Railway Cold Chain Freight Demand Forecasting with Graph Neural Networks: A Novel GraphARMA-GRU Model

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ABSTRACT

Accurate demand forecasting is imperative for efficient railway cold chain freight operation planning, resource optimization, and market responsiveness. Given the unique spatiotemporal characteristics and diversity of cold chain demands, the mismatch between capacity and demand has become a bottleneck, constraining the development of railway cold chain freight transportation. To tackle this challenge, we propose a graph neural network model with ARMA graph convolutional layer (ARMA Filter) and gated recurrent units (GRU), namely the GraphARMA-GRU Model, for adaptive and efficient short-term forecasting of railway cold chain freight demand. Our model can effectively capture temporal features, external factors, and the intricate spatiotemporal relationships influencing railway cold chain demands. The ARMA Filter is employed to grasp the spatial connectivity within the railway network, and GRU layers are utilized for refining temporal features. Furthermore, it also integrates external factors and refined temporal features in two graph convolutional layers to better capture multimodal characteristics. The proposed model is validated with real data of railway cold chain freight in China, whose results show an 18% improvement in prediction accuracy compared to the average performance of baseline models. In addition, interpretability methods are introduced to enhance the model’s transparency and promote future development for railway cold chain freight transportation, which may offer deep insights and support critical decisions for a smooth transition from road-based to railway-based cold chain freight transportation.

Keywords: Cold Chain Logistics; Graph Neural Networks; Freight Demand Forecasting

1. Introduction

Railway cold chain, characterized by its eco-friendliness and large capacity to transport fresh and temperature-sensitive goods, is gaining increasing prominence in China's evolving transportation sector and logistics industry. However, integrating cold chain freight transportation with passenger and general cargo flows on the same railway network may encounter intricate operational challenges. Thus, the optimal balance between efficient railway network utilization and the satisfaction of diverse demands for cold chain freight transportation is of crucial importance. In this regard, accurate forecasting of cold chain freight demands becomes imperative for planning efficient railway freight operations, optimizing resource allocation, and responsively adapting to market fluctuations (Jiang et al., 2014; Li et al., 2022; Marchetti and Wanke, 2020). In contrast to passenger transportation, freight transportation lacks autonomy. It heavily relies on preplanning and arrangements (Boysen et al., 2011), including the organization of car flow, freight train formation plan, and the utilization of empty cars (Barbour et al., 2018). This organizational dependence also applies to the operation of railway cold chain. The absence of accurate short-term freight demand predictions may lead to imbalances in railway freight supply, resulting in excessive resource wastage and increased costs or insufficient supply, causing cargo congestion and inadequate service (Milenkovic et al., 2023). Ultimately, this impacts freight transportation efficiency and customer satisfaction.

Moreover, considerable variations exist in the transport characteristics, transport needs, and required infrastructure across different types of cargo, i.e., facilities, equipment, and personnel. This is particularly evident in railway cold chain freight transportation, where the stringent requirements to maintain a low and constant temperature for cold chain cargo dramatically complicate and increase variability in the deployment of facilities, equipment, and personnel. The pronounced volatility in cold chain freight demands further amplifies the negative effects of inaccurate demand forecasting. Additionally, in comparison to road-based cold chain transportation, railway cold chain freight transportation not only offers higher efficiency and economic benefits but also helps significantly improve environmental performance (Li and Zhang, 2020), which positions it for broader prospects for development (Li et al., 2022). Due to these reasons, the accurate forecasting of cold chain freight demands has become an urgent need for railway transportation companies, decision-makers, and relevant stakeholders, which can help significantly enhance operational efficiency and railway network utilization, elevate the level of customer service, and further promote green and sustainable development.

Currently, the research on railway freight demand forecasting is relatively limited (Tang et al., 2022). Moreover, the existing models predominantly focus on the forecasting of railway freight demands at the macro level (Li et al., 2020), where the spatiotemporal characteristics of different cargo types cannot be adequately represented. In addition, the graph structural features of railway networks are not incorporated in these models. Influenced by various factors, e.g., macroeconomic conditions, supply capacity, geographical location, and network characteristics (Feng et al., 2018), the demand for railway cold chain cargo exhibits complex nonlinear characteristics and a certain degree of randomness. Furthermore, traditional time series models used in railway freight demand forecasting exhibit significant shortcomings when predicting frequently fluctuating demand, and handling high-dimensional predictive variables remains challenging (C. Liu et al., 2023). This complexity necessitates a more robust and sophisticated approach to accurately forecast demand.

Thus, to fill the literature gap, we propose a graph neural network model with ARMA graph convolutional layer (ARMA Filter) and gated recurrent units (GRU), namely the GraphARMA-GRU model, for short-term cold chain freight demand forecasting. The motivation for adopting the GraphARMA-GRU model stems from its ability to effectively capture the intricate structural information of the railway network, which is a significant limitation in existing models. By combining ARMA filters and GRU, the model can handle both spatial and temporal dependencies in the data, addressing the complex, nonlinear, and random characteristics of cold chain freight demands. Additionally, this model overcomes the challenges of traditional time series models, which struggle with frequently fluctuating demand and high-dimensional variables.To our knowledge, this paper is the first research that employs a graph neural network model in the field of freight demand forecasting. The effectiveness and applicability of the proposed model are validated with empirical railway freight data in China, and the analysis results indicate that this model exhibits significant advantages in railway freight demand forecasting. In addition, an interpretable method based on graph neural networks is introduced to explain the working principles of our original model. Through this interpretability analysis, a better understanding of the model's forecasting results can be obtained, based on which the recommendations for railway cold chain logistics operations and deep insights for freight organizations are provided.

The organization of the paper is as follows. Section 2 reviews the relevant literature and identifies the literature gaps. Section 3 introduces the model development and its interpretive methods. Section 4 presents the empirical data used, validates the model, and analyzes and discusses the results. Section 5 concludes the study.

2. Literature review

Based on the topic of our research, the relevant studies are reviewed in two domains. The first domain pertains to the development of forecasting models for railway freight demand, while the other one focuses on the application of graph neural network methods in transportation. Finally, the literature gaps are explicitly identified.

2.1 Railway Freight Demand Forecasting Methods

Railway freight has consistently been a focal point in transportation research. Existing studies have delved deeply into railway freight operations, typically employing operations research methods to optimize railway freight systems (Zhen et al., 2023). In this trend, Zhen et al. (2024) modeled and optimized railway transport volume and capacity allocation under uncertainty, while Li et al. (2024) optimized the railway cold chain freight service network. Some research indicates that accurate railway freight demand forecasting is the data foundation for establishing optimization models (Feng et al., 2018; Li et al., 2024). Railway freight demand forecasting has increasingly become a vital domain in the study of complex transportation systems (Yang and Yu, 2015). In recent years, numerous studies have been done to explore various methodologies for railway freight demand forecasting (Ghofrani et al., 2018).

These approaches can be primarily categorized into two classes, namely, traditional time-series analysis methods (Babcock et al., 1999) and regression analysis techniques (Tang et al., 2022). Within the realm of traditional methodologies, Babcock et al. (1999) employed an ARIMA model to capture the time-dependent nature of freight demand, enabling the prediction of quarterly loading and unloading quantities in U.S. railway grain transportation. He and Huang (2018) improved the grey Verhulst model through Fourier series correction and the particle swarm optimization algorithm for the annual forecasting of China's rail freight demand.

The second class is characterized as Artificial Intelligence (AI) based forecasting models, with a primary focus on using and developing neural network models, i.e., GRU (Tan and Zhang, 2020), LSTM (Cheng et al., 2020), and GRNN(Guo et al., 2019; Zhao et al., 2023). These studies employ either qualitative or quantitative analyses to identify the influencing factors of freight demand and then incorporate them into neural network models to achieve short-term or medium-term railway freight demand forecasting. For instance, Tan et al. (2020) applied the GRU model in conjunction with date, weather, and the daily average freight rate to predict short-term freight demands for railway cargo tickets. Cheng et al.(2020) utilized LSTM to forecast railway freight volume by taking into account several factors, including secondary industry value added, Gross Domestic Product (GDP), railway operation mileage, and highway freight volume. The distinctive gating mechanisms of GRU and LSTM models have been proven to be effective in capturing time-dependent patterns in the data and enhancing the accuracy of railway freight demand forecasting. Furthermore, the impact of hyperparameters on model performance and the improved accuracy through parameter adjustments have been investigated in several studies. For example, Wang et al. (2019) employed genetic algorithms to enhance the model parameters of the generalized neural network, which yielded improved prediction accuracy and accelerated convergence speed.

2.2 Graph Neural Network Research in Transportation

Over the years, an increasing trend has been witnessed for algorithm development, evolving from statistical methods to deep learning approaches and, recently to graph neural networks (GNNs) in the field of transportation (Jiang and Luo, 2022). The GNN is a deep learning model for graph-structured data that can effectively capture the complex relationships and local structures among nodes and adapt to the complex and variable data features and the rules of spatio-temporal changes. Due to the innate graph structure of transportation networks, GNNs have established a substantial research foundation that can be extensively used in different fields of transportation research, e.g., traffic flow (Guo et al., 2022), speed (Qiu et al., 2023), travel time prediction (Shen et al., 2022), as well as travel demand forecasting (Lin et al., 2018), and traffic signal control (Yang et al., 2021). Notably, traffic volume prediction is becoming a prominent subfield within the domain of traffic state prediction. Due to the fact that our research shares inherent similarities with traffic volume prediction, a comprehensive review of model development in this domain is provided.

Brimos et al. (2023) comparatively verified the effectiveness of using GNNs and Open Government Data (OGD) for real-time traffic flow prediction. Several studies investigate the use of feature engineering to enhance the predictive performance of GNNs. Sun et al. (2022). designed a three-dimensional mesh spatial structure based on GNN to characterize the dynamic graph and achieve effective prediction of dynamic traffic flow, which could help support emergency transportation planning. Lee and Rhee (2022) introduced the DDP-GCN, which took into account distance, direction, and positional relationship to predict urban traffic speeds. Li et al. (2021) constructed a graph convolutional network (GCN) by integrating data from multiple sensors with different time series. Li and Zhu (2021) proposed a spatio-temporal fusion graph neural network (STFGNN) that combines graph modules and gated convolution modules to learn hidden spatio-temporal dependencies and to process long sequences.

Furthermore, Guo et al. (2022) introduced a novel self-attention mechanism and proposed an Attention-based Spatial-Temporal Graph Neural Network (ASTGNN) for long-term traffic flow prediction. Liu et al. (2023) employed a structure similar to the attention mechanism and proposed a novel Spatial-Temporal Gated Hybrid Transformer Network (STGHTN). This method incorporates the gating mechanism and the global features of the Transformer to further enhance the effectiveness of traffic flow prediction. Besides, research focuses have also been given to combining other algorithms in the performance improvement of GNNs in traffic flow prediction. Jiang et al. (2022) proposed Bi-GRCN by combining GCN with Bi-GRU and modeled the spatial and temporal dependence of traffic flow to achieve accurate prediction of traffic flow. Xiong et al. (2020) designed Fusion Line Graph Convolutional Networks (FL-GCNs) by combining GNNs and Kalman filtering to predict dynamic origin-destination (OD) demand matrices of traffic flows considering spatial correlation, congestion, and time dependence. Zhang et al. (2020) investigated an RGC-LSTM model by combining the graph convolution operator with the residual LSTM structure to predict the traffic speed and the traffic flow of highways.

2.3 Literature summary

Based on the comprehensive review of the relevant literature, three gaps are identified as follows:

1. In the context of forecasting models, the majority of research has predominantly focused on passenger transport, with relatively less attention given to freight transportation. One reason for this lies in the inherent challenges and difficulties related to the acquisition of short-term railway freight data (Ghofrani et al., 2018). Furthermore, long-term freight volume data often suffers from insufficient sample sizes, which results in premature convergence of AI models and becomes practically infeasible.

2. Different types of commodities may exhibit significant spatiotemporal variations, say, distinct distribution and transportation patterns in time and space. However, the existing freight demand forecasting models are relatively generalized and are thus incapable of accounting for the characteristics and requirements of various cargo types. Such approaches cannot offer adequate information support for real-world logistics management. Thus, there is a pressing

need for the development of new freight demand forecasting models to better meet the unique requirements of different types of commodities.

3. There is no denying the fact that AI has the potential to fundamentally change every aspect of railway operations, e.g., capacity management, lifecycle costs, maintenance, and passenger flow forecasting, which may ultimately help to reduce errors and improve efficiency in the railway sector (Tang et al., 2022). Railways have distinct network characteristics. However, these graph-based structural features have not been considered by existing railway freight demand forecasting models. Furthermore, to our knowledge, there is also a lack of research that applies GNNs in railway freight demand forecasting.

Thus, this paper aims to fill these gaps and contribute to the literature by developing a novel GraphARMA-GRU Model that can better integrate the characteristics of railway cold chain freight transportation into demand forecasting.

3. METHODS

3.1 Introduction of the GraphARMA-GRU Model

3.1.1 Background

For the classic GNN models, there are typically several key definitions: $A \in \mathbb{R}^{N \times N}$ represents the adjacency matrix of a graph with N nodes, and $X \in \mathbb{R}^{N \times F}$ represents the features of the nodes on the graph. Let $D \in \mathbb{R}^{N \times N}$ be the diagonal matrix, the symmetric normalized Laplacian of the graph can be represented as $L = I_N - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$. The spectral decomposition of L is shown in Eq. (1), and the graph neural network modifies the expression of features X through the graph filters, the operation corresponding to the spectral domain can be expressed as applying the frequency response function $g(\cdot)$ to the eigenvalues, as shown in Eq. (2).

$$L = \sum_{n=1}^{N} \lambda_n \mu_n \mu_n^T$$

$$\bar{X} = \sum_{n=1}^{N} g(\lambda_m)\mu_n \mu_n^T X$$

Where λ_n and μ_n are the eigenvalues and eigenvectors of the Laplacian matrix, $\bar{X}$ is the features transformed by the graph filter, and the desired frequency response function $g(\cdot)$ can be approximated by a polynomial of order K, see Eq. (3).

$$g_{POLY}(\lambda) = \sum_{k=0}^{K} w_k \lambda^k$$

To express that polynomial filters are localized in the spatial domain, we first recall that the k-th power of any diagonalizable matrix, such as the Laplacian, can be computed by taking the power of its eigenvalues, i.e., $L^k = \mu diag[\lambda_1^k, \ldots \lambda_M^k]\mu^T$. It follows the filtering operation in Eq. (4).

$$\bar{X} = (w_0 I + w_1 L + w_2 L^2 + \cdots + w_k L^K)X = \sum_{k=0}^{K} w_k L^k X$$

A particular first-order polynomial filter has been proposed by Kipf and Welling (2017) for semi-supervised node classification. The model is called the Graph Convolutional Network (GCN), and the filtering operation is given in Eq. (5).

$$\bar{X} = \sigma(\hat{A}XW)$$

Where $\hat{A}$ is the modified adjacency, specifically the calculation is $\hat{A} = D^{-\frac{1}{2}}\tilde{A}D^{-\frac{1}{2}}$, with $\tilde{A} = A + I_N$. By this approach, the features of the node itself can be preserved during the filtering process, and $\sigma(\cdot)$ is a non-linear activation function (e.g. a tanh of sigmoid function). GCN is the most popular graph neural network and has been widely used in many fields.

A critical limitation of a single-layer GCN is that it only aggregates first-order neighborhood information, which restricts its ability to effectively capture larger graph structures. Even though stacking multiple GCN layers may help tackle this limitation, it may lead to excessive smoothing of node features when dealing with sparse data in predictions. This characteristic can significantly impact the quality of railway cold chain freight demand forecasting, as it inherently exhibits sparsity. To achieve effective adaptation, node features with significant differences are necessary, as excessive smoothing may result in decreased predictive performance or uniformly consistent output predictions.

3.1.2 Model components

In the previous Section, we presented the foundation of GNNs and pointed out the inadequacy of the GCN models for addressing the problem in this paper. To tackle the issue of sparse target set prediction, we introduce a novel graph neural network model called GraphARMA-GRU.

A. ARMA graph neural network layer

The ARMA graph neural network layer is inspired by the ARMA model's principles that enable the graph neural network layer to consider time series information between features and targets during computation. It can capture more comprehensive global structures and longer-term temporal dependencies (Bianchi et al., 2021). The spatial representation of the ARMA graph neural network layer is depicted in Eq. (6).

$$\bar{X} = (I + \sum_{k=1}^{K} q_k L^k)^{-1} (\sum_{k=0}^{K-1} p_k L^k) X$$

Where K represents the maximum neighborhood order aggregated by this layer. Rearranging Eq. (6) yields $(I + \sum_{k=1}^{K} q_k L^k)\bar{X} = (\sum_{k=0}^{K-1} p_k L^k) X$, The left-hand of the equation corresponds to the MA term, while the right-hand corresponds to the AR term, q_k and p_k are coefficients. The introduction of the AR term enhances the model's robustness against noise since it relies on the multi-step propagation of node features. This is crucial for effectively capturing long-term dependencies and global structures.

This approach increases computational complexity as evident in Eq. (6), which requires matrix inversion. In this study, we use an alternative method to approximate the ARMA filter using recursion.

Eq. (6) can be rewritten as a recursive fitting function $\bar{X}^{t+1} = \alpha M \bar{X}^{t} + \beta X$,where

$\alpha(|\alpha|<1)$ and β are fitting coefficients, and $M=\frac{1}{2}(\lambda_{\max}-\lambda_{\min})I-L$, the convergence properties of this recursive approximation can be analyzed and expressed as shown in Eq. (7).

$$\bar{X}=\lim_{t\to\infty}[(\alpha M)^t\bar{X}^0+\beta\sum_{i=0}^{t}(\alpha M)^t X]$$

Clearly, the eigenvectors of M and L are the same, but the eigenvalues of M become $\eta_m=(\lambda_{\max}-\lambda_{\min})/2-\lambda_m$ The first term in Eq. (7) goes to zero when $t\to\infty$, and the second term is a series that converges to $\beta/(1-\alpha\eta_m)$. We can write the approximated form of the ARMA filter as $g(\lambda_m)=\beta/(1-\alpha\eta_m)$. By performing the Laplacian decomposition on the matrix L, we can obtain the spectral analytical form of the ARMA filter, as shown in Eq. (8).

$$\bar{X}=\sum_{k=1}^{K}\sum_{m=1}^{M}\frac{\beta_k}{1-\alpha_k\eta_m}\mu_n\mu_n^T X$$

Where μ_n represents the eigenvectors of the Laplacian matrix, It can be observed that the approximated form and Eq. (6) are mathematically equivalent. We can express one layer of the ARMA graph neural network in the form of Eq. (9).

$$\bar{X}^{t+1}=\sigma(\tilde{L}\bar{X}^t W+XV)$$

Where W and V are trainable parameters, $\bar{X}$ is the feature of nodes, and $\tilde{L}$ is the modified Laplacian matrix. We denote the ARMA graph neural network layer of the K-th layer as ARMA_K, and its output can be represented by Eq. (10), where $\bar{X}^T$ denotes the output of the last layer in Eq. (9).

$$\bar{X}=\frac{1}{K}\sum_{k=1}^{K}\bar{X}_k^T$$

B. Gated Recurrent Unit (GRU)

Similar to data in other transportation fields, railway cold chain freight demand data exhibits temporal dependencies. Although the ARMA graph neural network layer shares some similarities with recurrent neural networks, when dealing with time series data, the absence of gating mechanisms may lead to the model learning excessively irrelevant temporal features, thus compromising its performance. To address this, we introduce the Gated Recurrent Unit (GRU) to further process the temporal data within the features.

$$z_t = \sigma(W_z \cdot [h_{t-1}, x_t])$$
$$r_t = \sigma(W_r \cdot [h_{t-1}, x_t])$$
$$\tilde{h}_t = \tanh(W \cdot [r_t * h_{t-1}, x_t])$$
$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

Eq. (11-14) describe the process of the GRU model, where z_t represents the update gate, and r_t represents the reset gate. The activation function $\sigma(\cdot)$ of both gate units is the sigmoid function, which allows the model to control information forgetting and updating through the gate mechanisms. h_{t-1} represents the hidden state passed from the previous time step, x_t represents the node input passed from the current time step. The reset gate controls how much information from the previous hidden state can be input into the candidate hidden state $\tilde{h}_t$. The update gate, on the other hand, controls the proportion of $\tilde{h}_t$ and h_{t-1} in the final output h_t. Through this approach, GRU can retain useful temporal information as input for the ARMA graph neural network layer.

3.2 Overall Architecture of the GraphARMA-GRU Model

The overall architecture of our proposed model is depicted in Figure 1. Firstly, the temporal features undergo multiple GRU units to output the final hidden layer. Secondly, we incorporate the external features of nodes and the temporal feature learned by GRU using two ARMA graph neural network (ARMAGNN) layers. As mentioned earlier, these ARMAGNN layers leverage adjacency information between nodes to enhance the capturing of relationships and patterns in graph data. Lastly, we concatenate the outputs of the two ARMAGNN layers and input them into the fully connected layer, reshaping the output to match the railway cold chain freight demand of nodes at time $t+1$. During training, the model's output is compared with the actual data using a loss function to calculate the error. The model can then update its parameters through the error propagation mechanism.

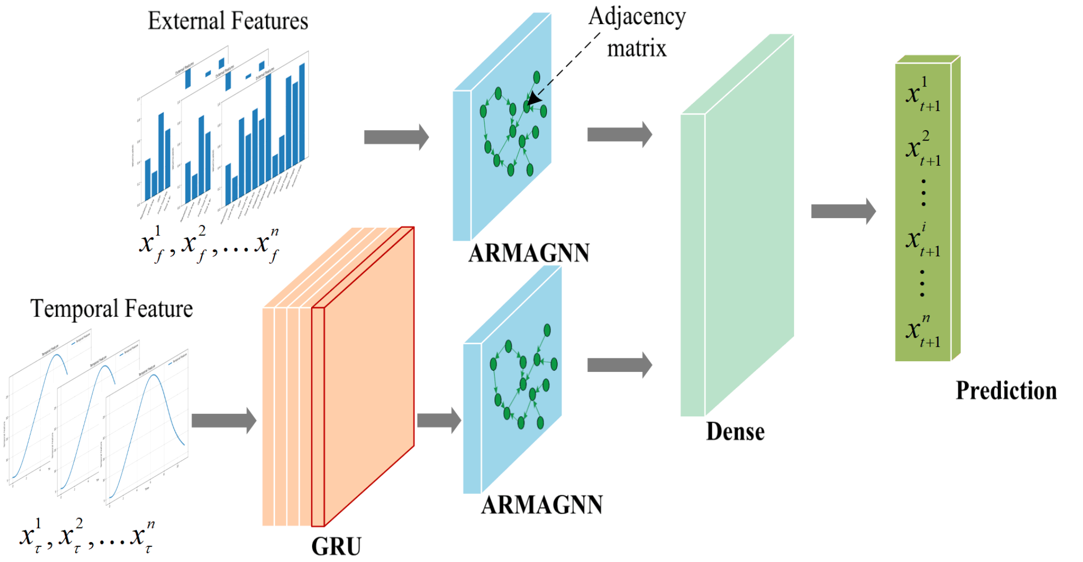


Figure 1. Overview of GraphARMA-GRU Model

The model's input consists of the time series data of cold chain freight demand for all nodes over the past τ time steps: $x_\tau^1, x_\tau^2, \ldots x_\tau^n$, where x_τ^1 represents $x_{t-\tau}^1, \ldots, x_t^1$, and this pattern continues for the remaining nodes. Additionally, the input includes the external features for all nodes, denoted as $x_f^1, x_f^2, \ldots x_f^n$ and the adjacency matrix A which represents the relationships between nodes. The model's output is the forecasted cold chain freight demand for all nodes in the next time step: $x_{t+1}^1, x_{t+1}^2, \ldots x_{t+1}^n$.

3.3 Model Interpretability

Emphasizing interpretability in deep learning applications cannot be overstated. It contributes to improving the transparency of models. To provide explanations for our model, we introduce the GNNExplainer method (Ying et al., 2019); and this method can address the following issues:

1) For a specific node, what are the important factors affecting its railway cold chain freight demand? 2) For a specific node, which nodes' features have a significant impact on it? 3) For a specific node, which edges play an important role in influencing that node?

When provided with a trained GNN model and a prediction, GNNExplainer generates an explanation by identifying a subgraph $G_i \subseteq G_c$ of the computation graph and a subset of node features $X_i = \{x_j \mid v_j \in G_i\}$ that significantly influence the model's prediction. The explanation highlights the key factors contributing to the GNN's decision-making process. Which utilizes mutual information to quantify this importance and can be expressed using the following optimization framework:

$$\max_{G_i} MI(O,(G_i, X_i)) = H(O) - H(O \mid G = G_i, X = X_i)$$

By applying the method proposed by Ying et al. (2019) to solve Eq. (15), we can obtain the explanation subgraph G_i and explanatory feature subset X_i, which will be used to interpret our GraphARMA-GRU Model. Figure 2. illustrates a simple example. The green nodes and edges represent elements that have a significant influence on the output, while the features marked with a cross on the right-hand indicate irrelevant features that have little impact on the output.

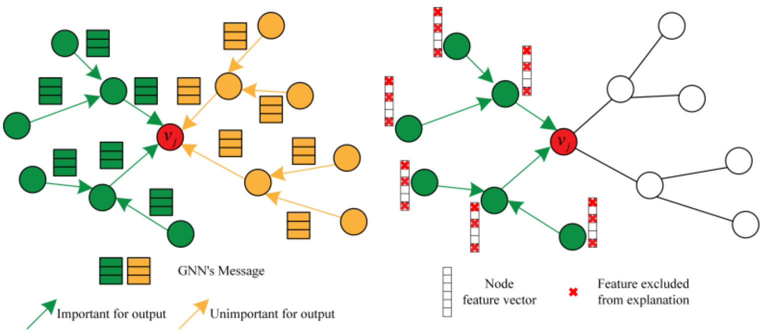


Figure 2. Example of an interpretable subgraph

4. Experiments

4.1 Data description

In this study, we utilized a real dataset from China Railway Special Cargo Logistics Co., Ltd., covering 43,497 records of railway cold chain freight volume from September 1, 2018, to September 30, 2019. The dataset includes 14 categories of goods, such as frozen meat, fruits, vegetables, and pharmaceuticals, with comprehensive coverage. To handle the data in a reasonable way, considering the periodic patterns in railway cold chain freight volume, we adopted cities as spatial objects (a total of 173 cities). We aggregated the data on a weekly basis. By this approach, we could reduce the noise and dimensionality of the time series data, which enhances the model's practicality.

Additionally, we obtained the railway adjacency relationships among the mentioned 173 cities (as shown in Figure 3), as required input for the model, by processing the topological relationships using the actual railway network map from OpenStreetMap (https://www.openstreetmap.org) in ArcGIS.

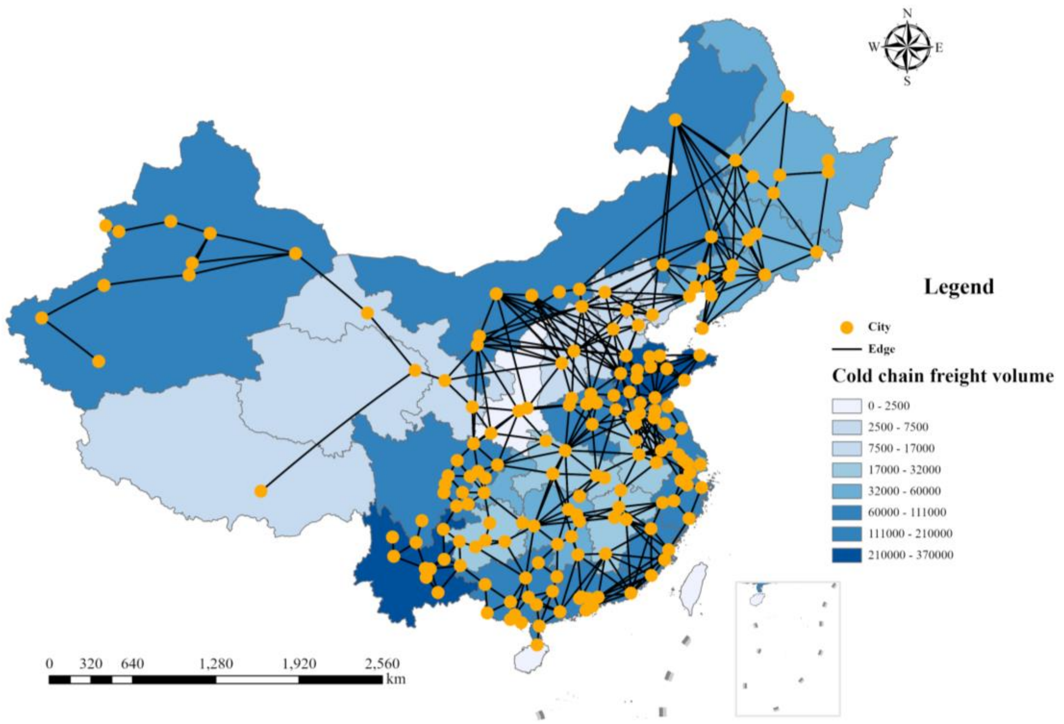


Figure 3. Railway adjacency topology graph

We visualized the weekly freight volumes of all 173 cities in a three-dimensional bar chart, as shown in Figure 4. It is evident that railway cold chain freight volume exhibits higher sparsity and volatility. To address this challenge, our model incorporates time series features and selects relevant external features tailored to the cold chain context. We collected indicators from national and city statistical yearbooks that have an impact on railway cold chain freight volume for these 173 cities, which is a common practice in existing studies(Barbour et al., 2018; He and Huang, 2018; Wang et al., 2019; Yang and Yu, 2015; Zhao et al., 2023). Furthermore, we gathered Point of Interest (POI) indicators related to cold chain freight transportation from the perspective of supply and demand, including Fresh Food Market POI, Food & Beverage POI, Shopping POI, and Fruit Market POI. Data for all 173 cities was collected using the Amap API (https://lbs.amap.com). The time series features encompass the freight volumes of railway cold chain cargo for the initial time steps in these 173 cities. In our experiments, multiple time steps were considered to determine the most appropriate model configuration.

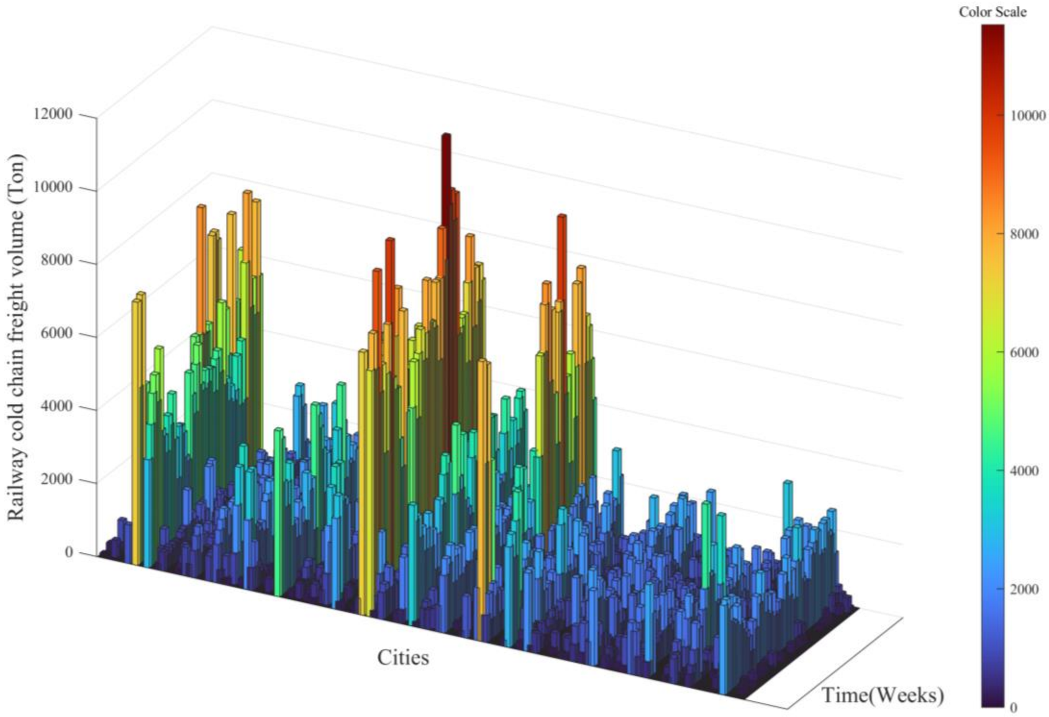


Figure 4. Overview of Railway Cold Chain Freight Volume

4.2 Model hyperparameter configuration

Optimizing model hyperparameters is crucial in building and training machine learning models (Peng et al., 2023). Hyperparameters are configurations set before the training process begins, directly influencing the model's learning capacity and generalization performance. These parameters cannot be learned from the data and must be carefully chosen based on domain knowledge, experimentation requirements, and data characteristics.

The hyperparameters of GNN models mainly include learning rate, weight decay, hidden size, dropout rate, and batch size. We adopted a method similar to Gridsearch to optimize the model's hyperparameters, evaluating the predictive performance of model variants using the R^2

score on the test set. This metric is widely used for assessing regression models, especially when comparing different model variants. It should be noted that exhaustively exploring all possible combinations of hyperparameters is impractical and unnecessary. Instead, we narrowed down the hyperparameter search to the most promising combinations. We trained over 300 model variants and visualized this process in Figure 5. The hidden size parameter has values of [16, 32, 64, 128, 256], but we selected the top three groups with higher R^2 values for simplification in the plot. The highest point (red dot) in Figure 5 represents the optimal hyperparameter values for our model. Therefore, the hyperparameters of our model are: learning rate of 0.005, weight decay of 0.008, and Hidden size of 128. The training set was 80% of the data, and the testing set was 20%. The model optimizer selected was Adam, which is a commonly used optimization algorithm.

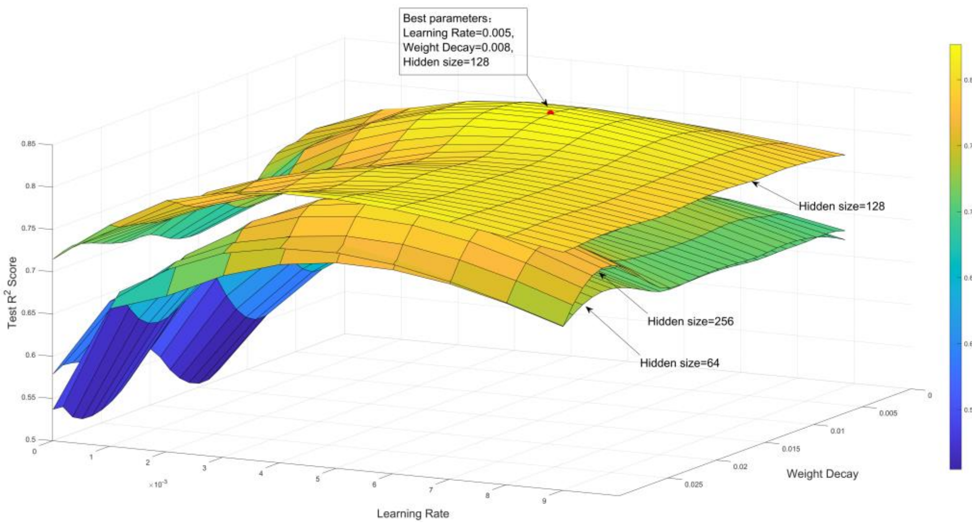


Figure 5. Hyperparameters adjustment process

Once the hyperparameters are determined, the model can be trained, and the various metrics during the training process are shown in Figure 6. It can be observed that as the number of epochs increases, both the RMSE (Root Mean Squared Error) of the training and testing sets gradually decrease. From the R^2 scores, show that both the training and testing sets exhibit the same upward trend, which indicates that the model's parameters are appropriately set, and the model successfully converges without overfitting.

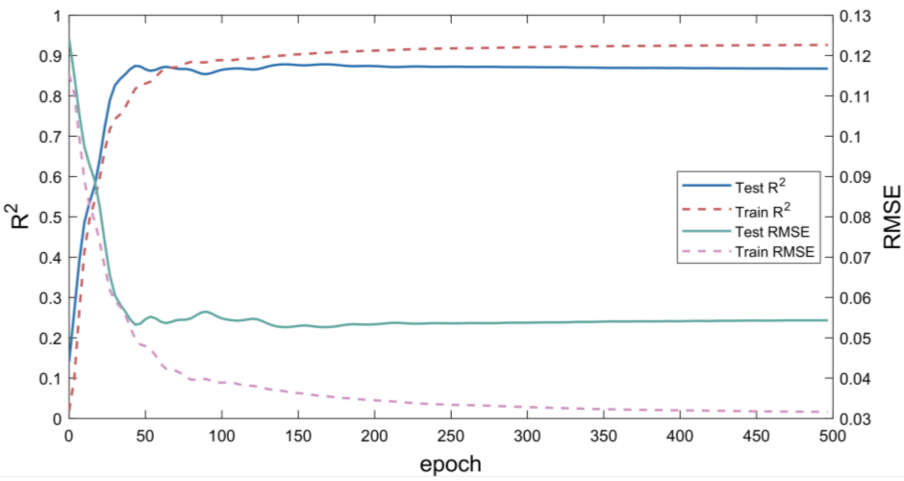


Figure 6. R^2 and RMSE variation curve

4.3 Performance of the Model

We compare the performance of our proposed GraphARMA-GRU model with the following baseline models:

(1) Graph Convolutional Network (GCN): GCN is one of graph neural networks' most widely used models. We use all features, including both temporal and external features, as input for the GCN model. The adjacency matrix input is consistent with the GraphARMA-GRU model. For more detailed information about the GCN model, please refer to Section 3.1.1.

(2) Gated Recurrent Unit (GRU): GRU is a constituent of the GraphARMA-GRU model. We use only the temporal features as input for the GRU model. For more detailed information about the GRU model, please refer to Section 3.1.2 B.

(3) Multilayer Perceptron (MLP): MLP is a standard baseline model in neural networks. We use temporal and external features as input for the MLP model.

(4) Random Forest (RF): RF is a classic machine learning model widely used in transportation. The input features for the RF model are consistent with the MLP model.

(5) Gradient Boosting Regression Tree (GBRT): GBRT is an ensemble learning model used for regression tasks. The input features for the GBRT model are consistent with the MLP model.

(6) ARIMA is a traditional time series model. We model each city individually, using the complete time series data for each city as input, and split the data into training and testing sets

in a 8:2 ratio.

We conduct comprehensive experiments to evaluate the performance of these baseline models and our proposed GraphARMA-GRU model. The comparison results are shown in Table 1.

Table 1. The prediction results of the GraphARMA-GRU model and other baseline models

Model		GraphARMA-GRU	GCN	GRU	MLP	RF	GBRT
Time step = 9	RMSE	**0.0536**	0.1437	0.0639	0.0821	0.0705	0.0682
	MAE	**0.0213**	0.0781	0.0334	0.0453	0.0411	0.0365
	R^2	**0.8670**	0.6521	0.7993	0.7143	0.7203	0.7417
Time step = 6	RMSE	**0.0552**	0.1483	0.0658	0.0844	0.0726	0.0702
	MAE	**0.025**	0.0804	0.0344	0.0466	0.0423	0.0376
	R^2	**0.8286**	0.6003	0.7725	0.7013	0.7072	0.7169
Time step = 3	RMSE	**0.0649**	0.1616	0.0663	0.0923	0.0793	0.0767
	MAE	**0.0312**	0.0878	0.0327	0.0509	0.0462	0.041
	R^2	0.7786	0.6336	**0.7825**	0.694	0.6998	0.7206

We evaluated the models' forecasting performance for the future one-time step's cold chain freight demand at different time steps. It can be observed that our proposed model outperformed other models across several time steps, confirming the effectiveness of our proposed railway cold chain freight demand forecasting model. The following is an analysis of Table 1 from different perspectives:

From the perspective of time steps, as the input time step increases, it implies that the overall feature quantity for each model also increases, leading to improved forecasting performance for all models. This indicates a strong temporal pattern in railway cold chain freight demand. Additionally, at each time step, the two best-performing models are GraphARMA-GRU and GRU. This is because these two models handle time series data differently from the other models. The mutual relationships between time sequence features are considered in these models, while the other models treat time series features and external features as independent and equivalent features, which limits their ability to capture temporal relationships effectively.

From the perspective of spatial relationships, only GraphARMA-GRU and GCN models consider the railway adjacency relationships between different cities. The performance of the GraphARMA-GRU model is better than the GRU model, which only considers time features. For the input with a time step of 9, the R^2 of GraphARMA-GRU is 4.67% higher than that of GRU. This is not surprising, as the railway adjacency relationships are indeed important factors influencing railway cold chain freight demand. However, it is noteworthy that the performance of the GCN model, which also considers spatial relationships, is surprisingly poor. This could be due to two reasons. First, as mentioned in Section 4.1.1, the GCN model faces the issue of excessive smoothing. Second, although GCN also takes time series feature data as input, it treats data from different time steps as independent features, making it challenging to capture time series patterns and thus reducing its predictive capability. Additionally, the ARIMA model results were excluded from Table 1 because each ARIMA model was tailored to individual cities with distinct parameters, rendering it impractical to standardize the time steps with the aforementioned baseline models. Despite our efforts to configure appropriate (p, d, q) parameters for each ARIMA model based on our Augmented Dickey–Fuller (ADF) tests, the model's performance was substantially poor, with R^2 values almost universally negative. This indicates that the ARIMA model's explanatory power for the data is exceedingly low, even inferior to simple mean predictions. The mean RMSE and MAE were 0.3421 and 0.2472, respectively, which are several times higher than those of the worst-performing model in Table 1. This outcome is not unexpected, as the railway cold chain freight volume data demonstrate significant temporal non-stationarity.

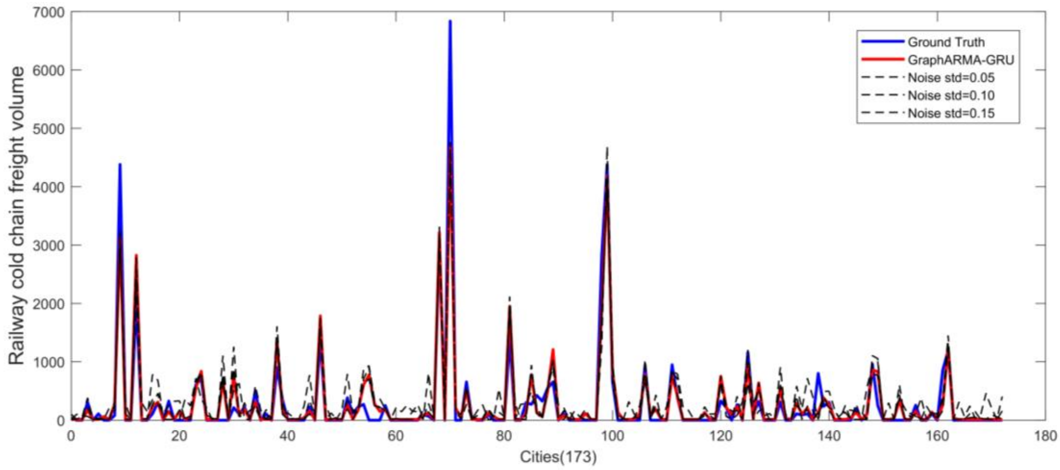
Examining the robustness of a model is equally crucial, especially in predictive modeling. Robustness refers to the stability and resilience of the model to noise, perturbations, or variations in the input data. In real-world applications, uncertainties and noise are inevitable, leading to changes and disturbances in the input data, affecting the model's predictive outcomes. To assess the model's robustness, we introduced Gaussian perturbations with a mean of 0 and standard deviations of 0.05, 0.1, and 0.15 to the normalized model inputs (standard deviations=0.17). Table 2 presents the observed model's predictive performance variations under these perturbations.

Table 2. Robustness analysis of GraphARMA-GRU

Gaussian Perturbation	GraphARMA-GRU		
	RMSE	MAE	R^2
Std=0.05	0.054	0.0264	0.8531
Std=0.1	0.06	0.0321	0.8263
Std=0.15	0.0614	0.0347	0.8164

As observed, with Gaussian noise(std=0.05), the predictive performance remains stable with minimal degradation. This implies that the model has good robustness to minor noise variations, which is highly beneficial for real-world datasets that often contain minor noise. For higher noise levels (std=0.1 and 0.15), there is a slight increase in RMSE and MAE and a decrease is observed in R^2 by 4.93% and 6.19%, respectively. This might imply that even with some degree of noise, the GraphARMA-GRU model can still explain the variability in the data effectively. This observation indicates that our model demonstrates a certain level of robustness.

We selected and presented the prediction results of cold chain freight demand for 173 cities in a specific time frame(week=14) from the test set. Additionally, we included the prediction results with added noise in the graph, as shown in Figure 7. Due to the data's sparsity and volatility, plotting too many time frames on a single graph may lead to visual clutter, affecting practical interpretation. Therefore, to ensure a high level of clarity and coherence in the results, the data from all time frames in the test set were not included in this particular graph. From Figure 7, it can be observed that the predictive curves of GraphARMA-GRU generally align well with the actual values. However, the predictive performance at a few extreme values is not as good as expected. This behavior might be attributed to the sparsity and complexity of the data. Dealing with extreme values can challenge for the model, mainly when the data exhibits substantial variations or non-linear relationships. Despite the slight limitations in predicting extreme values, the GraphARMA-GRU model can still accurately captures the overall trends in freight demand for most cases. Furthermore, the model exhibits robustness when confronted with noise, indicating its resilience in handling typical prediction tasks.



Figrue 7. The visualization results for prediction and robustness analysis

We also conducted a comparative analysis of the model's performance across different forecasting terms, as illustrated in Table 3. Overall, the differences between the two are not substantial. The results indicate an enhancement in the model's predictive capability for mid-term forecasts, as evidenced by higher R^2 values compared to short-term forecasts. However, the RMSE and MAE are slightly higher, suggesting a diminished capacity of the model to capture subtle changes. Furthermore, mid-term forecasts exhibit less sensitivity to variations in the time step relative to short-term forecasts. In summary, the GraphARMA-GRU model demonstrates considerable robustness in handling predictions across different granularities.

Table 3. Performance of GraphARMA-GRU on different forecast terms

Model		GraphARMA-GRU (weekly)	GraphARMA-GRU (monthly)
Time step = 9	RMSE	0.0536	0.0548
	MAE	0.0213	0.0332
	R^2	0.8670	0.8647
Time step = 6	RMSE	0.0552	0.0573
	MAE	0.025	0.0347
	R^2	0.8286	0.8589
Time step = 3	RMSE	0.0649	0.0601
	MAE	0.0312	0.0351
	R^2	0.7786	0.8375

4.4 Interpretability of the Model

In Section 2.4, we discussed that GNNExplainer could provides explanations for GNNs on a per-node basis. In contrast to traditional machine learning models, where samples are assumed to be independently and identically distributed, and predictions are made for the entire dataset, GNNs consider the interconnectedness between nodes, where node features can mutually influence each other.

Consequently, GNNExplainer's explanations are node-centric. By generating explanatory subgraphs for each node, GNNExplainer enables a deeper understanding of how the GNNs make predictions based on the underlying graph structure and how the features of each node and their relationships with neighboring nodes contribute to the prediction outcomes. For the specific task in this study, the node-centric explanations offer more granular insights, aligning closely with the reality of each city's uniqueness. The explanations consider the individuality of each node (city) and utilize the node's features and its neighbors' influence to make predictions. This approach allows the model to perform personalized analysis of the influencing factors for different cities rather than treating all cities as identical samples. By relying on node-centric explanations, we gain a better understanding of how the GNNs predict the cold chain freight demand for different cities and can further comprehend the significance and contribution of each city in the prediction process.

Given the large size of our dataset with 173 cities, providing individual explanations for each city is impractical. Therefore, to enhance the model's interpretability and facilitate meaningful analysis, two important cities from the northern and southern regions of China, namely Beijing and Hangzhou, are chosen for further analysis of interpretability. The feature importance of these cities can be found in Table 4.

Table 4. Feature Importance

Features	Feature Importance(%)	
	Beijing	Hangzhou
Time Series Feature	25.94	24.76
Population	11.99	11.06
Land Area	7.78	7.68
GDP	7.76	6.68
Fresh Food Market POI	11.14	11.24
Food & Beverage POI	4.06	4.18
Shopping POI	5.44	5.17
Fruit Market POI	7.74	8.63
Number of Enterprises	3.95	3.6
Total Retail Sales of Consumer Goods	3.90	3.58
Road Freight Volume	5.21	6.31

Waterway Freight Volume	1.6	5.81
Civil Aviation Cargo Volume	3.49	1.30

In the railway cold chain freight demand forecasting for Beijing and Hangzhou, the impact of time series features is the most significant, accounting for approximately 25.94% and 24.76%, respectively. This underscores the crucial role of historical time series data in demand forecasting, prompting industry practitioners to refine data collection and analytical frameworks, focusing on historical trends to mitigate uncertainties and streamline operational planning. As a result, the railway system can achieve higher efficiency through proactive resource allocation, minimizing underutilization or overcapacity issues during peak and off-peak periods. Population, land area, and GDP features are also important factors, accounting for around 12% to 7%. Furthermore, fresh food markets, and fruit market distribution levels also have considerable importance. These indicators, varying across different levels of the cold chain service supply chain, significantly influence railway cold chain freight demand, particularly from the perspective of supply and demand relationships. Integrating such macroeconomic elements into forecasting models is imperative as it arms policymakers and logistics strategists with a comprehensive analytical toolkit. This enriched perspective enables them to formulate well-informed decisions on infrastructural enhancements or expansions, thereby aligning investments with actual market needs and fostering a more responsive and efficient cold chain ecosystem.

An interesting observation is the significant difference in the importance of waterway freight volume between Beijing and Hangzhou, which are 1.6% and 5.81%, respectively. This is a realistic situation, and the reasons can be explained by the differences related to geographical locations and waterway transportation conditions. Beijing, as an inland city, has a much lower amount of waterway freight volume, resulting in the low importance of this feature. In contrast, Hangzhou benefits significantly from several waterway transportation routes, such as the Qiantang River and the Hangzhou-Ningbo Canal. The competition between waterway transportation and railway transportation has an impact on freight demand forecasting, and this relationship can be identified and reflected in the model's results. The difference in importance of civil aviation cargo volume is also worth noting; in comparison to Huangzhou, this indicator has a 2.68 times greater impact in Beijing. Similarly, this difference in importance can also be well explained. Beijing, being the capital of China and with two large international airports, has a much higher volume of air cargo transportation compared to Hangzhou. As mentioned earlier, this is due to the model being node-based, where the same feature's impact on different cities varies. Traditional machine learning models can, however, not achieve this, as they overlook the diversity of samples.

The model's interpretability also includes the weights of edges within the subgraph. The interpretable subgraphs for these two cities are visualized. For better understanding and visualization, we abstracted the topological structures onto maps, as shown in Figures 8 and 9. The interpretable subgraphs depict how the predicted values of the target nodes are generated during the model's forecasting process. From another perspective, they describe how the cold chain freight demand of the target city is influenced by other cities within the graph structure. The color of edges in the interpretable subgraphs represents the strength of their interactions, where darker-colored lines indicate stronger connections and lighter-colored lines indicate weaker connections.

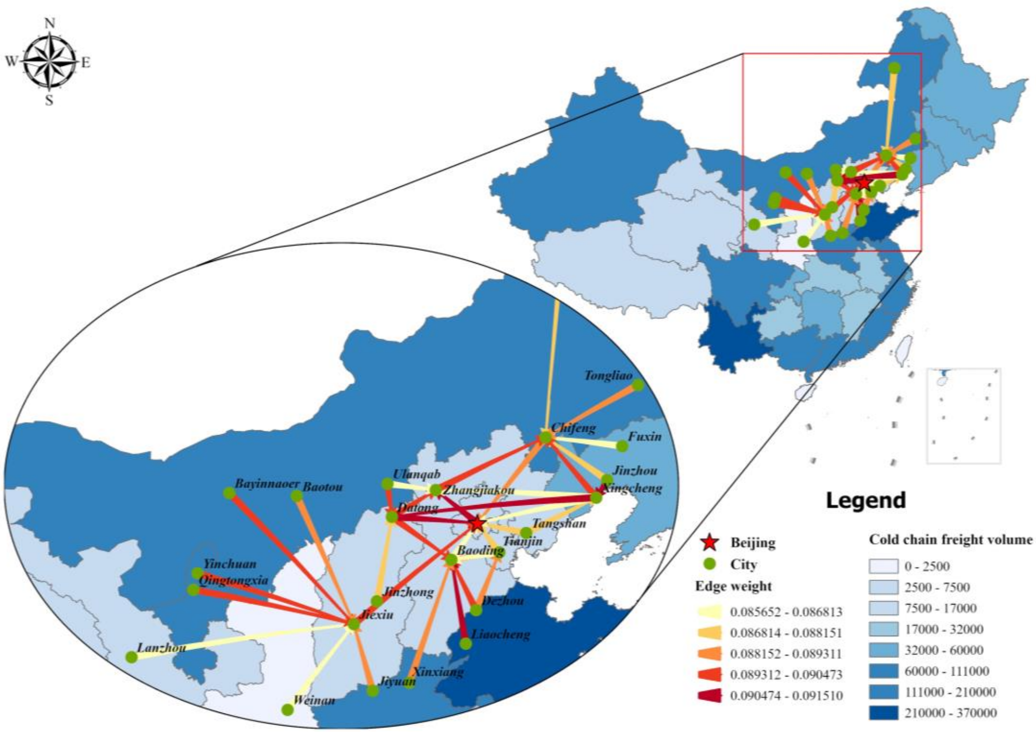


Figure 8. Explanatory Subgraph for Beijing City

It can be observed that Beijing, Jiexiu, Baoding, and Chifeng exhibit strong attraction for cold chain cargo from neighboring cities, and the distribution of freight shows an apparent agglomeration effect with these cities as central hubs. This phenomenon reflects the aggregation and grouping activities in the long-distance transportation of cold chain cargo, showcasing their geographical significance. For instance, Chifeng plays a pivotal role as a hub for cold chain freight transportation between the northeastern provinces of China and Beijing. Meanwhile, Datong and Jiexiu jointly handle freight flows from the western regions, mainly originating from Inner Mongolia, Gansu, and Shaanxi. The impact from the western regions on Beijing is more significant than that from the eastern regions, indicating the spatial imbalance in the distribution of supply and demand for cold chain cargo. This suggests that corresponding transportation organization plans for different types of cargo should be formulated.

Additionally, the economic activities in the Beijing-Tianjin-Hebei urban cluster are also reflected in this network. Baoding and Zhangjiakou, as two important pillars of Hebei's economic development, form the backbone of the regional transportation network between Beijing and Tianjin. The radiating effect of cold chain transportation services on the surrounding areas is built upon this framework.

Furthermore, it is also noteworthy that physical adjacency on the basic routes does not necessarily lead to direct connectivity for transportation services. Goods still need to be consolidated in intermediate cities before reaching their destination (or even taking detours), as seen in the case of Tianjin and Baoding in the graph. While this may be a result of maximizing the utilization of railway network capacity, shippers and transportation authorities should take this behavior into account during the shipment pooling process at the origin to achieve maximum transportation efficiency.

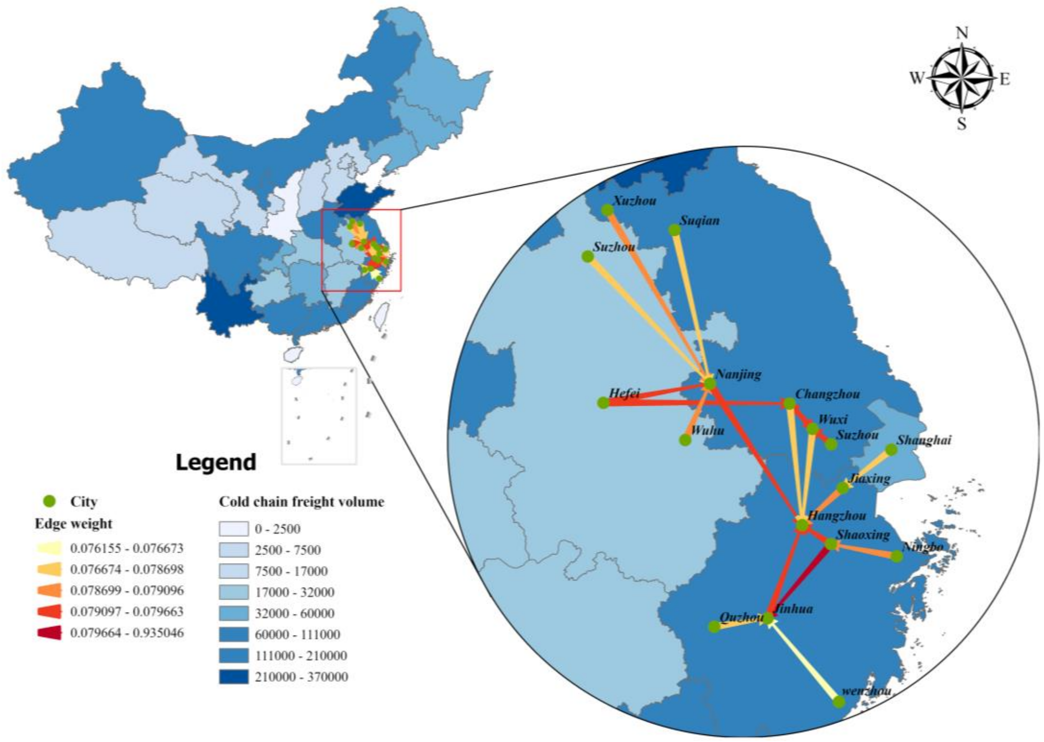


Figure 9. Explanatory Subgraph for Hangzhou City

Similar to Beijing, the explanatory subgraph of Hangzhou also exhibits a radiating network structure, with Hangzhou, Nanjing, and Jinhua aggregating the cold chain freight demand from surrounding cities. Nanjing primarily gathers freight flows from Jiangsu and Anhui provinces. The remaining cities concentrate on freight flows from various coastal cities in the eastern region.

Edges connecting Jinhua, Shaoxing, Nanjing, and Hangzhou have darker colors, with these three edges accounting for 45% of the entire explanatory subgraph. Considering the geographical proximity, Shaoxing and Jinhua have strong freight transportation connections with Hangzhou due to their location. The high-weighted edges between Hangzhou and Nanjing reflect the economic ties of the Yangtze River Delta urban cluster, which is one of the most economically dynamic and prosperous urban clusters in China. These cities are closely linked geographically and economically, forming a highly developed economic region. As two important major cities in the Yangtze River Delta urban cluster, their frequent economic activities are well-reflected in transportation, showcasing the derivativeness of railway transportation. This highlights the impact of the geographical location of specific cities and the changes in socio-economic indicators on freight demand, which needs to be focused on in future demand forecasting and freight planning.

Another observation is that the freight flow in Hangzhou seems to exhibit a longitudinal belt-like distribution, which differs from Beijing's horizontal distribution. This reflects that Hangzhou has relatively weaker connections with its western provinces in the cold chain-related industries and underscores the spatial imbalance in supply and demand relationships.

An important aspect is that our model's input data only includes each city's cold chain freight volume rather than intercity OD freight volume. During the training process, our model can adaptively adjust the information flow between nodes, allowing for a characterization of the impact of other cities on the target city. This is an exciting approach that provides valuable insights.

In the explanatory subgraph, adjacent edges typically have higher weights, indicating the importance of considering the transportation demand and supply chain between these cities in freight planning. Additionally, the high connectivity and frequent interaction between cities enhance the sensitivity of the cold chain market. Therefore, relevant authorities should prioritize these routes when organizing transportation activities.

At the same time, it is equally important to focus on some significant non-adjacent edges, as they reveal indirect connections between cities and trends in freight movement. When preparing freight plans, it is necessary to consider these different types of transportation routes and carefully arrange the transportation paths and transfer points for goods. Furthermore, the influence of city clusters must be taken into account. Economically developed regions like the Beijing-Tianjin-Hebei and Yangtze River Delta areas have formed close geographical and economic ties, which promote logistics development and the flow of goods. In freight planning, considering the effects of city clusters is crucial for reallocating regional transportation resources and fulfilling the demands of economic and social development.

In summary, through explanatory analysis, the predictive and influence patterns of railway cold chain freight demand can be better understood, which may further help optimize resource allocation and transportation efficiency and enhance the operational performance of the freight railway network. Our explanatory approach can make the model's forecasting result more interpretable, which helps provide specific recommendations and effective solutions for cold chain freight railway transportation organization and logistics order allocation. From a practical standpoint, the model's ability to uncover hidden relationships and the influence of non-adjacent cities guides policymakers in identifying critical corridors for investment and infrastructure development. It facilitates the anticipation of potential bottlenecks, enabling proactive measures to avoid disruptions in the cold chain supply. Moreover, the model's insights encourage collaboration among cities and regions, fostering a coordinated approach to logistics planning that considers the dynamics of city clusters. This cooperation can lead to shared logistics facilities, synchronized transportation schedules, and optimized freight flows, collectively enhancing the resilience and sustainability of the cold chain network. In essence, the interpretability of the model not only enhances our theoretical comprehension of cold chain freight dynamics but also translates into practical strategies. These strategies can drive operational efficiency, economic growth, and environmental sustainability in the railway cold chain sector. By offering actionable intelligence, the model equips stakeholders with the tools to make informed decisions that directly impact economic performance and public interest.

5. Conclusion and discussion

In this study, we propose a GraphARMA-GRU model for demand forecasting of railway cold chain freight transportation, which simultaneously takes into account network structure, time features, and external characteristics. Through empirical validation with real data in China, the effectiveness and applicability of the model in tackling the predictive challenges posed by sparse data are illustrated. In literature, most existing research combines GCN layers with established neural network layers to create new models. However, this study, on the other hand, integrates ARMA graph neural network layers with GRU layers and demonstrates their efficacy. On the application level, most models for freight demand forecasting have been developed based on machine learning algorithms, but the use of neural network models has not been extensively investigated. In this regard, our paper provides the first research that uses GNN models for railway cold chain freight demand forecasting, and our experimental results show the suitability and effectiveness of this method. Furthermore, the incorporation of interpretability methods enhances the transparency of the model's forecasting process, which may push forward the frontier of using GNNs for transportation research. Through interpretability analysis, deep insights, managerial implications, and practical recommendations can be obtained for better decision support in the planning of future railway cold chain freight transportation.

We believe the model proposed in this study is not limited to the current scenario. It is applies equally to transportation networks with distinct network structures, such as road, water, and air transport. Future research endeavors could explore the applicability of the GraphARMA-GRU model in multi-modal transportation networks, considering integration with road, water, and air transport. Dynamic adaptation methods could be investigated to ensure the model remains relevant and accurate amid evolving transportation networks or changing characteristics of goods. Additionally, the analysis of interpretable subgraphs contributes to a deeper understanding of potential issues in the cold chain freight transportation process, including but not limited to problems related to empty containers and cars. By providing explanations at the node level, it becomes possible to analyze the direction and intensity of freight flow specifically, offering more concrete and substantiated decision support for cold chain freight transportation. This detailed analysis aids in formulating effective management strategies, improving resource utilization efficiency, reducing waste, and optimizing the overall operation of the cold chain freight transportation network.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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CrediT authorship contribution statement

Tao Peng: Writing-original draft, Methodology, Conceptualization, Software, Writing – review & editing. Mi Gan: Conceptualization, Investigation, Funding acquisition, Writing-original draft. Qichen Ou: Writing-original draft, Formal analysis, Resources. Xiaoyuan Yang: Writing-original draft, Visualization. Lifei Wei: Writing-original draft. Henrik Rødal Ler: Writing-original draft. Hao Yu: Writing-original draft, Funding acquisition.

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