defined as

$$\alpha_k = \frac{\exp(w^T z^{(k)})}{\sum_{j=1}^{K} \exp(w^T z^{(j)})} \tag{13}$$

where $w$denotes a learnable parameter vector and Krepresents the total number of omics modalities. Based on the computed attention weights, the model performs a weighted aggregation of multi-omics features to obtain a unified feature representation. The fused representation can be expressed as

$$z_{fusion} = \sum_{k=1}^{K} \alpha_k z^{(k)} \tag{14}$$

where z_{fusion} represents the integrated feature embedding after attention-based fusion. After obtaining the fused feature representation, MLP is employed as the prediction module to estimate the biogeochemical activity indicators of marine microbial communities. The prediction can be formulated as

$$\hat{y} = W_2 \sigma(W_1 z_{fusion} + b_1) + b_2 \tag{15}$$

where $W_1$and W_2denote the weight matrices of the neural network layers, $b_1$and $b_2$represent bias terms, and $\sigma(\cdot)$denotes the nonlinear activation function. The research content of this paper can be represented by Figure 1.

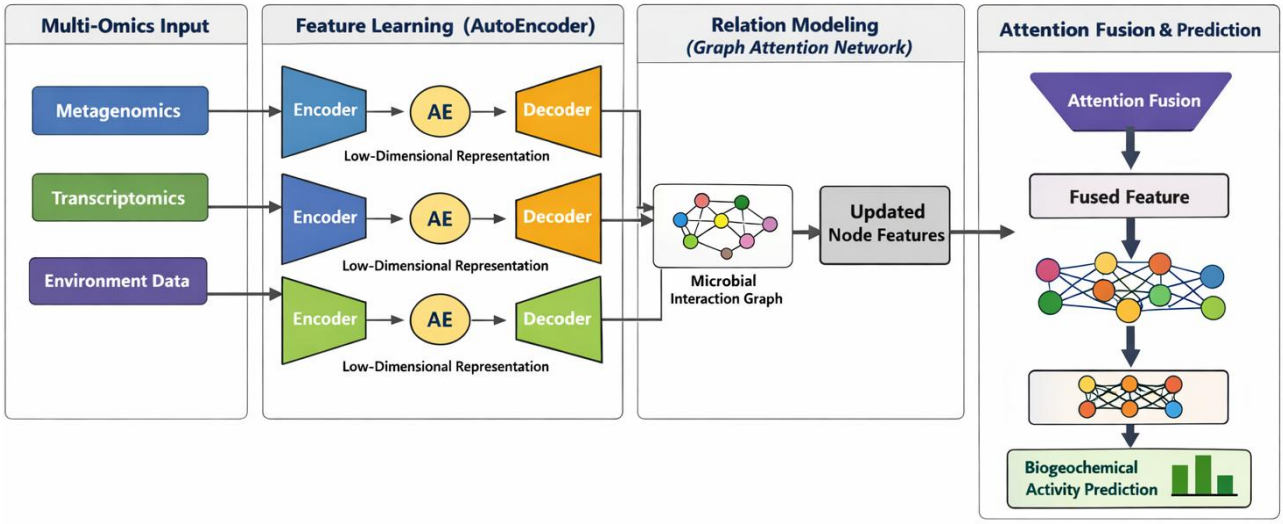

Figure 1. Overall Flowchart

4. Experiments and Results

4.1. Experimental Settings

This study constructs a task for predicting marine microbial biogeochemical activity based on multi-omics feature data. Each sample consists of multimodal features, including microbial functional features, transcriptomic features, and environmental variable information. After data processing, a total of 3,200 samples were obtained, each containing three types of modal features. The microbial functional features have a 512-dimensional dimension, the transcriptomic features have a 256-dimensional dimension, and the environmental variable features have a 32-dimensional dimension. All features are uniformly organized according to sample dimensions to form a multimodal input matrix for subsequent model training.

In the data preprocessing stage, all input features are first Z-score standardized to eliminate the influence of differences in feature scales. Regarding data partitioning, following common machine learning experimental settings, the data is randomly divided into training, validation, and test sets, with proportions of 70%, 15%, and 15%, respectively.

The experiments were implemented in a Python 3.9 environment, using the PyTorch 2.0 deep learning framework. The experiments were conducted on a computing platform equipped with an Intel Xeon processor, 32 GB of memory, and an NVIDIA RTX 3090 GPU. During model training, the Adam optimizer was used for parameter updates, with an initial learning rate of 0.001, a batch size of 64, and a maximum of 200 training epochs. An Early Stopping strategy was also introduced, terminating training when the validation set error no longer decreased over 20 consecutive epochs to prevent overfitting.

Regarding model structure parameters, an autoencoder was used for multi-omics feature representation learning, with a hidden layer structure of 512–256–128–256–512. The GAT contained a two-layer attention propagation structure, with four attention heads per layer and a hidden dimension of 128. In the multi-omics fusion stage, an attention fusion mechanism was introduced to adaptively weight and integrate features from different modalities. The final prediction module, MLP, had a hidden layer dimension of 64.

To comprehensively evaluate model performance, this paper uses multiple regression metrics to analyze the prediction results, including Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and Coefficient of Determination(R^2).

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i| \tag{16}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2} \tag{17}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2} \tag{18}$$

4.2. Performance Comparison with Baseline Methods

To verify the effectiveness of the proposed model in predicting marine microbial biogeochemical activity, this paper compares the proposed method with the previously mentioned SVM, RF, MLP, and AE-MLP model which incorporates autoencoder feature learning. To further evaluate the impact of graph structure modeling on prediction performance, this paper also introduces GCN and GAT as comparative methods.

Table 1. Comparison of prediction performance of different models

Method	MAE	RMSE	R^2
SVM	0.218	0.296	0.812
RF	0.205	0.281	0.826
MLP	0.192	0.264	0.842
AE-MLP	0.178	0.243	0.861
GCN	0.167	0.229	0.879
GAT	0.159	0.218	0.892
Proposed AE-GAT-AFNet	0.141	0.197	0.914

As shown in Table 1, different models exhibit significant performance differences in predicting marine microbial biogeochemical activity. SVM and RF can accomplish the prediction task to some extent, but their prediction accuracy is relatively low due to their difficulty in fully modeling the complex nonlinear relationships in multi-omics data. The RF model achieves better performance than SVM, mainly due to its ensemble learning structure's advantage in handling complex data features.

The introduction of GCN methods significantly improved model performance. The GCN model, by constructing a microbial relationship graph, incorporates structural information between samples into the prediction model, thereby enhancing prediction accuracy. The GAT model, by introducing an attention mechanism, assigns different weights to different neighboring nodes, enabling it to more accurately capture the complex relationships between microorganisms, thus outperforming the GCN model.

In summary, the proposed AE-GAT-AFNet model achieves the best performance across all evaluation metrics. Specifically, it reduces MAE by approximately 26.6% and RMSE by approximately 25.4% compared to traditional MLP models, while improving the correlation coefficient to 0.914. These results demonstrate that by combining autoencoder feature learning, graph attention network structure modeling, and multi-omics attention fusion mechanisms, the model can effectively integrate multimodal information and capture the structural relationships of microbial communities, thereby significantly improving the accuracy and stability of marine microbial biogeochemical activity prediction.

4.3. Ablation Study

To further validate the effectiveness of the key modules in the proposed model, this paper designs a series of ablation experiments to progressively remove different components from the model and analyze their impact on prediction performance. Specifically, this study mainly examines the following three core modules: w/o AE: Removes the autoencoder module and directly uses raw features for modeling. w/o GAT: Removes the graph attention network and uses only feature representations for prediction.w/o AF: Removes the attention fusion mechanism and uses simple feature concatenation for multi-omics fusion. The results of the ablation experiment are shown in Table 2.

Table 2. Comparison of ablation test results

Model	MAE	RMSE	R^2
w/o AE	0.176	0.241	0.865
w/o GAT	0.168	0.232	0.878
w/o AF	0.158	0.220	0.894
Proposed AE-GAT-AFNet	0.141	0.197	0.914

In summary, the complete model AE-GAT-AFNet achieved the best results across all evaluation metrics. This result demonstrates that combining autoencoder feature learning, graph attention network structure modeling, and multi-omics attention fusion mechanisms can effectively enhance the model's ability to represent complex multi-omics data, thereby significantly improving the accuracy and stability of marine microbial biogeochemical activity prediction.

Figure 2 shows the prediction results on the test set. Significant differences exist in the fit between the predictions and the actual values for different models on the test set. Overall, all models can capture the changing trends of biogeochemical activities to some extent, but their prediction accuracy and stability vary.

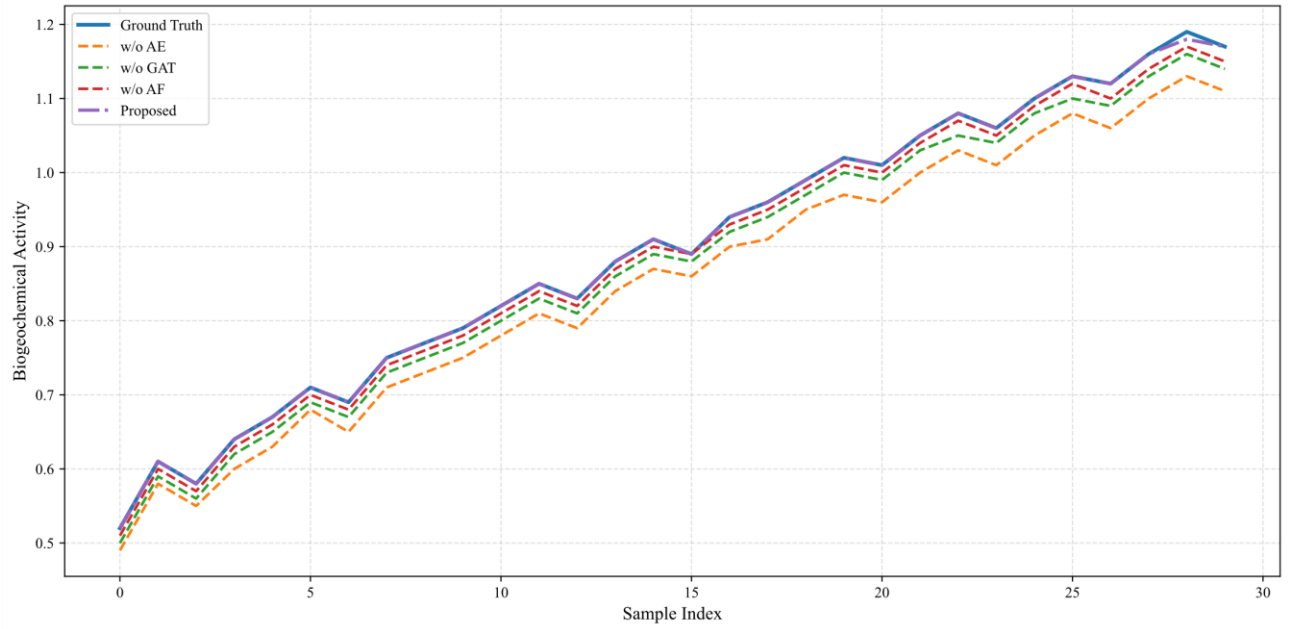

Figure 2. Results of different ablation experiments on the testing machine

For models without an autoencoder module (w/o AE), their prediction curves deviate significantly from the actual values in several intervals, indicating that the autoencoder (AE) plays a crucial role in high-dimensional multi-omics feature compression and representation learning. For models without a graph attention network (w/o GAT), although the overall trend fits the actual values well, significant fluctuations still occur in some intervals, suggesting that structural relationships between microorganisms have a significant impact on the prediction task. For models without an attention fusion module (w/o AF), their prediction performance is improved, but some local bias still exists, indicating that simple feature splicing cannot fully utilize the complementary information between multi-omics data.

In contrast, the proposed AE-GAT-AFNet model showed better fitting performance throughout the entire test interval, and its prediction curve was basically consistent with the actual value. This indicates that the model can effectively integrate multi-omics features and capture the relationship of microbial community structure, thereby significantly improving the accuracy and stability of biogeochemical activity prediction.

5. Conclusion

This paper proposes a deep learning prediction framework, AE-GAT-AFNet, based on multi-omics data fusion for predicting the biogeochemical activity of marine microbial communities. This method uses an AE to perform feature compression and representation learning on high-dimensional multi-omics data, effectively reducing redundant information and noise interference. Subsequently, GAT is used to construct a microbial relationship graph, modeling the potential structural relationships between microbial communities. Based on this, AF is introduced to adaptively weight and integrate

different omics modalities, and the final prediction task is completed through a MLP. This framework can simultaneously utilize multi-omics feature information and microbial structural relationship information, thereby improving the model's ability to represent complex ecosystem data.

Comparative experiments with various baseline methods show that the proposed model achieves superior performance on multiple evaluation metrics. Experimental results demonstrate that AE-GAT-AFNet exhibits significant advantages in prediction accuracy and stability compared to traditional machine learning methods and general deep learning models. Meanwhile, ablation experiments further validated the effectiveness of key modules in the model. The autoencoder effectively enhanced feature representation, the graph attention network captured structural relationships between microorganisms, and the attention fusion mechanism more effectively integrated information from different omics systems. These results demonstrate that reasonable feature learning, structural modeling, and multimodal fusion play crucial roles in improving predictive performance.

Although the proposed method achieved good predictive results in the experiments, there is still room for improvement. Future research can be expanded in several ways, such as introducing more complex graph structural modeling methods to further characterize the relationship networks between microorganisms, combining temporal modeling methods to analyze the dynamic changes of microbial communities over time, and exploring more efficient multimodal fusion strategies to improve the model's generalization ability. Through these studies, it is hoped that the application potential of artificial intelligence methods in marine ecosystem analysis and biogeochemical process prediction can be further enhanced.

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