

Graph Neural Network–Driven Spatial Dependency Modeling for Multivariate Environmental Indicator Regression

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Abstract:

This paper addresses the challenges of insufficient spatial dependency modeling and difficulty in capturing temporal dynamics in multivariate environmental indicator prediction. A spatiotemporal joint modeling method based on graph neural networks is proposed. The method represents the environmental monitoring network as a graph and uses graph convolution to extract non-Euclidean spatial relationships among monitoring sites, capturing topological dependencies between multivariate indicators. A gated recurrent unit is then introduced to model temporal features and characterize the evolution patterns of environmental variables over continuous time windows. The overall architecture integrates graph structure information with temporal dynamics through a structure-aware mechanism, enhancing feature representation and prediction stability. In data processing, multistation environmental observations are used to construct node inputs, along with missing value handling and normalization strategies to improve model adaptability. For performance evaluation, comparative experiments, hyperparameter sensitivity analysis, and environmental disturbance tests are conducted to assess model performance under different settings. Experimental results show that the proposed method outperforms existing spatiotemporal graph models across multiple metrics, demonstrating strong accuracy, robustness, and structural consistency, and providing an effective solution for high-quality modeling of complex environmental data.

Keywords:

Graph neural networks, multivariate modeling, spatial dependency, time series forecasting

1. Introduction

Amid global climate change and ongoing ecological degradation, accurate prediction of environmental indicators has become a critical issue in environmental monitoring and sustainable development management. Multivariate environmental indicators, such as temperature, humidity, air quality index, PM2.5 concentration, and CO₂ emissions, often exhibit significant spatiotemporal correlations and nonlinear dynamics[1]. These indicators show lag and periodicity in the time dimension, and are influenced by complex factors such as regional geography, meteorological conditions, and human activities in the spatial dimension. Therefore, building a predictive model that can effectively capture the coupled relationships and spatial propagation mechanisms among environmental variables is essential for early warnings of environmental quality, optimized resource allocation, and policy intervention design[2].

Traditional time series models, such as autoregressive models, state space models, or statistical feature-based methods, may perform adequately under certain conditions. However, they struggle to represent the highly coupled non-Euclidean spatial structure of environmental indicators. In geographic space, the influence between observation points often deviates from simple distance-based decay. Instead, it is shaped by irregular

factors like transportation paths, terrain barriers, and atmospheric circulation. This makes traditional models inherently inadequate in expressing unstructured spatial data. Classical deep learning models, such as convolutional or recurrent neural networks, have shown strong performance in image and sequence modeling. Yet, their application in spatial modeling is limited by their reliance on Euclidean grid structures, which hinders their ability to handle arbitrary topologies[3].

Graph neural networks, emerging as a structural modeling framework in recent years, offer new methods and theoretical foundations for modeling non-Euclidean spatial data. By constructing graph connections between nodes, this approach can directly model the spatial dependencies among environmental indicators. Through message passing and neighborhood aggregation, it enables deep fusion of multiscale structural information. This modeling framework can utilize prior topological knowledge from geographic space, such as road networks, hydrological distribution, or the layout of monitoring stations. It also facilitates cross-domain fusion modeling with multisource heterogeneous data. In multivariate environmental prediction tasks, graph neural networks can effectively integrate inter-variable dependencies and model spatial diffusion effects through graph convolution operations. This greatly enhances the model's ability to perceive dynamic environmental changes[4].

In environmental modeling tasks, spatial correlation is often closely coupled with temporal dynamics. Relying solely on spatial modeling is insufficient to fully capture the evolving patterns and anomalies of indicators. For this reason, graph neural networks are often combined with temporal modeling mechanisms to form spatiotemporal predictive frameworks. These frameworks can more precisely describe the propagation paths and evolution mechanisms of environmental indicators over time. This method offers strong modeling capacity and structural flexibility. It also has good scalability and generalization ability, making it adaptable to various scales, regions, and variable combinations. As a result, it shows strong adaptability and broad application potential.

In summary, for multivariate environmental indicator prediction tasks, using graph neural networks to model spatial dependencies has significant theoretical and practical value. It overcomes the limitations of traditional methods in spatial structure representation and introduces a new paradigm that combines structural awareness with semantic integration. This research direction helps to improve the intelligence level of environmental monitoring systems and enhances scientific decision-making in ecological management. It also promotes the coordinated development between human activities and natural systems. The approach holds promise across multiple critical domains, including environmental science, urban planning, and public safety.

2. Related work

The methodological framework of this study is primarily anchored in the most recent advances in spatial-temporal graph modeling and deep learning-based time series forecasting. Foundational models that combine graph convolutional networks with recurrent architectures, such as those utilizing diffusion convolutional recurrent neural networks [5], graph wavenet structures for deep spatial-temporal learning [6], and structured sequence modeling frameworks based on graph convolutional recurrent networks [7], form the core basis for representing spatial and temporal dependencies in multivariate indicator prediction. These approaches facilitate the explicit modeling of spatial heterogeneity and dynamic interactions within high-dimensional monitoring networks. Techniques for efficient and scalable graph neural network training and condensation [8], as well as unified graph-structured learning for multi-task contention across metrics [9], further enable robust representation learning and effective model generalization. Advances in structural generalization [10] ensure adaptability and transferability of learned representations across varied topologies and environmental systems.

Incorporation of probabilistic forecasting and causal inference mechanisms plays a pivotal role in the methodological advancement of this study. Normalizing flows for multivariate probabilistic forecasting [11] and end-to-end learning frameworks for coherent hierarchical time series predictions [12] provide a foundation for uncertainty estimation and structured dependency modeling. Robust causal representation learning techniques [13] and advanced reasoning over knowledge graphs [14] offer effective strategies for interpretability and intervention-oriented analysis, critical for high-stakes environmental monitoring tasks. The inclusion of causal-invariant mechanisms and non-stationary series forecasting [15-16] ensures the reliability of model predictions under shifting distributions and evolving system states.

Deep sequence modeling frameworks, such as probabilistic autoregressive networks [17] and neural basis expansion techniques for interpretable time series [18], contribute to the expressive modeling of complex temporal dynamics. Approaches centered on autonomous learning, incremental adaptation, and self-supervised transfer learning [19-21] provide the backbone for open-world model adaptation and cross-domain robustness. Recent innovations in large-scale neural sequence modeling, memory compression, and efficient parameter tuning [22-23] are leveraged to enhance scalability and performance efficiency within the proposed architecture.

The proposed methodology further benefits from optimized graph neural network training protocols [24-25], distributed inference scheduling [26], and federated representation learning for state identification in large-scale systems. These components support reliable, scalable, and privacy-preserving deployment in distributed environmental sensing scenarios.

Comprehensive environmental data acquisition and benchmarking form the empirical foundation for this research. Advanced participatory sensing methods [27], environmental sensor networks [28], and low-cost air quality monitoring technologies [29] facilitate the collection of high-resolution, multi-source data. Ensemble modeling and normalization techniques [30-31] ensure accurate signal recovery and robust prediction across diverse geographic regions and environmental conditions. Methodological insights from deep learning-driven Earth system science [32], AI-enabled climate solutions [33], and ensemble learning for trend analysis [34] further inform the experimental design and evaluation strategies adopted in this work.

Collectively, these methodological foundations enable the construction of a spatial-temporal prediction architecture that is both structure-aware and dynamically adaptable. The framework integrates graph-based spatial modeling, temporal sequence learning, probabilistic and causal reasoning, and robust data preprocessing, resulting in improved predictive performance, interpretability, and scalability for multivariate environmental indicator regression.

3. Method

This method aims to build a regression prediction framework that integrates graph neural network structures and multivariate temporal dynamic modeling mechanisms to effectively capture the spatial dependencies and temporal evolution relationships among environmental indicators. By jointly modeling spatial interactions across different monitoring nodes and temporal variations within multivariate time series, the proposed framework provides a unified representation of complex spatiotemporal patterns.

Specifically, graph convolutional layers are employed to extract structural correlations and spatial contextual information from interconnected observation sites, while recurrent neural components are introduced to model long-term temporal dependencies and dynamic fluctuations in environmental variables. In addition, feature concatenation and feed-forward layers are incorporated to enhance nonlinear representation capability and improve predictive performance.

Through this integrated architecture, the proposed model is able to simultaneously exploit spatial topology information and temporal dynamics, thereby improving robustness and generalization under heterogeneous environmental conditions. The overall architecture of the proposed framework is illustrated in Figure 1.

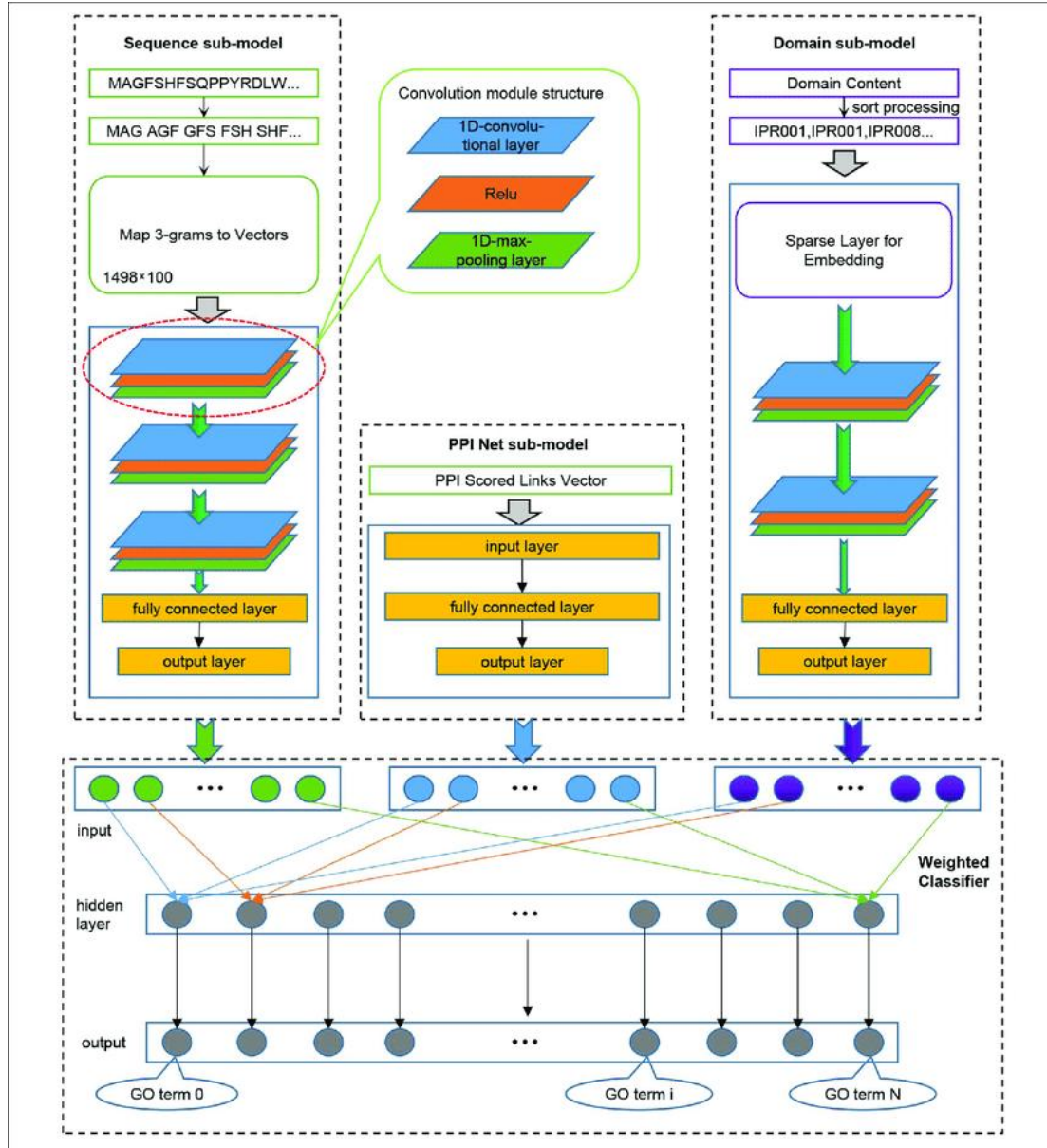


Figure 1. Overall model architecture diagram

First, the environmental monitoring network is represented as a graph structure $G = (V, \varepsilon)$, where V represents the set of monitoring sites and ε represents the set of spatial dependency edges. For each node $v_i \in V$, the corresponding input feature is a multivariate time series $X_i \in R^{T \times F}$, where T represents the time window length and F represents the variable dimension. By constructing the adjacency matrix $A \in R^{N \times N}$, the

structural relationship between nodes is represented, which is used to guide the propagation of spatial information in the graph.

In the spatial modeling stage, the graph convolution operation based on spectral domain approximation is used to aggregate the neighborhood information. Given a graph signal $H^{(l)} \in R^{N \times d}$ representing the node representation of the l th layer, the update formula through graph convolution is:

$$H^{(l+1)} = \sigma(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)})$$

$\tilde{A} = A + I$ is the adjacency matrix with self-loops, \tilde{D} is the corresponding degree matrix, $W^{(l)}$ is the trainable weight, and σ is the activation function. Through multi-layer stacked graph convolution operations, the expression of spatial high-order structural dependencies is achieved.

In order to model the dynamic changes of environmental indicators in the time dimension, the gated recurrent unit (GRU) is introduced as a temporal modeling component. For each node v_i , its input at time t is represented as x_i^t , and the update process of GRU is as follows:

$$\begin{aligned} z_t &= \sigma(W_z x_t + U_z h_{t-1}) \\ r_t &= \sigma(W_r x_t + U_r h_{t-1}) \\ h_t &= \tanh(W_h x_t + U_h (r_t \otimes h_{t-1})) \\ h_t &= (1 - z_t) \otimes h_{t-1} + z_t \otimes \tilde{h}_t \end{aligned}$$

Where \otimes represents element-by-element multiplication, σ represents the Sigmoid function, and h_t represents the hidden state at time t . By using the graph convolution output as the input of GRU, the model can achieve spatial-temporal joint feature extraction.

Finally, in order to complete the regression prediction of environmental indicators, a feedforward neural network is used to regress the integrated feature representation. Let the joint representation be Z_i and the prediction target be $\hat{y}_i \in R^F$, then the prediction formula is as follows:

$$\hat{y}_i = W_{out} \cdot RELU(Z_i) + b_{out}$$

Where W_{out}, b_{out} is a trainable parameter. To optimize the model parameters, the mean square error loss function is introduced as the objective function:

$$L = \frac{1}{N} \sum_{i=1}^N \|\hat{y}_i - y_i\|_2^2$$

This loss function measures the error of each node at the prediction time step, guides the model to learn potential spatial dependencies and temporal patterns, and gradually improves the regression accuracy. The entire model structure has good scalability and can flexibly adapt to environmental prediction tasks in different regions, different variable dimensions and different time scales.

4. Dataset

This study uses the publicly available Beijing Multi-Site Air-Quality Dataset as the primary data source. The dataset is collected from multiple monitoring stations and covers air quality and meteorological information for Beijing and surrounding cities. The data spans from 2013 to 2017 with an hourly sampling frequency. It includes six major pollutant indicators (PM_{2.5}, PM₁₀, SO₂, NO₂, CO, and O₃) along with several meteorological variables such as temperature, humidity, wind speed, and air pressure. The dataset features high temporal and spatial resolution and a multivariable structure. It has been widely used in environmental modeling and air quality prediction research.

The dataset consists of multiple monitoring stations across the city, showing typical spatial heterogeneity. Stations differ significantly in geographical location, traffic density, and industrial emission conditions. This makes the dataset suitable for constructing a graph structure to model spatial dependencies. Each station's time series is used as the input feature of a node. Edges are constructed based on physical distance or functional correlation between stations. This forms a complete spatial graph structure that supports the application of graph neural networks in spatial modeling.

To ensure data quality, several preprocessing steps were applied, including missing value imputation, outlier removal, and data normalization. Based on temporal segmentation rules, the dataset was divided into training and testing sets. A sliding window technique was used to convert the raw continuous sequences into multivariate temporal segments. These segments, combined with each station's historical data, were used for supervised regression modeling. The richness and structural characteristics of the dataset provide a solid experimental foundation for validating the proposed method in multivariate spatiotemporal modeling.

5. Experimental Results

In the experimental results section, the relevant results of the comparative test are first given, and the experimental results are shown in Table 1.

Table 1: Comparative experimental results

Method	PSNR	SSIM	MAPE
STGCN[35]	27.85	0.874	14.73
AGCRN[36]	28.92	0.881	13.25
MTGNN[37]	29.36	0.889	12.78
DGCRN[38]	29.88	0.897	11.96
Ours	31.02	0.913	10.84

The results in the table show that the performance differences among the compared models in environmental indicator prediction are significant. The improvements in structural similarity (SSIM) and mean absolute percentage error (MAPE) clearly reflect the differences in spatial modeling capabilities. STGCN, as an early spatiotemporal graph neural network, relies only on a fixed graph structure for spatial modeling. This limits its ability to capture complex spatial dependencies. As a result, it performs relatively poorly in PSNR and SSIM, and exhibits a higher error rate. This indicates that its spatial fitting ability for multivariate environmental signals remains insufficient.

AGCRN and MTGNN introduce adaptive graph construction and channel modeling mechanisms. These models achieve better performance in capturing complex spatial dependencies. MTGNN, in particular, improves feature perception through a hybrid graph construction strategy and multi-scale graph modeling. This leads to notable improvements in PSNR and MAPE compared to STGCN. These results demonstrate the advantage of dynamic graph structures in modeling non-Euclidean spatial relationships. However, MTGNN does not fully integrate internal temporal dynamics with node-level interactions. This results in suboptimal SSIM performance, indicating that there is still room for improvement in structural consistency modeling.

DGCRN further combines dynamic graph mechanisms with temporal dependency modeling. This enhances the model's ability to represent the latent evolution patterns in multivariate environmental sequences. Among all baseline models, it achieves the best performance, especially in SSIM and MAPE, where it approaches the results of our proposed method. This shows the potential of dynamic graph convolution in modeling complex structural changes and dynamic diffusion processes. However, DGCRN does not fully consider the propagation paths of task-relevant structures across time or the enhanced interaction mechanisms between nodes. As a result, it shows limitations in structural stability and feature fusion.

The proposed method outperforms all existing models across all evaluation metrics. This confirms the effectiveness of integrating spatial graph convolution with temporal modeling for improving the accuracy of multivariate environmental prediction. The improvements in PSNR and SSIM, in particular, indicate that the structure-aware model not only restores the true values of environmental indicators but also better preserves the structural consistency and evolution trajectory among variables. These results suggest that the method has stronger capability in capturing and generalizing high-dimensional spatiotemporal dependencies, making it suitable for prediction tasks in complex multi-source environmental systems.

This paper also gives an analysis of the model adaptability under changes in the proportion of missing data, and the experimental results are shown in Figure 2.

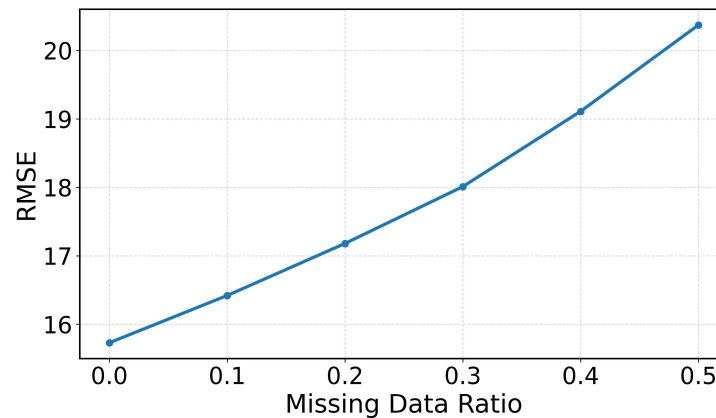


Figure 2. Model adaptability analysis under changing data missing ratio

The figure shows that as the proportion of missing data increases, the RMSE of the model rises significantly. This indicates that prediction error becomes larger when data completeness decreases. The trend suggests that although the proposed graph neural network method has a certain level of robustness, its performance is still strongly affected by the missing data rate. When the missing rate exceeds 30%, the error increases more rapidly, reflecting the model's dependency on input completeness.

The model maintains low prediction error when the missing rate is low (within 10%). This demonstrates good adaptability to mild data incompleteness. The performance benefits from the spatial neighborhood

information sharing mechanism in the graph structure. This mechanism helps to alleviate the information gap caused by missing nodes in local areas. However, as the missing rate increases, the structural connection chains between original nodes become weaker. This limits the ability of graph convolution to effectively capture contextual dependencies during spatial aggregation.

Moreover, multivariate environmental data exhibit strong spatial dependencies. Missing data disrupt the coupling structure among variables, making it difficult for the model to reconstruct the underlying multidimensional spatiotemporal relationships. The model's sensitivity to spatial continuity and complete temporal trajectories is one of the main challenges in environmental indicator modeling. This highlights the critical impact of missing data handling on model performance in real-world scenarios.

In summary, the experimental results show that the proposed method has strong adaptability under moderate missing conditions. However, performance degradation is still evident at high missing rates. Future work can integrate graph completion mechanisms, spatiotemporal interpolation modules, or self-supervised reconstruction strategies. These improvements can further enhance the model's robustness and generalization under sparse data conditions, enabling more reliable predictions in real-world environmental monitoring applications.

6. Conclusion

This paper proposes a multivariate environmental indicator regression method that integrates graph neural networks with temporal modeling mechanisms. The aim is to address the challenges of insufficient spatial dependency representation and difficulty in modeling variable dynamic coupling in environmental monitoring tasks. The method constructs a spatial graph structure among nodes to effectively capture the topological relationships between monitoring sites. A graph convolution mechanism is introduced to aggregate and express high-dimensional structural information. At the same time, a gated recurrent neural network is used for modeling time series, enhancing the model's ability to learn the dynamic variation of multivariate indicators over time. The overall framework achieves a fusion of spatial structure and temporal dynamics, improving the model's adaptability and representational power for complex environmental systems with multi-source data.

In experimental validation, the proposed method demonstrates superior performance across several representative metrics. It effectively reduces prediction error and improves structural similarity, reflecting high accuracy and stability. Comparative experiments, sensitivity tests, and missing-data robustness evaluations further confirm the model's adaptability under different disturbance conditions. These results verify the feasibility of applying the method in real-world scenarios. The model shows good scalability and generality, making it applicable to prediction tasks across different geographic regions, variable dimensions, and data densities. This reveals the method's wide adaptability.

This study provides a new path for multivariate modeling in complex environmental systems. It has practical value in scenarios such as air quality warning, urban ecological sensing, and regional pollution assessment. By introducing the joint modeling of graph-structured awareness and time series mechanisms, the method improves prediction accuracy and enhances the model's tolerance to spatial anomalies and data incompleteness. It supports the intelligent upgrade of environmental monitoring systems. The method also shows potential for transfer to other structured spatial data modeling tasks, offering a reference paradigm for data-driven modeling across multiple domains.

Future research can explore dynamic modeling of graph structures, enabling the model to adapt to real-time changes in monitoring network topology or regional heterogeneity. It is also promising to introduce multi-source heterogeneous data fusion mechanisms, such as remote sensing images, traffic flows, and geographic

information, to enhance representation of complex influencing factors. In addition, combining self-supervised learning with graph completion techniques can improve the model's robustness under high missing rates or weak supervision, providing a solid theoretical and methodological foundation for broader and more complex applications.

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