SPEED PREDICTION FOR FREIGHT TRANSPORT: A GRAPH NEURAL NETWORK APPROACH

SPEED PREDICTION FOR FREIGHT TRANSPORT: A GRAPH NEURAL NETWORK APPROACH

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Lay Abstract

Predicting how fast freight moves through a transportation network is key for efficient logistics and supply chains—vital components of global trade. While traditional prediction methods based on statistical analysis have their merits, they fall short when grappling with the complexities of today's fast-paced and ever-changing road networks. This study explores these traditional methods and then goes a step further, introducing an advanced model based on Graph Neural Networks (GNNs). This advanced model is adept at understanding the intricate interplay of factors affecting traffic speeds. It integrates cutting-edge techniques such as diffusion-convolutional layers and multi-head attention mechanisms with Gated Recurrent Units (GRUs) for our predictions. This method competes with older models, bringing greater accuracy and efficiency to the prediction process. This means better management of the routes freight takes, leading to more reliable and resilient supply chains worldwide.

Abstract

The accuracy in predicting the speed of freight within a transportation network is a cornerstone for achieving optimality in logistics and supply chain management. Given the critical role of freight transport in maintaining the efficiency of global supply chains, this study highlights the necessity for innovative predictive models capable of navigating the multifaceted and dynamic nature of transportation systems. Traditional methodologies, primarily rooted in statistical analysis and linear modeling, have provided foundational insights but are not adequate in addressing the multifaceted and dynamic nature of modern transportation systems. This research proposes a three-fold approach, firstly, analyzing conventional traffic speed prediction methodologies to understand their theoretical foundations, data utilization, and performance metrics and further, advancing a GNN-based model that effectively captures the complex relationships and dynamics within road networks to enhance the precision of vehicular speed predictions.

This study aims to contribute to the domain of transportation and freight logistics by offering a robust, adaptive, and accurate tool for speed prediction, leveraging advanced techniques such as diffusion-convolutional layers and multi-head attention mechanisms integrated with Gated Recurrent Units (GRUs). This novel approach advances conventional models by providing superior predictive accuracy and efficiency, thus addressing key challenges such as the need for real-time adaptability and the ability to capture intricate network dynamics. By enhancing the precision of freight speed predictions, the study not only aims to improve the operational efficiency of freight networks but also to contribute to the optimization of global trade and supply chain management, ultimately supporting the resilience and reliability of global logistics operations. Importantly, the analysis assumes that the average speeds recorded in the METR-LA dataset, which primarily reflects mixed vehicular traffic, are representative of freight vehicles, providing a basis for generalizing findings to freight transport scenarios.

Keywords: Speed Prediction, Graph Neural Network, Machine Learning, Freight Transport, Intelligent Transportation Systems, Spatiotemporal models.

Acknowledgments

I stand at the culmination of a journey that has been as challenging as it has been enlightening, a journey that has sculpted not just a body of research, but also a period of profound personal growth. This thesis, while a manifestation of my academic pursuit, is a mosaic of the countless contributions, encouragements, and sacrifices of many, to whom I owe my deepest gratitude.

My advisors, Dr. Saiedeh Razavi and Dr. Susan Tighe deserve my foremost appreciation. Not only for their scholarly guidance but also for the confidence they instilled in me.

I extend my sincere thanks to my research committee, whose insights sharpened the focus of my research and challenged me to broaden my academic horizons. Their rigorous scrutiny ensured that this work met the standards of scholarly excellence.

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My family has been an unfaltering source of love, support, and encouragement. To my parents and my beloved husband, Sandeep, whose sacrifices have paved the way for my achievements, I am forever indebted.

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List of Abbreviations and Symbols

MAB-STGNN	Multi-head Attention Built-in Spatial Temporal Graph Neural Network
GNN(s)	Graph Neural Network(s)
GRU	Gated Recurrent Units
CNN	Convolutional Neural Network
ARIMA	Autoregressive Integrated Moving Average
SARIMA	Seasonal Autoregressive Integrated Moving Average
KNN	K-Nearest Neighbors
SVM	Support Vector Machine
RL	Reinforcement Learning
RNN	Recurrent Neural Network
LSTM	Long Short-Term Memory
STGCN	Spatial-Temporal Graph Convolutional Networks
TGCN	Temporal Graph Convolutional Network
HA	Historical Average (commonly used in time-series forecasting)
SVR	Support Vector Regression

STL-GRU	Seasonal-Trend Decomposition using Loess-Gated Recurrent Unit (Hybrid model combining STL decomposition with GRU)
MTL-GRU	Multi-Task Learning Gated Recurrent Unit
AST-GCN	Attention-Based Spatial-Temporal Graph Convolutional Networks
AST-MTL	Attention-Based Spatial-Temporal Multi-Task Learning
FNN	Feedforward Neural Network
AGNN	Attention-based Graph Neural Network
GCN	Graph Convolutional Network
EAGNN	Edge Attention-based Graph Neural Network
GAT	Graph Attention Network
SVC	Support Vector Classification
ML	Machine Learning
AI	Artificial Intelligence
FHWA	Federal Highway Administration
NTAD	National Transportation Atlas Database
BTS	Bureau of Transportation Statistics
ATRI	American Transportation Research Institute
METR-LA	Metropolitan Transportation Authority Los Angeles (dataset)

SYMBOLS

y_{ij}	Actual recorded traffic speed for road segment j at temporal interval i
y'_{ij}	Predicted traffic speed for road segment j at temporal interval i
N	Total number of road segments within the traffic network or nodes within the graph
M	Number of temporal intervals within the prediction horizon
A	Weighted adjacency matrix representing road connectivity
X	Feature matrix representing traffic speeds over time
k	Number of diffusion steps in the diffusion-convolutional layer
h	Number of attention heads in the multi-head attention mechanism
d_{GRU}	GRU hidden state size
$\odot$	denotes element-wise multiplication
W_z, W_r, W_h	Weight matrices for update gate, reset gate, and candidate state in GRU
U_z, U_r, U_h	Weight matrices for update gate, reset gate, and candidate state in GRU applied to the previous hidden state
b_z, b_r, b_h	Bias terms for the update gate, reset gate, and candidate state in GRU

z_t	Update gate vector at time step t in GRU
r_t	Reset gate vector at time step t in GRU
h_t	Hidden state vector at time step t in GRU
H	Output feature matrix of the diffusion-convolutional layer
$\theta^{(k)}$	Trainable weight matrices associated with each diffusion step
σ	Sigmoid or other activation function
X	Normalized feature matrix after Min-Max scaling
h_t	Past temporal horizon for historical data input
T_f	Future temporal horizon for traffic signal prediction
T_h	Traffic signals over past time steps
X'	Road Length Adjustment factor
$\bar{S}$	Average speed recorded by sensor
n	Total number of vehicles (including both trucks and passenger vehicles) for which the speed was recorded.
s_i	Speed of the i^{th} vehicle.

Declaration of Academic Achievement

I hereby declare that the research presented in this thesis is the result of my own original work conducted as part of my advanced study program. I affirm that all sources of material not originated by me have been appropriately cited and acknowledged within this work.

The advancement of the Multi-head Attention Built-in Spatial-Temporal Graph Neural Network (MAB-STGNN) model, its application to traffic speed prediction, and the results thereof, as reported in this thesis, are my contributions to the field of machine learning and traffic forecasting. This work was carried out with adherence to ethical research standards under the guidance of my academic supervisors.

I also acknowledge the contributions of my research colleagues and other collaborators whose insights and expertise have played a significant role in shaping this research.

Any software, frameworks, or tools not originally developed by me, and utilized during my research, have been duly credited, and their use has been strictly for the purpose of this academic endeavor within the bounds of legal and ethical guidelines.

In my thesis, I used ChatGPT, an AI language model by OpenAI, for proofreading and to gain clarity on specific topics, ensuring all AI contributions were critically evaluated and cited. ChatGPT also assisted in enhancing the coherence of the textual content in this thesis, helping to improve the overall quality of the presented work. All empirical data, including the METR-LA dataset utilized for model training and testing, have been applied in a manner consistent with the terms of use and with proper attribution to the respective sources.

1 INTRODUCTION

Motivation

Freight transport plays a pivotal role in maintaining the seamless operation of supply chains in the global economy. The complexities inherent in transportation infrastructure, compounded by the multifaceted nature of international trade and logistics, necessitate innovative approaches to enhance freight transport efficiency (S. Li et al., 2022). The rapid pace of urbanization, particularly in emerging economies, introduces additional complexities in freight transport, necessitating adaptive and resilient predictive models. These models must account for a wide array of variables, including but not limited to, traffic congestion, disruptions, transport network capacities, and the environmental sustainability of freight operations. In an era characterized by an ever-increasing need for operational efficiency, environmental sustainability, and safety, accurate prediction of freight speed stands as a cornerstone in the transformative landscape of logistics and transportation (Otte et al., 2020).

As global trade expands and freight networks become increasingly complex, the need for accurate and dynamic speed and travel time prediction models has become a pressing issue. The pursuit of accurate and reliable predictions of freight transport travel time or speed is not just a logistical concern but a critical factor in the overall efficiency and resilience of global supply chains (Tsolaki et al., 2022). However, accurate and reliable prediction of freight travel time or speed is a paramount challenge, considering the dynamic and interconnected nature of global logistics networks (Petropoulos et al., 2022) (Çatay & Eshtehadi, 2023). Addressing this challenge requires advanced predictive models that can adapt to the dynamic nature of transportation networks, necessitating further research and technological advancements.

Traditional models, while useful, often fall short of capturing the intricate, non-linear relationships within transportation networks, leading to suboptimal decision-making and planning [6] (Díaz et al., 2019). The integration of advanced technologies such as artificial intelligence and Machine Learning (ML) into predictive models holds promise in addressing these challenges, offering more accurate and timely insights into freight dynamics. This thesis is motivated by the potential of Graph Neural Networks (GNNs) to advance speed prediction in freight networks by leveraging their unique ability to model complex network structures and dynamics.

Problem Statement

The problem statement of this research revolves around the development of an effective and reliable method for predicting freight transport speeds within a complex road network. Traditional methodologies for freight speed prediction, are inadequate for several reasons:

- Inability to Capture Network Complexities: Freight networks are inherently complex, characterized by numerous interacting components, including various modes of transport, diverse routes, and dynamic operational conditions. Traditional models struggle to account for these complexities, leading to predictions that lack accuracy and reliability (Díaz et al., 2019).
- Limited Adaptability to Real-Time Changes: The dynamic nature of freight networks, influenced by factors such as traffic conditions, weather, and unforeseen disruptions, necessitates models that can adapt to real-time changes. Existing methodologies often fail to incorporate real-time data effectively, hindering their adaptability and responsiveness (H. Zhao et al., 2023).
- Inadequate Representation of Interdependencies: The components of freight networks are not independent but are interconnected in complex ways. Traditional speed prediction models often overlook these interdependencies, resulting in a significant gap in accurately predicting freight speeds (Wang et al., 2019).

In summary, the problem statement indicates a critical need for a more efficient approach to accurate freight speed prediction, capable of navigating the complexities of modern freight networks.

Proposed Research

This thesis proposes an advanced approach to speed prediction in freight networks using Graph Neural Networks. The objectives of this research are as follows:

- To conduct a comprehensive analysis of conventional methodologies in freight traffic speed prediction, encompassing their theoretical underpinnings, application in real-world scenarios, the spectrum of data sources leveraged, and performance metrics for traffic speed prediction research.
- To develop an advanced model that adeptly delineates the complex relationships and dynamic attributes within the freight networks, thereby enhancing the precision of vehicular speed predictions.
- To evaluate the performance of the proposed model in real-world scenarios, comparing its predictive accuracy, efficiency, and adaptability against traditional speed prediction methods.

To pursue these objectives, the proposed research aims to leverage GNN models to overcome the limitations of traditional freight speed prediction methods. GNNs are particularly well-suited for this task due to their ability to model complex, non-linear relationships within graph-structured data, which is a natural representation of transportation networks. The main advantages of using GNNs for this purpose include:

- Capability to Model Complex Systems: GNNs can capture the intricate relationships and dependencies within freight networks, providing a more holistic and accurate representation of the system (K. Xu et al., 2018).
- Flexibility and Adaptability: By incorporating real-time network data, GNNs can adapt to changes in the network, leading to more dynamic and responsive speed predictions (Z. Wu, Pan, Chen, et al., 2019; Zhou et al., 2018).

- Enhanced Predictive Accuracy: Through the deep learning capabilities of GNNs, the proposed model is expected to offer superior predictive accuracy compared to traditional models, taking into account a wider range of influencing factors and their interactions (Dwivedi et al., 2023; K. Xu et al., 2018)

By adopting a GNN-based model, this research seeks to provide a robust, adaptive, and accurate tool for freight speed prediction, contributing to the optimization of logistics and supply chain operations and enhancing the efficiency of global trade networks.

The scope of this research will encompass the design and implementation of the predictive framework, approach speed prediction through the lens of network-based learning, and the validation of the model using real-world freight network data.

Research Contributions

This research makes contributions to the domain of freight logistics through the development and implementation of a Graph Neural Network (GNN)-based model for predicting freight speeds, designed to overcome the constraints of conventional prediction methods. The key contributions of this study are outlined as follows:

a. Advancing Two-Phase Model Design: At the heart of our contribution is advancing a two-phase model that integrates a diffusion-convolutional layer as its foundational phase. This layer is adept at capturing the spatial dependencies inherent in freight networks, offering intuitive interpretations of these complex relationships. Its efficient computational framework ensures that the model can be applied to large-scale networks without compromising on performance, marking a significant advancement over traditional models that often struggle with the high-dimensional nature of traffic data.

b. Integration of Multi-Head Attention with Gated Recurrent Unit (GRU) Mechanism: The second phase of the model introduces a multi-head attention mechanism combined with a GRU to adeptly manage the spatiotemporal features within the freight network. This dual-component layer is engineered to focus on diverse aspects of the spatiotemporal space, enhancing the model's ability to discern critical patterns and trends that influence freight speed. This attention to detail facilitates a more nuanced understanding of the dynamic interplay between various factors affecting freight movement, thus enabling more accurate and reliable predictions.

c. Empirical Validation with Real-World Data: The efficacy of the proposed model has been rigorously tested using the METR-LA dataset, a comprehensive real-world dataset derived from the Los Angeles loop detector system. The application of GNN-based approach to this dataset has yielded significant improvements over existing baseline methods, underscoring the model's practical utility and effectiveness in real-world settings. This empirical validation not only demonstrates the superiority of the proposed model in terms of predictive accuracy but also highlights its potential applicability across different geographic and operational contexts within the freight logistics sector.

d. Broader Impact: The proposed model can help city planners, policymakers, and government agencies make better tactical and strategic infrastructure decisions by gaining insights to identify critical infrastructure needs for a more efficient freight transport. The proposed model represents a pivotal innovation for supply chain and logistics organizations, offering a foundation upon which these entities can refine their operational strategies, enhance customer satisfaction, advocate for sustainability, and fortify their supply chains against unforeseen disruptions. The ripple effects of these enhancements are bound to resonate across the global economy, underscoring the indispensable role of accurate freight speed prediction in the modern logistics and supply chain ecosystem.

In this thesis, the METR-LA dataset is utilized, which predominantly contains traffic speed data collected from various locations across the Los Angeles metropolitan area. It is important to note that this dataset primarily reflects the general vehicular traffic and does not distinguish between different types of vehicles, such as passenger cars and freight trucks. To adapt this dataset for freight speed prediction, specific assumptions about truck vehicles are made. These assumptions are critical as they allow for the approximation of the behavior of freight trucks based on the average speed data recorded for mixed traffic.

It is assumed that the speeds recorded by the sensors are representative of all vehicles on the road, including freight trucks. This simplification is guided by the hypothesis that the average speeds, although is reflective of a diverse mix of vehicle types, provide a reasonable proxy for truck speeds under similar traffic conditions. This approach acknowledges the limitations inherent in the dataset but leverages statistical assumptions to extrapolate freight-specific insights. Details on these assumptions and how they influence the predictive modeling are discussed comprehensively in Chapter 4, where the integration of these assumptions into the analysis is addressed to ensure that the predictions remain relevant and grounded in the practical realities of freight transport in urban settings.

By employing these assumptions, the research aims to bridge the gap between general traffic speed data and specific freight speed predictions, thereby enhancing the applicability of the findings to real-world freight logistics and management challenges.

Overall, the findings of this research are poised to enhance the way freight speeds are predicted, offering a more adaptable, efficient, and intelligent framework for managing freight transportation systems. By pushing the boundaries of what is possible with advanced machine learning techniques in freight transport, this study paves the way for future innovations that could further enhance the operational efficiency and responsiveness of freight networks globally.

Thesis Organization

This thesis is organized into the following several key sections, each designed to address specific aspects of the research and contribute to the advancement of freight speed prediction in network environments.

- Chapter 1 provides an Introduction: An overview of the research topic, motivation, objectives, and contribution.
- Chapter 2 provides a Literature Review: An examination of existing speed prediction methods in freight networks and an introduction to Graph Neural Networks.
- Chapter 3 provides Methodology: A detailed description of the GNN model design, algorithms, data preparation, and the formulation of the speed prediction problem.
- Chapter 4 provides Research Experiment and Data: Implementation details of the GNN model, including the software, and computational resources used. Details about the data, the experimental setup, and evaluation metrics.
- Chapter 5 provides Results and Analysis: Comparison with traditional speed prediction models, model performance, analysis of the results, and the implications for freight network management.
- Chapter 6 provides Conclusions, and Recommendations for Future Work: Summary of the research findings, contributions, limitations, and suggestions for future research directions.

2 BACKGROUND AND LITERATURE REVIEW

This chapter explores the current state of traditional freight speed prediction methods, the advent of machine learning in freight transport data analysis, and the innovative application of GNNs within this domain.

Figure 1 outlines various traffic prediction models for freight networks, categorized into three main groups: Statistical and Probabilistic Models, Traditional Machine Learning Models, and Neural Network-Based models. Under Statistical and Probabilistic Models, it lists ARIMA (Autoregressive Integrated Moving Average), SARIMA (Seasonal Autoregressive Integrated Moving Average), Kalman Filter, Bayesian Network, and Regression. The Traditional Machine Learning Models include KNN (K-Nearest Neighbors), and SVM (Support Vector Machines). The Neural Networks-based category, features CNN (Convolutional Neural Networks), RNN (Recurrent Neural Networks), GRU (Gated Recurrent Units), GNN (Graph Neural Networks), and Hybrid models that combine various neural network architectures. This classification indicates a range of approaches from traditional statistical, probabilistic, and machine learning models to advanced deep neural network-based models for predicting traffic in freight networks. The further sub-sections provide a comprehensive review of the above models.

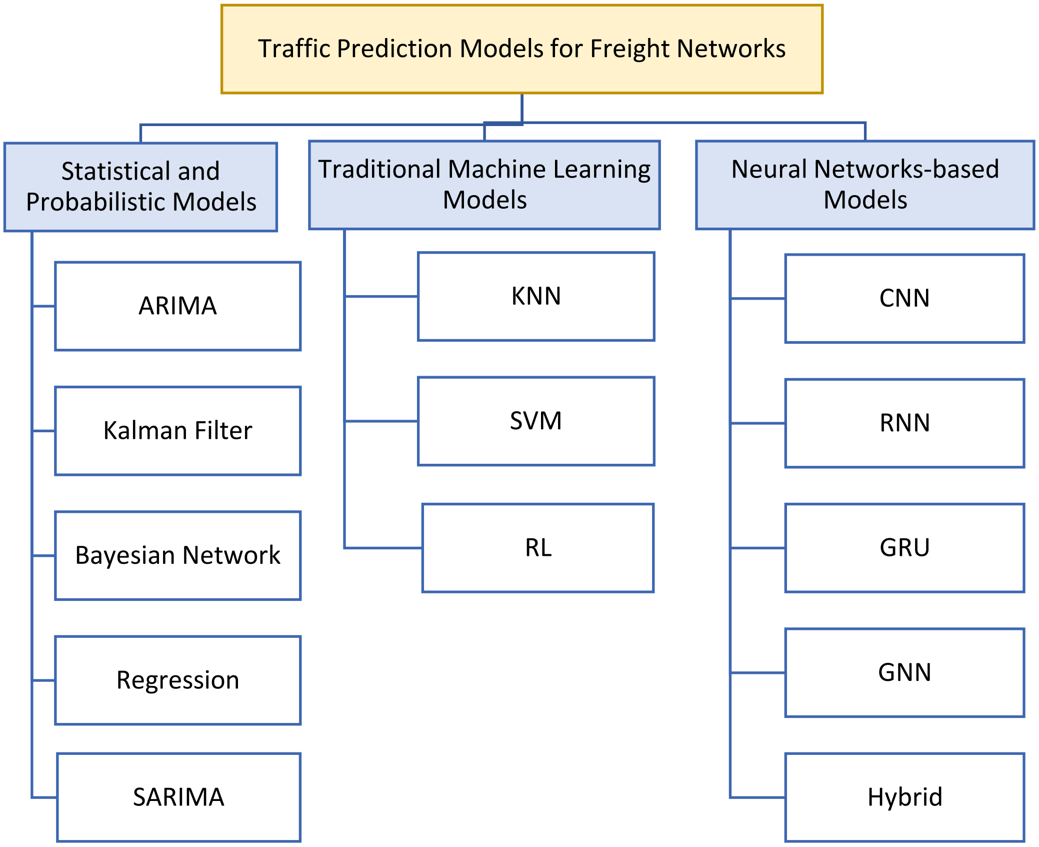
Traffic Prediction Models for Freight Networks
Statistical and Probabilistic Models
Traditional Machine Learning Models
Neural Networks-based Models
ARIMA
Kalman Filter
Bayesian Network
Regression
SARIMA
KNN
SVM
RL
CNN
RNN
GRU
GNN
Hybrid

Figure 1 Traffic Prediction Models for Freight Networks

Statistical and Probabilistic Models in Traffic Speed Prediction

Traditional approaches to traffic speed prediction have predominantly relied on statistical and probabilistic models and simulations. These methods, while foundational, often fall short of capturing the dynamic interplay of variables within complex freight networks.

Traditional statistical models have played a pivotal role in predicting general vehicle and truck traffic speeds, leveraging a variety of methodologies to enhance the accuracy and reliability of traffic forecasts. Table I provides a summary of key studies from 2006 to 2023, comparing various predictive models like Regression, ARIMA, and Kalman Filtering in freight transportation, highlighting their methodologies and identifying specific gaps, such as data dependency and model adaptability in diverse conditions.

For instance, a study in 2006 explored the efficacy of Regression, ARIMA, Kalman Filter, and Neural Networks in short-term traffic speed prediction, finding that Kalman Filtering and Neural Networks provided more accurate and realistic predictions [14]. However, the study highlighted the need for model improvements during non-peak hours and varying weather conditions, noting that models based on Neural Network and Kalman Filter require extensive data for effective training. Similarly, in 2008, a Regression-Time Series Analysis Model incorporating Seasonal ARIMA errors was developed, significantly improving short-term freight prediction precision by considering seasonal variations and historical trends [15]. The Seasonal ARIMA (SARIMA) model was employed to enhance short-term freight prediction precision by factoring in both seasonal variations and historical trends within the freight transport data. This model, though innovative, faced challenges in adequately accounting for sudden changes in freight demand due to external factors and had limitations in generalizing across different freight transportation modes or routes [20].

Table I Statistical Traffic Speed Prediction Models

Article	**Year**	**Method**	**Gaps**
(Lee et al., 2006)	2006	Regression, ARIMA, Kalman Filtering, Neural Networks	Kalman Filtering models require extensive data for training
(C. Chen et al., 2019)	2008	Regression-Time Series Analysis Model, SARIMA	May not adequately account for sudden changes in freight demand due to external factors. Limitations in generalizing across different freight transportation modes or routes.
(D. Xu et al., 2017a)	2017	ARIMA and Kalman Filter	Model performance may degrade in the face of sudden, non-recurring congestion events. Challenges in scaling the model across different geographic regions.
(Molnar et al., 2022)	2017	Kalman Filtering Technique	The technique's performance in highly dynamic or congested traffic conditions, particularly for trucks with different driving patterns than passenger vehicles, is not fully explored.
(Benninger et al., 2022)	2022	Extended Kalman Filter	The model's reliance on cloud-based traffic information may limit its effectiveness in areas with poor connectivity or data coverage.
(Molnar et al., 2022)	2022	Kalman Filter and Traffic Flow Models	The study's focus is on connected vehicles, which may not fully address the unique speed prediction challenges faced by trucks, such as different acceleration and deceleration behaviors.
(Ferreira et al., 2023)	2023	ARIMA, SARIMA	Limitations in handling non-linear and complex data patterns; need for more adaptive models.

By 2017, a model combining ARIMA and Kalman Filter demonstrated high accuracy in real-time road traffic state predictions using both historical and real-time data (D. Xu et al., 2017b). Despite its success, the model's performance was susceptible to degradation in the face of sudden, non-recurring congestion events, and it faced challenges in scaling across different geographic regions.

The implementation of an Extended Kalman Filter model utilized live traffic speeds from cloud-based services for speed prediction in traffic jam situations, achieving a notable 18% improvement in accuracy (Benninger et al., 2022). This model's reliance on real-time data and cloud-based services represented a significant step forward in leveraging technology for traffic speed prediction. However, the model's effectiveness could be limited in areas with poor data connectivity or coverage, suggesting an avenue for further development in ensuring the model's robustness across different environments.

Additionally, research on the Kalman Filter and Traffic Flow Models in 2022 introduced an onboard traffic prediction algorithm for connected vehicles, tested in real-world traffic conditions (Molnar et al., 2022). This study highlighted the potential of integrating vehicle-to-vehicle communication and advanced traffic flow modeling for individualized speed predictions. Despite its innovative approach, the study's primary focus on connected vehicles raised questions about the model's adaptability to trucks with distinct driving behaviors, pointing to the need for tailored models that can accommodate the unique characteristics of freight traffic. In 2023, (Ferreira et al., 2023) discussed ARIMA and SARIMA (Seasonal ARIMA) models in the context of network traffic prediction, highlighting their limitations in handling non-linear and complex data patterns, and the need for more adaptive models to better capture the intricacies of network dynamics.

A comprehensive review of existing literature reveals a diverse range of methodologies employed in predicting speed for both freight and passenger transport. Numerous studies have explored this domain, shedding light on the strengths and limitations of various approaches (Grubesic et al., 2008; Tsolaki et al., 2022; United Nations Conference on Trade and Development, 2021; X. Yang et al., 2022). These studies collectively underscore the continuous evolution of statistical and probabilistic models in traffic speed prediction, highlighting their strengths in leveraging historical and real-time data to improve forecasting accuracy, while also acknowledging the ongoing challenges in data requirements, model adaptability, and applicability to diverse transportation contexts.

Traditional Machine Learning Methods in Freight Transport

The integration of machine learning techniques in predicting freight network speeds is an emerging frontier that promises to address the multifaceted challenges faced by the logistics and transportation sector. The use of modern methods in AI and ML has the promise of enhancing the accuracy and adaptability of speed prediction models. The application of ML in this domain has been explored through various methodologies, objectives, and findings across numerous studies and this section provides a broader review of the use of ML in freight transport and logistics literature.

M. Mansoursamaei, et al. (Akbari & Do, 2021) conducted a comprehensive review of ML in logistics and supply chain management, emphasizing the shift towards mathematical models and simulations, with a notable focus on neural networks for predictive and optimization purposes. This systematic review underscores the evolving landscape of ML applications in logistics, highlighting the potential for enhanced predictive accuracy in freight speed and logistics operations. J. Wojtusiak et al., in (Wojtusiak et al., 2012), delve into the application of machine learning in agent-based stochastic simulations, providing a foundational understanding of how these techniques can enhance inferential theory and evaluation in logistics. This is further supported by (Guermazi et al., 2020), who explores machine learning-based entity matching approaches for validation in logistics, underscoring the versatility of machine learning in improving logistical operations.

J. Sierra-Gracia et al., in (Sierra-Garcia & Santos Peñas, 2022) explored the synergy between reinforcement learning and conventional control to enhance the tracking of complex trajectories by automatic guided vehicles (AGVs) within logistics environments. Their intelligent hybrid control scheme, which amalgamates reinforcement learning-based control with conventional PI regulators, showcases the adaptive capabilities of ML in managing the intricacies of freight movement, particularly in navigating abrupt path changes and kinematic constraints. Lin K et al. (Lin et al., 2022) discuss the use of Q-learning, a type of reinforcement learning, for optimizing the speed trajectory of freight trains considering safety, energy efficiency, punctuality, and stopping accuracy. The proposed method showed a reduction in energy consumption compared to traditional approaches. (Salais & Saucedo, 2022) delved into demand forecasting for freight transport, applying RNN Encoder-Decoder to logistic distributions. Their work highlights the critical role of

ML in forecasting and managing freight demands, ensuring efficient logistics operations, and addressing the dynamic requirements of freight networks.

Machine learning (ML) models have become increasingly significant in the field of transportation logistics, particularly for their capability to accurately predict traffic flow, thereby saving substantial labor and material resources (Mansoursamaei et al., 2023). The inherent non-linear and stochastic nature of urban mobility data makes it particularly suitable for ML techniques, which can effectively extract patterns and construct robust forecasting models from complex datasets (Cho et al., 2014). These models are adept at handling the heterogeneity of data sources, types, and characteristics, quantifying space-time dependencies, and addressing the strong non-linear characteristics of traffic flow along with various dynamic and static factors that affect it.

For instance, (Furtlehner et al., 2022) utilized Support Vector Machines (SVM) to forecast traffic congestion by analyzing data from multiple sensors, showing high levels of accuracy in their predictions. However, the model's effectiveness could be compromised by data delays from previous processes, and the continuous influx of information could increase the complexity of the data. Similarly, (Cheng et al., 2018) introduced an adaptive KNN model that considered the spatial characteristics of road networks, demonstrating superior efficiency with low error metrics compared to other techniques. In (Liu et al., 2017), the study proposed an improved KNN model that incorporated a novel dynamic distance measure to better capture the spatiotemporal correlation in traffic networks, showing greater precision than traditional models. These studies underscore the potential of ML in enhancing traffic flow prediction in urban environments, though challenges such as computational costs for real-time applications and the need for models to adapt to high-intensity fluctuating traffic remain areas for further development.

Neural Network-Based Methods in Freight Transport

Neural network-based methods, particularly deep learning techniques are distinguished by their multilayered structures capable of extracting high-level features from complex datasets, making them suited for handling the multifaceted nature of transportation logistics data. The proliferation of sensor devices across urban landscapes has led to an abundance of diverse data types, from which deep learning models can unearth intricate spatial and temporal dependencies. Among the array of deep learning approaches, Convolutional Neural Networks (CNN), Long Short-Term Memory networks (LSTM), Gated Recurrent Units (GRU), and Graph Convolutional Networks (GCN) have proven efficacy in navigating the complexities of vehicular flow forecasting (Ferreira et al., 2023; Grubesic et al., 2008; Staudemeyer & Morris, 2019; Zeng et al., 2021; L. Zhao et al., 2018). These models excel in digesting heterogeneous datasets from varied sources, offering enhanced prediction accuracy in vehicular traffic flow by adeptly mapping space-time interdependencies (Guo et al., 2021).

The application of CNN, for instance, has been pivotal in deciphering spatial features within traffic data, while LSTM and GRU models have been instrumental in understanding temporal dynamics. A notable study in (Y. Wu et al., 2018) leveraged a CNN-based model combined with GRU to dissect traffic flow data, integrating multi-periodicity elements to enhance prediction accuracy. This model's proficiency, validated through metrics like MAE and RMSE, underscored its superior performance against traditional methods, though it encountered limitations at certain prediction intervals. It was observed that the model's predictive accuracy diminished under specific circumstances, potentially attributable to anomalies in traffic events, alterations in traffic dynamics not encapsulated within the training dataset, or intrinsic limitations of the model's architectural framework in encapsulating certain temporal variations. Similarly, (Fouladgar et al., 2017) proposed a decentralized CNN-based framework, emphasizing scalability and real-time information dissemination, crucial for expansive network applications. This approach reduced the need for historical site data, and highlighted adaptability, albeit with potential shortcomings in modeling individual events due to the deep learning architecture's complexity.

On the other hand, (S. Zhang et al., 2018) the introduction of deep residual learning to manage historical trajectory, weather, and event data further exemplifies the depth of analysis achievable with deep learning. Their method, employing a robust CNN structure, adeptly managed spatial characteristics among nodes and integrated external data sets to refine predictions. While these advanced models have significantly contributed to traffic prediction, they also highlight a common challenge: the balance between model complexity and interpretability. As deep learning continues to evolve within transportation logistics, future research must navigate these intricacies, aiming for models that not only provide high accuracy but are also adaptable and interpretable for real-world applications.

C. Furtlehner et al., in (Mansoursamaei et al., 2023) reveals the multifaceted applications of ML not only in speed prediction but also in enhancing green practices within maritime logistics, addressing emissions, and energy consumption issues. This study focused on promoting environmental sustainability in maritime ports through ML, illustrating the application of polynomial regression models and recurrent neural networks (RNNs) including long short-term memory (LSTM) networks.

In the realm of freight speed prediction, Recurrent Neural Networks (RNN) and Long Short-Term Memory (LSTM) networks have been recognized for their proficiency in handling sequential data and discerning temporal dependencies. Chen, Chen, et al. (Y. Chen et al., 2020) implemented RNN and LSTM to forecast the speed distribution of freight vehicles traversing mountainous terrains. A key finding from their research was the superior capability of LSTM models in accurately capturing the spatial-temporal dynamics of vehicle speeds, outperforming conventional regression models not only in predictive accuracy but also in providing a deeper interpretative understanding of vehicular speed behaviors. However, a noted limitation was the LSTM model's intensive computational requirements, particularly in processing large datasets, and the potential for overfitting when not properly regulated (Y. Chen et al., 2020).

Expanding on this, Lu et al. (Lu et al., 2020) introduced a graph LSTM (GLSTM) framework tailored for road speed forecasting, which merges LSTM's temporal analysis with a graph-based approach for spatial feature aggregation. The innovative integration of graph neural networks (GNNs) with LSTM allowed for a more nuanced capture of the complex interplay between spatial and temporal traffic flow variables. A pivotal discovery was GLSTM's enhanced prediction accuracy, showcasing its potential in surpassing existing methodologies.

Despite the advancements in transportation technologies and data analytics, the accurate prediction of freight speed remains an area demanding further research and innovation. The existing methodologies often fall short of capturing the complex dynamics of freight transport networks, leading to suboptimal speed predictions.

Graph Neural Networks: A Paradigm Shift

Recent advancements in machine learning, notably Graph Neural Networks (GNNs), have exhibited superior efficacy across a range of tasks within non-Euclidean domains (Z. Wu, Pan, Long, et al., 2019)

(Wu Lingfeiand Cui, 2022)

. GNNs adeptly navigate graph-structured data, translating graph inputs into quantifiable numerical representations. These networks dynamically adapt their architecture to mirror the structure of the input graph, employing iterative information aggregation across vertices to encapsulate the intricate interdependencies prevalent in freight transportation and logistics networks

(Tygesen et al., 2023). This adaptability facilitates precise predictions for individual nodes, connections, or entire graphs, thereby supporting informed decision-making within complex logistical frameworks.

GNNs leverage graph theory principles, where nodes and edges possess distinct attributes conducive to convolutional or aggregation operations, reflecting various facets of freight networks such as velocity, timestamps, rail connections, cargo volumes, and lane counts. The capability to infer dynamic graphs from evolving data sets enables the modeling of transient spatial relationships, with the potential to construct and employ super-graphs and sub-graphs within hierarchical traffic systems. This innovative approach positions GNNs at the forefront of addressing the challenges faced by traditional deep learning techniques in processing diverse sensor data within heterogeneous environments

(Bruna et al., 2014; Tygesen et al., 2023; Wu Lingfeiand Cui, 2022)

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In recent years, Graph Neural Networks (GNNs) have emerged as a transformative solution for addressing the limitations of conventional methods in predicting speed for freight and passenger transport (Rahmani et al., 2023a). GNNs excel in capturing the inherent graph structure of transportation networks, allowing them to adaptively learn spatial, temporal, and contextual dependencies. By iteratively aggregating information across nodes and edges, GNNs offer a holistic view of the interconnected elements within the transportation network. This enables more accurate predictions of speed, taking into account factors such as traffic flow, route topology, and historical patterns. The shift towards GNNs signifies a paradigmatic advancement in the field of transportation prediction, opening avenues for more nuanced and adaptable models capable of meeting the evolving challenges of freight transport in our interconnected world (Petropoulos et al., 2022). Graph Neural Networks (GNNs) represent a paradigm shift in modeling complex systems by directly addressing the limitations of traditional methods. GNNs are designed to process data structured as graphs, making them inherently suitable for representing transportation networks where nodes (e.g., distribution centers).

Figure 2 illustrates the overarching structure of a Graph Neural Network (GNN) framework tailored for modeling freight or supply chain networks. At the core of this architecture is the graph's initial representation, established in the input layer, which assigns feature representations to the graph's nodes and edges, encapsulating essential data elements.

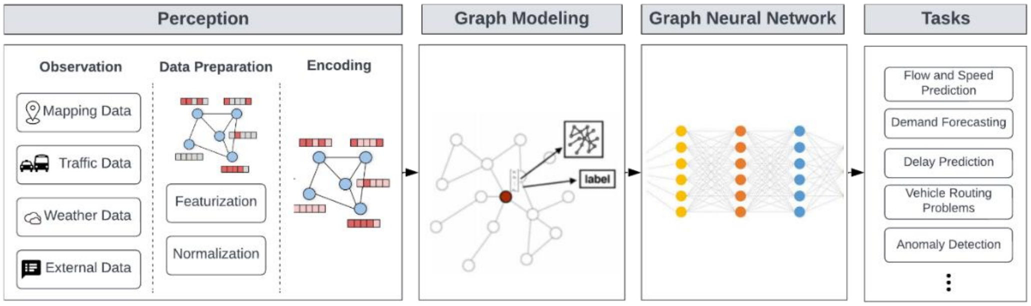

Figure 2 General Graph Neural Network architecture to model freight and supply chain networks [43]

This initial setup is pivotal for graph modeling, which meticulously captures the intricate interactions within the network. For example, in the context of truck speed prediction, the road network can be conceptualized as a graph, with nodes symbolizing various traffic-related attributes of trucks over specific time intervals, and edges depicting the connectivity between different road segments. The essence of graph modeling lies in the nuanced representation of these nodes and their interconnections. The GNN layer then refines these initial representations by leveraging node and edge information. The GNN's kernels synthesize comprehensive embeddings that encapsulate the dynamic interactions within the network by integrating information from neighboring nodes and edges. This capability to apprehend spatial dependencies, represented through complex, non-Euclidean graph structures, enables GNN models to excel in various freight transportation and logistics applications, including traffic flow prediction, demand forecasting, delay estimations, solving vehicle routing problems, and anomaly detection [50].

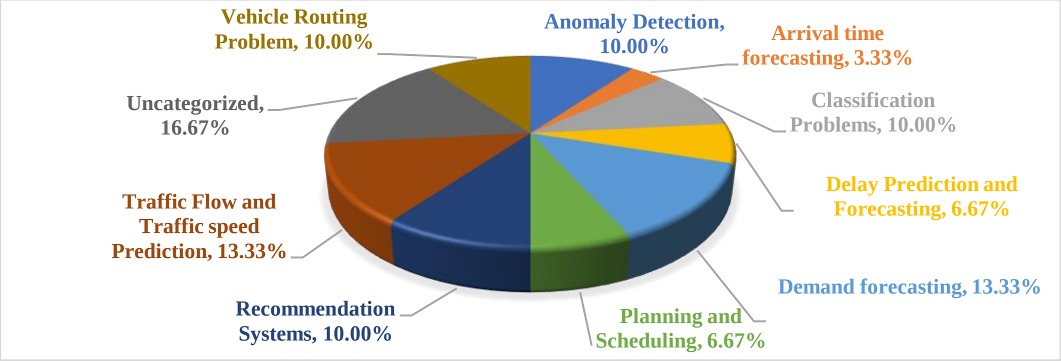

Figure 3 Application categories in Freight Transportation, SCM, and Logistics (adopted from authors' prior work [50])

Figure 3 offers a visual depiction of journal articles published between January 2018 and February 2022. It categorizes the applications of Graph Neural Networks

(GNN) within the fields of freight transportation, Supply Chain Management (SCM), and logistics.

Key Features of GNNs in Transportation Analysis:

- *Topology Awareness:* GNNs inherently consider the layout and structure of the network, allowing for the modeling of spatial relationships and dependencies between nodes and links in a transportation network.
- *Dynamic Data Integration:* They can incorporate real-time information, adapting predictions to current network states and external conditions.
- *Complex Pattern Recognition:* Leveraging deep learning, GNNs can identify intricate patterns and non-linear relationships within the network data, surpassing the capabilities of traditional linear models.

Implementation of GNNs for Freight Speed Prediction

The application of GNNs in freight transportation speed prediction involves several critical steps, from data collection and preprocessing to model training and validation

(Tygesen et al., 2023; Wu Lingfeiand Cui, 2022)

. Key considerations include:

- *Graph Representation*: Constructing a graph representation of the transportation network, where nodes and edges are defined based on geographical locations and pathways, respectively, and are attributed with relevant features (e.g., node capacity, edge speed limits, traffic conditions).

- *Feature Engineering:* Identifying and integrating relevant features that influence freight speed, including historical performance data, environmental conditions, and network characteristics.
- *Model Architecture and Training:* Designing a GNN architecture tailored to the specific characteristics of the transportation network and employing advanced training methodologies to optimize model performance.

The investigation into traffic flow and speed prediction has been a focal point of scholarly discourse, as evidenced by a significant body of the literature within our reviewed documents. Recognizing the inherent challenges associated with these prediction tasks, particularly in accounting for contextual and temporal variables such as weather conditions, time of day, and holidays, a prevalent approach involves conceptualizing the traffic system as a spatiotemporal graph.

Recognizing the intricacies of freight speed prediction, which inherently involves spatiotemporal dependencies influenced by contextual factors such as weather conditions, time of day, and other environmental variables, GNNs offer a nuanced and effective solution. By representing the freight network as a spatiotemporal graph, GNNs facilitate the incorporation of spatial dependencies shaped by the underlying topological structure (Rahmani et al., 2023a). This enables the model to discern and capture the dynamic relationships between different entities within the transportation system, providing a holistic understanding of the factors influencing freight speed (Yu et al., 2020). As a result, GNNs stand as a robust computational tool, contributing significantly to the advancement of predictive modeling within the realm of freight transportation, and offering valuable insights for optimizing logistics and resource allocation (Ramhormozi et al., 2022).

Taxonomy of GNNs

Data structured in graphs can be dissected and interpreted across various dimensions, namely at the node, edge, and graph levels, as illustrated in Figure 5. Each dimension targets distinct inquiries and necessitates unique algorithmic approaches for analysis. Beyond graph-specific tasks, machine learning methodologies further diverge into supervised, semi-supervised, and unsupervised categories. This amalgamation of graph-centric tasks with diverse learning paradigms offers considerable versatility in tackling intricate challenges. This discourse initially presents an overview of machine learning endeavors on graph data (Wu Lingfeiand Cui, 2022), followed by a detailed taxonomy of Graph Neural Networks (GNNs), serving as a guide in the architectural design of graph-based deep learning systems, particularly for novel problem settings.

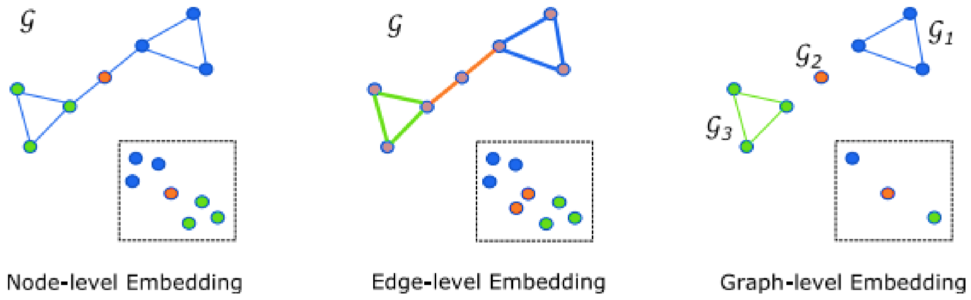

Figure 4 Graphic depiction of the three distinct granularity layers within graphs: a) representation at the node level, b) representation at the edge level, and c) representation at the graph level. (adapted from (Rahmani et al., 2023b)).

At the node level, within a given graph $G = (V, E)$, the objective is to comprehend the attributes of specified nodes $v \in V$. This domain encompasses tasks such as node classification, regression, and clustering. Node classification endeavors to assign nodes to distinct categories, whereas node regression predicts a continuous attribute for each node. Node clustering, as seen in Figure 4. (a), seeks to segregate nodes into cohesive groups based on similarity metrics, ensuring that analogous nodes congregate within the same cluster (K. Xu et al., 2018). Node classification/regression emerges as a prevalent machine learning pursuit within graph data, pertinent to the field of transportation. These tasks often involve scenarios where only a subset of nodes is labeled for training, with the aim to extrapolate features across all nodes $v \in V$. A notable distinction in graph-based node classification from conventional classification paradigms lies in the non-independent and identically distributed nature of nodes within graphs (W. L. Hamilton et al., 2017) , as opposed to the independent or dependency-modeled data points in traditional settings.

On the edge level, as seen in Figure 5 (b), the focus shifts to learning tasks applied to individual edges $e \in E$ of the graph $G = (V, E)$. This includes edge classification/regression and link prediction, with the former task involving the categorization of edge types or the prediction of edge attributes, and the latter aiming to infer the existence of a link between two specified nodes (Tygesen et al., 2023). Link prediction, also known as relation prediction or graph completion, is tasked with unveiling unseen or absent connections among nodes, utilizing a known subset of relationships $E_{train} \in E$ for training.

At the graph level, in Figure 5 (c), the challenge lies in formulating machine learning algorithms for an entire graph within a dataset comprising multiple (n) graphs. This category encompasses classification/regression and clustering tasks at the graph-wide scale. Here, the goal is to predict an overarching attribute or label for the entire graph rather than its constituent elements (nodes or edges). For instance, one might aim to classify the overall traffic condition within a city or region or assess the safety level of an intersection by considering the dynamics among various participants (vehicles, cyclists, pedestrians) (Tygesen et al., 2023). This multi-level approach to graph-based machine learning tasks underscores the depth and breadth of potential applications, from urban traffic management to safety assessments in complex interaction environments.

Table II Examples of GNN Structure for Different Applications (adopted from authors' prior work (Renuka Mandlik; Saiedeh Razavi; Susan Tighe, 2023))

Area	**Problem Identification**	**Graph Models**	**Nodes**	**Edges**	**Graph Type**	**Evaluated algorithm***	**Baseline Models**	**Article**
Marine	regional vessel flow prediction, Vessel volume prediction	STDGNN	ship position/ vessels	sailing pattern	vessel graph network	MAE, MAPE, RSME	GRU, STGCN, Graph Wavenet, TGCN	(C. Zhao et al., 2022)
Road	joint truck speed and flow prediction	MT-C2G	trucks	road segment	road network graph	MAE, RMSE	HA, ARIMA, SVR, STL-GRU, STL-GCN-GRU, MTL-GRU, TGCN, AST-GCN, AST-MTL	(H. Zhu et al., 2022)
Logistics	retail road network traffic flow; short-term traffic flow prediction	RTS-GAT	traffic flow	road segment	spatiotemporal graph data	MAE, MAPE, RSME	HA, ARIMA, FNN, AGNN, GCN, EAGNN, GAT	(Luo, 2022)
Logistics	assessing and predicting travel time reliability of trip (delivery)	TGCN	Traffic zone	study area	road network graph	MAE, MAPE, RSME, ACC	HA, ARIMA, SVC, random forest, FNN and STGCN	(Fang et al., 2022)

***MAE**- mean absolute error**,** **RMSE** - Root-mean-square error, **MAPE** - mean absolute percentage error

For an in-depth examination of GNN models and their diverse applications within freight transportation and logistics, further exploration of the GNN frameworks delineated in Table II is recommended.

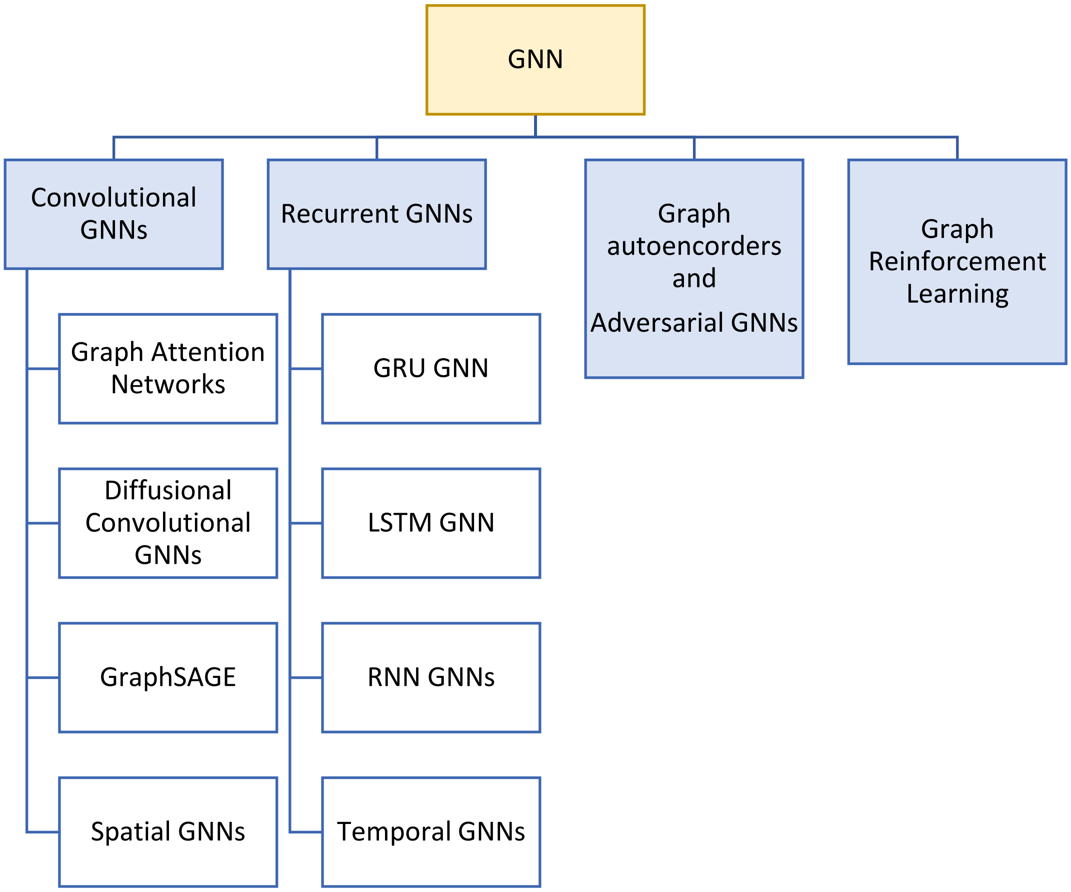

Figure 5 Various GNN models used for Freight Transportation and Logistics studies

Figure 5 illustrates a hierarchical taxonomy of Graph Neural Networks (GNNs), categorizing them into three principal branches based on their architectural traits and functional objectives. The first branch, Convolutional GNNs' (L. Zhao et al., 2018), includes subtypes such as Graph Attention Networks (Veličković et al., 2017), which leverage attention mechanisms to weigh the significance of nodes during feature aggregation, and Diffusional Convolutional GNNs (Y. Li et al., 2017), which simulate the diffusion process for feature propagation across the graph. GraphSAGE (Z. Chen et al., 2022) and Spatial GNNs are also convolutional variants that handle feature extraction based on the graph's spatial structure.

The second branch, Recurrent GNNs, comprises models that introduce temporal dynamics into graph processing. This includes GRU+GNN (Grubesic et al., 2008) and LSTM+GNN(Lu et al., 2020), which incorporate gated recurrent units and long short-term memory units, respectively, to capture temporal dependencies in graph data. RNN GNNs and Temporal GNNs also fall into this category, emphasizing the importance of sequence and time in graph representation.

Lastly, the third branch encompasses Graph autoencoders and Adversarial GNNs, which are typically employed for unsupervised learning tasks such as graph embedding and network generation, and Graph Reinforcement Learning, which combines GNNs with reinforcement learning principles to enable decision-making and policy learning in graph-based environments. This organizational schema serves as a conceptual map for researchers and practitioners to navigate the complex landscape of GNN architectures and their applications.

The conventional deep learning models often overlook the unique properties of transportation networks, such as the non-Euclidean spatial correlations inherent in these systems. This gap is where Graph Neural Networks (GNNs) have proven to address, integrating graph structures with deep learning to effectively model the complex, interconnected nature of transportation networks (Rahmani et al., 2023b). Initial forays into utilizing GNNs for traffic forecasting, such as (J. Yang et al., 2022)'s graph-oriented model, highlighted the potential of these networks to account for spatial-temporal correlations among traffic sensor data within transportation networks. Subsequent innovations, such as diffusion-convolutional recurrent neural network (DCRNN) (Y. Li et al., 2017) and the spatial-temporal graph convolutional network (STGCN) (Heglund et al., 2020; M. Wu et al., 2020a) proposed by others, have further refined the application of GNNs in traffic forecasting. These models have demonstrated the ability to capture the dynamic spatial dependencies present in traffic networks through novel convolutional processes and have shown promising results in real-world datasets when compared to traditional benchmark models.

Recent advancements, including the integration of attention mechanisms and the development of models like the Graph Multi-Attention Network (GMAN) (C. Zheng et al., 2020), have addressed challenges such as dynamic spatial correlations, nonlinear temporal relationships, and error propagation in multi-step traffic forecasting. Another study introduces the Attention Temporal Graph Convolutional Network (A3T-GCN) (Bai et al., 2021) for traffic forecasting, aiming to capture both global temporal dynamics and spatial correlations within traffic flows. The A3T-GCN employs gated recurrent units for short-term trends and graph convolutional networks for spatial dependencies, enhanced by an attention mechanism to weigh the significance of different time points. This approach improves prediction accuracy, as demonstrated on real-world datasets.

These sophisticated GNN frameworks have outperformed existing models, particularly in predicting future traffic conditions over extended horizons. As GNNs continue to evolve, they offer a versatile and powerful tool for dissecting the multidimensional and dynamic patterns present in traffic datasets, heralding a new era in traffic forecasting research.

Current Limitations and Gaps of GNN Applications in Speed Prediction

The existing literature on applying Graph Neural Networks (GNNs) to traffic speed prediction highlights several research gaps:

- Handling of Heterogeneous Data: Freight networks involve diverse data types, including vehicle speeds, traffic volumes, and environmental conditions. Existing models might not effectively integrate this heterogeneous data to inform speed predictions.
- Dynamic Traffic Patterns: Many existing GNN models assume static graph structures and fail to account for dynamic changes in traffic patterns.
- Scalability and Computational Efficiency: As freight networks can be extensive and complex, scalability remains a challenge for current GNN models.
- Spatial-Temporal Correlations: While some GNN models consider spatial dependencies, they may not adequately capture the temporal correlations crucial for freight speed prediction.

- Generalization Across Networks: The ability of GNNs to generalize across different freight networks without extensive retraining is limited.
- Interpretability and Trust: The "black box" nature of many deep learning models, including GNNs, poses challenges for interpretability.

This investigation endeavors to bridge a multitude of identified gaps:

Firstly, there is a noticeable gap in the comprehensive analysis of conventional methodologies, particularly in their theoretical foundations, practical implementations, and the diversity of data sources utilized. Many existing studies focus narrowly on specific aspects of prediction methodologies without a holistic evaluation of their performance across varied real-world scenarios.

Secondly, existing models often fall short of capturing the intricate and dynamic relationships within freight networks, leading to a gap in the development of advanced models that can accurately reflect these complexities. This study seeks to fill this gap by proposing a model designed to understand and predict the nuanced interactions and variables influencing freight traffic speeds more effectively.

Lastly, there is a gap in the rigorous evaluation of new models against traditional methods, particularly in terms of predictive accuracy, efficiency, and adaptability to different traffic conditions and network configurations. This research aims to comprehensively assess the proposed model's performance in real-world settings, providing a clear comparison with established methodologies and demonstrating its potential advantages in enhancing freight traffic speed prediction.

3 METHODOLOGY

In response to the identified gaps in the existing literature on freight speed prediction, this research proposes the development and application of a Multi-head Attention Built-in model for Spatial-Temporal Graph Neural Network, which we abbreviated as MAB-STGNN.

By integrating attention mechanisms, the MAB-STGNN is designed to distinguish the varying significance of nodes and edges within the complex network from the real world, ensuring a nuanced analysis of diverse data types, including traffic volumes, vehicle speeds, and environmental factors. The dynamic nature of traffic patterns, crucial for accurate freight speed forecasting, will be addressed through temporal attention mechanisms, enhancing the model's adaptability to real-time changes. Moreover, the MAB-STGNN aims to overcome scalability challenges by optimizing computational efficiency. By synthesizing spatial and temporal correlations and fostering model generalization across network topologies, the MAB-STGNN approach promises not only theoretical advancements in GNN applications but also substantial practical improvements in freight transportation management. Additionally, the development of transparent attention mechanisms within the MAB-STGNN framework is anticipated to enhance model interpretability, thereby building trust among industry stakeholders and facilitating informed decision-making in freight logistics operations.

In the ensuing segment of this methodology chapter, we will embark on an exploration of the Multi-attentional Built-in Spatial-Temporal Graph Neural Network (MAB-STGNN) model, focusing on its capacity to amalgamate spatial and temporal data for enhanced traffic speed prediction. The discussion will unfold the operational intricacies of the diffusion-convolutional layer and its synergy with the multi-head attention mechanism, delineating how these components coalesce to capture and interpret complex traffic dynamics. Furthermore, we will elucidate the normalization preprocessing steps critical for optimizing the adjacency matrix and feature matrix, ensuring that the model's inputs are appropriately scaled and structured for effective learning and prediction outcomes.

Problem Definition

This research is dedicated to the prediction of traffic information within a specified temporal domain by leveraging historical data pertaining to similar road segments. The term "traffic information" encompasses variables such as traffic speed, flow, and density, with a particular focus on traffic speed as a representative measure in the experimental context. The methodology articulated herein applies to diverse traffic information types, ensuring its generalizability.

Definition 1 (Traffic network) G: The urban road network can be modeled as a directed graph $G = (V, E)$, where $V = \{v_1, v_2, \ldots, v_N\}$ denotes the set of nodes, each representing a road, totaling N roads, and E represents the set of directed edges that signify the roads junction. In our model, intersections, including both signalized and unsignalized junctions, are defined as edges. This methodology is selected for its ability to accurately map the unidirectional movement of vehicles on roads (represented as nodes) through their connecting junctions (edges), offering a detailed representation of traffic flow and the network of connectivity within the urban road network.

The connectivity among these roads is encapsulated in the adjacency matrix A of dimensions $N \times N$, where each entry delineates the presence or absence of a direct link between any two roads. Specifically, in the neighborhood of a road node, v_i all directly accessible roads from its immediate network vicinity. The structure of A is such that its rows and columns correspond to individual road nodes, with the matrix elements reflecting the existence of a direct route between them. For an unweighted graph, this relationship is binary, marked by 0 (no direct connection) and 1 (direct connection present). Conversely, in this weighted graph scenario, the non-zero elements of A not only confirm the presence of a connection but also quantify the strength or capacity of that link, with the convention of setting the matrix's diagonal elements to 0, indicating no self-loops within the network.

Each directed edge in E originates from one node and points to another, effectively illustrating the direction of vehicular movement from one road segment to another through their connecting junction.

Definition 2 (Feature Matrix) $X^{N\times P}$: Let the road network graph G be abstracted such that each road corresponds to a node within the graph. The traffic speed on each road, serving as an attribute of its respective node, can be encapsulated within a feature matrix $X \in R^{(N \times P)}$. In this representation, $X^{N \times P}$, N denotes the total count of roads or nodes within the graph, and P signifies the dimensionality of the feature space, corresponding to the length of the historical traffic speed time series for each node. Consequently, the matrix X_t representing the vector of traffic speeds across all roads at a given time t, serves as a temporal snapshot within this multidimensional feature space.

If P is set to 1, implying that the only feature considered is speed, then X_t as a vector of traffic speeds across all roads at time t would be consistent with the definition of X. However, if $P > 1$, indicating multiple features per road, X_t would need to encompass all these features for each road at time t, not just speed.

To clarify, if speed is the sole feature under consideration for this model, the definition of X as $X^{N \times P}$ would imply P=1, making, X_t a vector representing speeds across all *N* roads at time *t*. If there are multiple features, then X_t would represent a matrix slice of *X* at time *t*, containing all features for each road at that moment.

Definition 3 (Traffic Speed Prediction): In this study, the urban road network, denoted as G, is characterized by spatial features derived from the road topology, while the temporal features are represented by the traffic speed observed on these roads. A mapping function f, is employed to forecast future traffic speeds at a future time T. The calculations are presented in Equation (1):

$$[X_{t+1}, \dots, X_{t+T}] = f(X_{t-M+1}, \dots, X_t, A) \tag{1}$$

The predictive model is articulated through a specific equation, where T denotes the duration over which predictions are made, and M represents the extent of the historical data series utilized for the analysis. The term X_t encapsulates the average traffic speed attributes of the roads at time t, serving as the temporal feature set. Additionally, A is defined as a weighted adjacency matrix that encapsulates the spatial connectivity and relationships between the roads within the network.

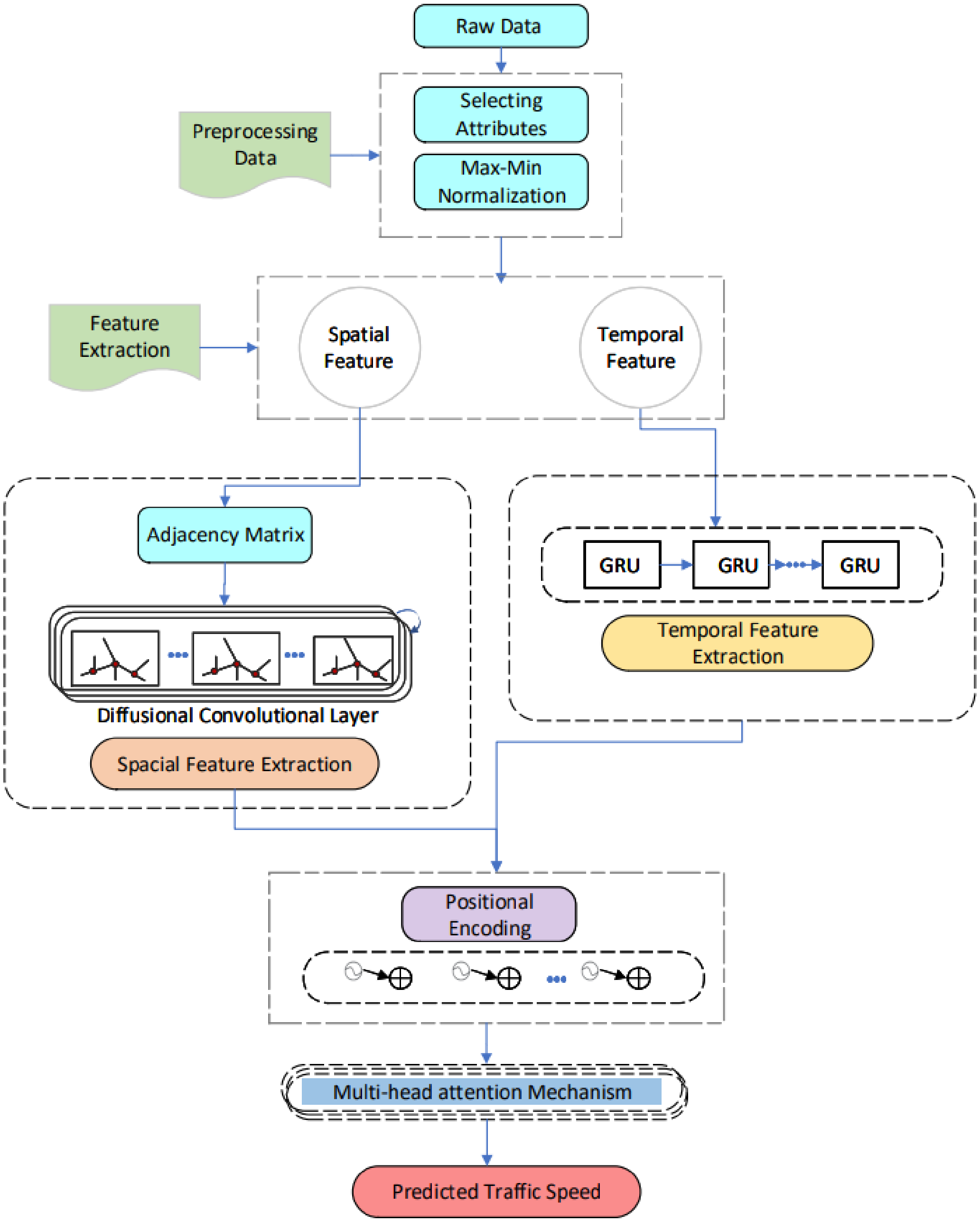

Figure 6 Proposed architecture of MAB-STGNN

The overarching architecture and operational mechanics of the proposed predictive framework, MAB-STGNN, are graphically depicted in Figure 6, providing a comprehensive overview of the model's structure and its functional components.

The proposed traffic forecasting framework amalgamates spatial and temporal dimensions to forecast traffic speed. The proposed architecture is an advanced model of the earlier discussed GNN model (Bai et al., 2021). The MAB-STGNN architecture employs a diffusion-convolutional layer, as introduced by (Bai et al., 2021) in tandem with a multi-head attention mechanism that incorporates positional encoding for the prediction of future traffic speed. This diffusion-convolutional layer is instrumental in enabling the cyclic propagation of information throughout the nodes in the graph network. Concurrently, the Gated Recurrent Unit (GRU) (Ramakrishnan & Soni, 2018; Shu et al., 2022) component of MAB-STGNN meticulously processes temporal attributes, assimilating the effects of both historic and future time series data. The incorporation of a multi-head attention framework, which computes an aggregate of the outputs from various attention heads, is pivotal in discerning the overarching trends in traffic fluctuations across the network. This study leverages the spatial attributes of urban road infrastructures along with historical traffic speed data, integrating features from both the spatial and temporal domains to refine the accuracy of traffic speed forecasts.

The spatial feature extraction model, a key component of the proposed framework, addresses the challenging task of extracting spatial features by employing diffusion-convolution layers. These layers play a critical role in capturing and discerning spatial patterns within input data, emphasizing the diffusion process to enhance the model's spatial awareness and its ability to represent intricate relationships embedded in the spatial domain (Atwood & Towsley, 2016). The nuanced approach to feature extraction underscores the significance of the diffusion process in augmenting the model's understanding of complex spatial structures within the dataset.

Computational Resources Setup

The computational experiments crucial to the development and validation of the Multi-head Attention Built-in Spatial-Temporal Graph Neural Network (MAB-STGNN) were conducted using a high-performance computing setup. This setup was specifically chosen to meet the demanding processing requirements of graph neural network algorithms. The core of this system comprised an 11th Gen Intel® Core™ i7-11800H processor, clocked at 2.30GHz, paired with 32GB of RAM, which facilitated the efficient handling of large datasets and complex computations. This computing environment ran on a 64-bit Windows 10 operating system, ensuring compatibility with a wide range of software libraries used throughout the research.

To ensure the reproducibility of the research findings and maintain the integrity of the computational experiments, detailed records of computation times were meticulously maintained. These records were particularly focused on the model training and evaluation phases, providing clear benchmarks for each critical operation. To ensure the reproducibility of the research findings and maintain the integrity of the computational experiments, detailed records of computation times were meticulously maintained. The total computational time for training the MAB-STGNN model was substantial due to the complexity of the model and the volume of data processed. Specifically, each training cycle, encompassing one pass through the METR-LA dataset, took approximately 20 to 30 minutes, with the model requiring about 100 epochs to converge fully. This resulted in a total training time of approximately 33 to 50 hours. Such detailed documentation supports the assessment of the model's computational efficiency and scalability, demonstrating the significant resources necessary to achieve robust predictive performance.

The selection of this specific hardware configuration was guided by its ability to perform parallel processing, a vital feature for reducing the computational load during extensive data operations and model training sessions. Additionally, the system's robust processing capabilities allowed for rapid iteration over multiple training cycles, which was instrumental in achieving the optimization of the MAB-STGNN model parameters.

Overall, the computational resources allocated were integral to the research's success, providing the necessary power to execute complex algorithms and handle extensive simulations required to advance the state of traffic speed prediction using graph neural networks.

Selecting Attributes

Attribute selection is a critical step in the development of predictive models like the MAB-STGNN. The primary goal of attribute selection is to maintain the most informative variables while eliminating redundancy that may complicate the model without contributing to its predictive power. In the context of the MAB-STGNN model, attribute selection would proceed by examining the correlations among various spatial and temporal features.

The correlation coefficient, which ranges from -1 to 1, is a statistical measure used to assess the strength and direction of the linear relationship between two attributes. A correlation coefficient close to 1 indicates a strong positive correlation, meaning that as one attribute increases, the other also increases. Conversely, a coefficient close to -1 implies a strong negative correlation, where an increase in one attribute corresponds to a decrease in the other. A coefficient around 0 suggests no linear correlation (Atwood & Towsley, 2016).

In the process of fine-tuning the MAB-STGNN, let's consider a scenario where we have a set of attributes such as 'Average Speed' (AvgSpd), 'Traffic Flow' (TF), 'Time of Day' (ToD), and 'Day of the Week' (DoW). If the correlation coefficient between 'Traffic Flow' and 'Average Speed' is found to be 0.96, this would indicate a high redundancy between these two attributes. Including both could lead to overfitting and unnecessarily complex models. To streamline the model and enhance its performance, we have opted to exclude one of these attributes. The decision on which attribute to remove is dependant on their individual predictive power and relevance to the model's objectives.

For example, if 'Average Speed' is more closely related to the prediction target, 'Traffic Flow' may be excluded. Additionally, if 'Time of Day' and 'Day of the Week' have a lower correlation with 'Average Speed', they would be retained since they likely offer unique insights that aren't captured by 'Average Speed' alone. The attributes selected should contribute to a comprehensive understanding of traffic dynamics without overlapping information.

Attribute selection in MAB-STGNN ultimately aims to create a model that not only accurately forecasts traffic conditions but also operates efficiently. The model's inputs are chosen to provide a detailed yet concise representation of traffic.

Normalization Preprocessing

The impact of road length on the adjacency matrix A, can be systematically addressed via normalization preprocessing. Before the application of Graph Convolutional Networks (GCNs) for the extraction of spatial attributes, it is imperative to subject the adjacency matrix A to a preprocessing regimen. After a thorough review of diverse research works (Han et al., 2012; Hashemkhani Zolfani et al., 2020; Tian et al., 2023; A. Zheng & Casari, 2018), we propose using the max-min normalization technique. Min-max normalization is a common preprocessing technique used across various data domains, including graph datasets, to scale feature values to a specific range, typically [0, 1]. This method is particularly useful in adjusting the scales of different features to a uniform range, enhancing the stability and performance of machine learning algorithms. The equation for the min-max normalization of a value x is given by:

$$x' = \frac{x - \min(x)}{\max(x) - \min(x)} \tag{2}$$

Where, x' denotes normalized data, x denotes original input data, and $\max(x)$, $\min(x)$ denotes maximum and minimum input data value respectively.

This technique ensures that all features contribute equally to the model's learning process, preventing features with larger scales from dominating those with smaller scales. In the context of graph datasets, min-max normalization can be applied to node features such as traffic volume, road length, or any other quantitative attribute, as well as to edge weights representing distances, capacities, or other metrics.

In the present examination, the solitary feature under consideration is the average speed. To employ Min-Max normalization for a univariate dataset comprising average traffic speed, the methodology delineates as follows:

Determine Min and Max Values: Identify the minimum (Min) and maximum (Max) values of the average speed from the entire dataset. These extremities serve as pivotal benchmarks for the normalization process.

Scale Each Data Point: Subsequently, each datum of the average speed feature undergoes transformation through the Min-Max normalization equation:

$$Normalized\ speed_i = \frac{speed_i - \min\ speed}{\max speed - \min\ speed} \tag{3}$$

Where, $speed_i$ represents the original average speed value of the i^{th} data point, Min Speed Min Speed denotes the minimum average speed value across the dataset, and Max Speed symbolizes the maximum average speed value across the dataset.

Apply Normalized Data to GNN: Using normalized average speed values as input to the GNN model. This standardized input helps an ML model efficiently learn the patterns and dynamics of traffic speed across the network.

Reconversion of Predictive Outputs: Post-prediction by the GNN, it may be requisite to revert the normalized predictive values to their original speed scale. This can be achieved by applying the inverse of the min-max normalization formula:

Original Speed = (Normalized Speed × (Max Speed − Min Speed)) + Min Speed

This step ensures that the model's output is interpretable and can be directly compared to real-world speed values.

Normalization, particularly through Min-Max scaling, is an indispensable preprocessing step that significantly augments the model's ability to navigate and interpret the variability in speed levels across distinct road segments, thereby enhancing the predictive accuracy of GNNs in traffic speed forecasting tasks (Beeking et al., 2023).

Diffusion-Convolutional Layer

The diffusion-convolutional layer, as applied within the spatial-temporal graph neural network model, embodies a mechanism designed to encapsulate spatial relationships inherent in graph-structured data, guided by the analogy of diffusion processes(Atwood & Towsley, 2016). This layer is pivotal for models aimed at interpreting dynamic systems such as traffic networks, where understanding the spatial interdependencies is crucial for accurate predictions. The foundational concept behind the Diffusion-Convolutional Layer is rooted in Graph Convolutional Networks (GCNs) (Atwood & Towsley, 2016; L. Zhao et al., 2018, 2020)(Atwood & Towsley, 2016). The diffusion process in graphs is an analogy to physical diffusion processes, where entities spread out from a source to the surrounding area over time. In the context of a graph, this process can be thought of as information propagating from one node to its neighbors, then to the neighbors' neighbors, and so forth. Mathematically, this process can be modeled using the graph Laplacian or adjacency matrices, which encode the connectivity structure of the graph. The operation of a diffusion-convolutional layer can be formalized as follows:

Given a graph $G = (V, E)$ with nodes $v \in V$ and edges $(v, w) \in E$, and a node feature matrix $X \in R^{(N\times P)}$ where N is the number of nodes and P is the number of features per node, the diffusion-convolution operation at each layer can be represented as:

$$H^{(k+1)} = \sigma(\textstyle\sum_{k=0}^{K} \theta^{(k)} (A^k X)) \tag{4}$$

where:

$H^{(k+1)}$ is the output feature matrix of the layer,

σ denotes a non-linear activation function (e.g., ReLU),

K is the number of diffusion steps,

$\theta^{(k)}$ are the trainable weight matrices associated with each diffusion step k,

A is the adjacency matrix of the graph, possibly normalized or augmented with self-connections to include the node's own features,

A^k represents the k^{th} power of the adjacency matrix, capturing the k-hop neighbors' influence.

Given that $P = 1$, due to the consideration of only traffic speed as the feature, the feature matrix X will consist of a single column representing the historical traffic speeds at each node (sensor location). The setup for the diffusion convolution operation remains as described but is applied specifically to this speed-centric feature matrix.

In traffic networks, the diffusion-convolutional layer allows the model to capture the spatial dependencies that dictate how traffic conditions in one region of the network influence or are influenced by conditions in other regions. This capability is crucial for forecasting tasks like traffic speed prediction, where the model must understand complex spatial-temporal patterns to make accurate future predictions. By leveraging the diffusion-convolutional layer, spatial-temporal graph neural networks can effectively model the intricate dynamics of systems like urban traffic, providing valuable insights and predictions to inform traffic management and planning strategies.

In this study, a two-layer diffusion-convolutional architecture is constructed, entailing the sequential application of two diffusion-convolution operations upon the feature set of the input graph. This serves to augment the model's capacity for encapsulating spatial dependencies, achieved through the expansion of each node's receptive field. This expansion facilitates the incorporation of informational cues from proximally distant nodal entities within the graph, thereby enriching the model's spatial interpretative capabilities. Incorporating the Rectified Linear Unit (ReLU) activation function after each diffusion-convolutional layer's output serves to instill non-linearity within the architectural framework of the model.

This methodology facilitates the model's proficiency in discerning intricate patterns inherent within the dataset by exclusively permitting the propagation of positive activation values. Consequently, this enhances the model's adeptness in assimilating non-linear relationships, a critical aspect for comprehending the multifaceted dynamics present in datasets, particularly those characterized by complex spatial-temporal interactions. This can be expressed in an Equation by:

$$f(X, A) = \sigma(\hat{A}\ ReLU(\hat{A}XW_o)W_1) \tag{5}$$

where:

X denotes the matrix of input features for each node in the graph,

A is the adjacency matrix of the graph, representing the connections between nodes,

$\hat{A}$ is the normalized adjacency matrix, often augmented with self-connections to include each node's own features in the convolution process. It is commonly computed as $\hat{A} = D^{-\frac{1}{2}}(A + I)D^{-\frac{1}{2}}$, where, I is the identity matrix and D is the diagonal node degree matrix of $A + I$,

W_o *and* W_1 are the weight matrices for the first and second diffusion-convolutional layers, respectively, which are learned during the training process,

$ReLU(.) = \max(0,.)$ is the Rectified Linear Unit activation function applied element-wise to introduce non-linearity after the first layer of diffusion-convolution,

$\sigma(.)$ represents an optional activation function applied to the output of the second diffusion-convolutional layer, which could be another non-linear function such as ReLU, or a different activation function depending on the specific requirements of the model.

This equation succinctly captures the essence of the two-layer diffusion-convolutional architecture, highlighting the role of ReLU in instilling non-linearity and enhancing the model's ability to capture complex spatial dependencies and intricate patterns within the graph-structured data. Through this formulation, the model leverages the expanded receptive field of each node, incorporating information from both immediate and more distant neighbors, thereby enriching its spatial interpretative capabilities.

Gated Recurrent Unit Model

Incorporating a Gated Recurrent Unit (GRU) model after the two-layer diffusion-convolutional architecture, as delineated for traffic speed prediction, epitomizes a sophisticated approach to capturing temporal dependencies within the data. The

GRU, a variant of the recurrent neural network (RNN), is adept at processing sequential data, making it particularly suited for temporal analysis in datasets with inherent time-based progressions, such as traffic speeds over time. The GRU model, illustrated in Figure 7, is characterized by its gating mechanisms, which are designed to mitigate the vanishing gradient problem commonly encountered in standard RNNs, thereby enhancing the model's capacity for learning long-term dependencies (C. Zheng et al., 2020),(Atwood & Towsley, 2016)The key operations within a GRU are defined by the following equations:

Update Gate

The update gate decides the extent to which the information from the previous state is carried over to the current state. It is calculated as:

$$z_t = \sigma(W_z x_t + U_z h_{t-1} + b_z)) \tag{6}$$

where:

z_t is the update gate vector at time step t

W_z is the weight matrix for the update gate applied to the input.

U_z is the weight matrix for the update gate applied to the previous hidden state.

x_t is the input vector at time step t

h_{t-1} is the hidden state vector from the previous time step $t-1$

b_z is the bias term for the update gate.

σ represents the sigmoid function, ensuring the gate values are in the range (0,1).

Reset Gate

The reset gate determines how much of the past information to forget, which influences the candidate activation:

$$r_t = \sigma(W_r x_t + U_r h_{t-1} + b_r)) \tag{7}$$

where:

r_t is the reset gate vector at time step t

W_r is the weight matrix for the reset gate applied to the input.

U_r is the weight matrix for the reset gate applied to the previous hidden state.

b_r is the bias term for the reset gate.

Candidate Hidden State

The candidate activation is computed using the reset gate to blend the past information with the new input:

$$\tilde{h}_t = \tan h\,(W_h x_t + U_h(r_t \odot h_{t-1}) + b_h)) \tag{8}$$

where:

$\tilde{h}_t$ is the candidate hidden state at time step t

W_h and U_h are the weight matrices applied to the input and the gated previous hidden state, respectively.

b_h is the bias term for the candidate hidden state.

$\odot$ denotes element-wise multiplication.

$\tan h$ is the hyperbolic tangent function, introducing non-linearity.

Final Hidden State

The final hidden state is a weighted sum of the previous hidden state and the candidate hidden state, with the weights determined by the update gate. This step effectively allows the GRU to decide how much of the new information to keep and how much of the past information to pass through.

$$h_t = (1 - z_t) \odot h_{t-1} + z_t \odot \tilde{h}_t \tag{9}$$

Where, h_t is the updated hidden state at time step t.

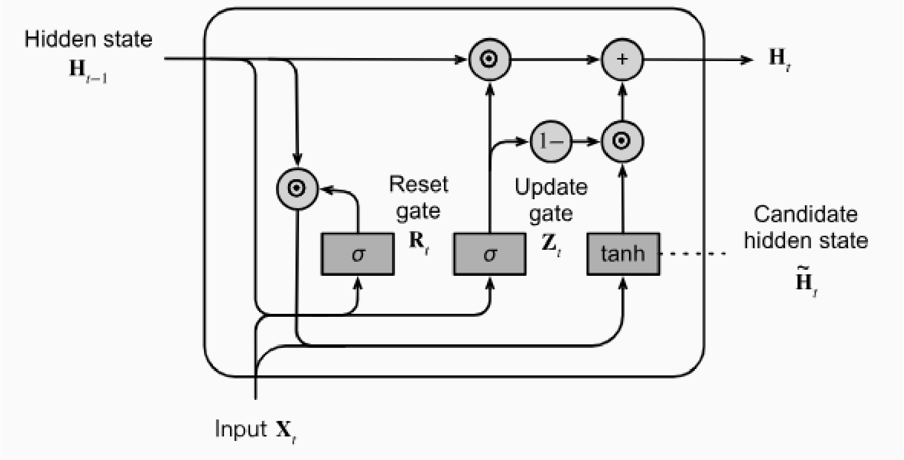

Figure 7 Architecture for Gated Recurrent Unit (adapted from (Grubesic et al., 2008)

The Gated Recurrent Unit (GRU) model as featured in Figure 7 is intricately designed to delineate the latent state embedded within the historical sequence of traffic speed data. Our framework integrates the GRU to meticulously analyze the temporal attributes inherent to roadway dynamics, thereby elucidating the intricate interplay between temporal progression and vehicular velocity. This process concludes with the generation of a latent state for each discrete temporal instance. Inherent to the GRU's design, the derived hidden state exerts influence on the computation of subsequent temporal features, while concurrently being preserved for integration into the multi-head attention framework. This dual functionality underscores the GRU's efficiency in temporal information propagation and its pivotal role in enhancing multi-head attention mechanism with rich, contextually informed states.

Positional Encoding

In the MAB-STGNN model, positional encoding plays a pivotal role in enhancing the model's ability to comprehend and leverage the inherent sequential nature of traffic data. Positional encoding is a technique used to inject information about the order of the data points in the sequence, which is crucial for models that need to understand temporal relationships, especially in the absence of inherent sequence-aware mechanisms like those in recurrent neural networks (Lv et al., 2018).

For the MAB-STGNN, positional encoding is implemented by adding a unique encoding to the feature vector of each time step in the input sequence. This encoding is designed to increase linearly along the temporal axis, ensuring that the model can differentiate between earlier and later time steps in the traffic speed data. Specifically, sine and cosine functions of different frequencies are used for positional encoding, following the Equation 10 and 11:

$$PE_{(pos,2i)} = \sin\left(\frac{pos}{10000^{\frac{2i}{d_{model}}}}\right) \tag{10}$$

$$PE_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{\frac{2i}{d_{model}}}}\right) \tag{11}$$

where pos is the position in the sequence, i is the dimension, d_{model} and is the dimensionality of the model's input. This approach, inspired by the methodology used in the Transformer model by Vaswani et al. (Vaswani et al., 2017) allows the MAB-STGNN to capture temporal patterns by providing it with explicit positional information. This encoding can capture the temporal information in traffic data sequences, helping the model distinguish between different time steps effectively (Y. Li et al., 2017).

The chosen frequencies for the sine and cosine functions ensure that each position in the sequence has a unique encoding, thus enabling the model to learn and leverage the positional information effectively. This is particularly important for traffic speed forecasting, where the significance of traffic conditions can vary significantly depending on the time of day, making the model's understanding of sequence position critical for accurate predictions(Y. Li et al., 2017).

The MAB-STGNN model utilizes sinusoidal positional encoding, as introduced in the seminal work on the Transformer model by Vaswani et al. (Vaswani et al., 2017). This form of positional encoding allows the model to use fixed-frequency functions to encode the position of a node within a sequence. The encoding adds information about the relative or absolute position of the tokens in the sequence, which is vital for the model to recognize patterns that depend on the sequence order. In our case, this encoding is particularly important for handling the spatial-temporal graph data, where the spatial configuration of the traffic network remains constant, but the traffic condition, like vehicle speed, changes over time.

By incorporating positional encoding, the MAB-STGNN model is endowed with a deeper understanding of temporal dynamics, significantly enhancing its ability to forecast traffic speeds with high accuracy, particularly in scenarios where the timing and order of data points are crucial for prediction accuracy.

Multi Head Attention Mechanism

Within the ambit of spatial-temporal graph neural networks tailored for traffic speed prediction, the integration of a multi-head attention mechanism constitutes a pivotal second phase, following the initial diffusion-convolutional layer. This multi-faceted attention paradigm, when amalgamated with the Gated Recurrent Unit (GRU) mechanism, endows the model with the capacity to discern and prioritize a diverse feature across both spatial and temporal dimensions.

The essence of the multi-head attention mechanism lies in its ability to concurrently process data through multiple attention 'heads' (Cho et al., 2014; Veličković et al., 2017). Each head independently attends to information from different representation subspaces, thereby enabling the model to capture a more nuanced and comprehensive understanding of the spatial-temporal dependencies inherent in the traffic speed data. This is particularly beneficial in complex graph-structured data where the relevance of features may vary significantly across different contexts and time frames.

Algorithm 1: The overall learning algorithm for MAB-STGNN

```
Input: The traffic signals over past $T_h$ time steps: $X$, adjacency matrix: $A$, number of diffusion steps: $k$, number of attention heads: $h$, GRU hidden state size: $d_{GRU}$
Output: Prediction of traffic signals $Y$ in $T_f$ future time steps.
   i.   Calculate the adjacency matrix $A$ by normalization preprocessing.
  ii.   Introduce the diffusion-convolution layer $H^{(k+1)} = \sigma(\sum_{k=0}^{K} \theta^{(k)} (A^k X))$
 iii.   GRU temporal processing (for each node sequence):
$h_t = (1 - z_t) \odot h_{t-1} + z_t \odot \widetilde{h}_t$
Where,
$z_t = \sigma(W_z x_t + U_z h_{t-1} + b_z))$ (update gate)
$r_t = \sigma(W_r x_t + U_r h_{t-1} + b_r))$ (reset gate)
$\widetilde{h}_t = \tan h (W_h x_t + U_h (r_t \odot h_{t-1}) + b_h))$ (candidate state)
  iv.   Road Length Factor Adjustment
            $X' = x/length$ (road)
   v.   Multi-head attention
            For each head, $i$, $1 \le i \le h$;
            $Q_i = X'W_i^Q; \quad K_i = X'W_i^K; \quad V_i = X'W_i^V$
            $Head_i = Attention\ (Q_i, K_i, V_i) = softmax\left(\frac{Q_i K_i^T}{\sqrt{d_k}}\right) V_i$
            $H^{(2)} = concat(Head_1, \ldots, Head_h) W^0$
  vi.   Feature Fusion and Prediction
```

$\boldsymbol{H} = \boldsymbol{concat}(\mathbf{H}^{(\mathbf{1})}, \mathbf{H}^{(\mathbf{2})})$

$\widehat{\boldsymbol{Y}} = \boldsymbol{MLP}\ (\boldsymbol{H})$

vii. Backpropagation: update parameters to minimize the prediction errors between $\widehat{\boldsymbol{Y}}$ and the true traffic signals $\boldsymbol{Y}$ in $\boldsymbol{T_f}$ future time steps.

In the above formulation, $ReLU$ and σ denote the rectified linear unit and sigmoid activation functions, respectively. $\Theta_{k}^{(1)}$, W^{Q}, W^{V}, W^{K} and W^{O} are trainable weight matrices for the diffusion-convolution, query, key, value, and output linear projection in the attention mechanism, respectively. d_k represents the dimensionality of the key vectors in the attention mechanism, and MLP denotes a multi-layer perceptron used for the final traffic signal prediction. This stepwise formulation encapsulates the model's workflow, from spatial feature aggregation and temporal sequence processing to the nuanced attention-driven feature weighting and prediction.

Data Post-Processing for Freight Speed Forecasting

Upon acquisition of the forecasted traffic speeds from the MAB-STGNN model, a paramount step involves the conversion of these generalized traffic data into freight-specific speed estimations. This adjustment is crucial due to the distinct speed characteristics of freight vehicles as compared to passenger vehicles, attributed to variables such as vehicle dimensions, payload, and regulatory speed limitations.

An effective method to tailor the forecasted speeds to freight vehicles involves the application of a correction coefficient, which is derived from empirical analyses that juxtapose the average speeds of freight vehicles against passenger cars under analogous traffic conditions. For example, research conducted by (Kim & Jeong, 2012) revealed that on urban freeways, the speed of freight vehicles is approximately 90% of that of passenger cars during non-peak hours, with this ratio diminishing in peak traffic scenarios. Such a correction factor can be applied to the model's output to yield a more accurate representation of freight speeds.

Furthermore, the influence of traffic congestion on freight mobility is an essential factor. Investigations such as (Forbes & Simpson, 1968) have demonstrated that freight vehicles exhibit a higher degree of speed variability under congested conditions compared to passenger cars. Implementing a congestion-based adjustment, leveraging congestion indices or real-time traffic density metrics could enhance the precision of freight speed predictions.

In summary, this research delineates the development of a Multi attentional built-in mechanism Spatial-Temporal Graph Neural Network (MAB-STGNN) model, specifically architected for the prediction of traffic speed. At the core of this model lies the strategic incorporation of diffusion-convolution layers, adept at distilling spatial attributes from the intricate network of traffic data. Complementarily, the Gated Recurrent Unit (GRU) is employed to meticulously parse the temporal dynamics, capturing the sequential variability inherent in traffic flow patterns.

4 RESEARCH EXPERIMENTS AND DATA

Data Description

A real dataset, METR-LA has been selected for this experiment. This dataset has been used in previous studies (Y. Li et al., 2017; M. Wu et al., 2020b; Z. Wu, Pan, Long, et al., 2019; Yu et al., 2018, 2020; Y. Zhang et al., 2022) and can be accessed at (https://github.com/deepkashiwa20/MegaCRN/tree/ main/METRLA, n.d.). The METR-LA dataset is a comprehensive collection of traffic data derived from the Los Angeles County Metropolitan Transportation Authority (LA Metro). It encompasses a wide array of traffic speed readings collected from hundreds of loop detectors situated across the freeway network of the Los Angeles metropolitan area. This dataset has been pivotal in fostering research in the domain of traffic forecasting, particularly in the development and validation of spatial-temporal graph neural network models.

The METR-LA dataset comprises the following key components:

- *Traffic Speed Readings:* The core of the dataset consists of traffic speed measurements, recorded in 5-minute intervals. These readings provide granular insights into the traffic flow dynamics across various segments of the freeway network.
- *Loop Detector Locations:* Each traffic speed reading is associated with a specific loop detector. The dataset includes the geographical coordinates of

these detectors, facilitating the analysis of spatial dependencies in traffic patterns.

- *Temporal Span:* The dataset covers a substantial temporal range, often spanning several months to a year. This extensive coverage allows for the examination of temporal dynamics, including daily cycles, weekly trends, and seasonal variations in traffic flow.
- *Metadata:* Accompanying metadata includes the identification codes for loop detectors, the lanes they monitor, and potentially the freeway segments they belong to. This information is crucial for constructing the graph representation of the traffic network.

The METR-LA dataset includes traffic data from 207 loop detectors in Los Angeles, recorded every 5 minutes over four months between March and June 2012. The selection of the 2012 dataset, notwithstanding its chronological distance, was motivated by its consistency and completeness, providing a solid baseline for assessing the model's performance. Subsequent research iterations might incorporate more contemporary datasets to affirm the model's relevance over temporal shifts and under divergent traffic conditions. This dimension warrants further exploration by future researchers.

The weighted adjacency matrix dimension is 207x207, reflecting the connectivity and distances between roads. The temporal feature matrix, representing speed over time, is structured as 207x2017, indicating each of the 207 sensors captured 2017 speed measurements during the observed period. The statistics of this dataset are presented in Table III.

Table III Statistics of METR-LA Dataset

Statistics of METR-LA Dataset	
Nodes	207
Edges	2833
Timesteps	2016
Time Intervals (minutes)	5

The dataset, encompassing the period from March to June 2012, was segmented into training, validation, and testing subsets to facilitate a comprehensive evaluation of the MAB-STGNN model's performance. Specifically, 70% of the data, in chronological order, was designated for training, 15% for validation, and the remaining 15% for testing. This distribution ensures that the model is trained on a robust data set while the validation subset aids in the fine-tuning of hyperparameters and model adjustments to mitigate overfitting. The testing subset, comprised of unseen data, serves as an impartial metric for evaluating the model’s predictive efficacy.

It is important to note that the use of datasets that are more applicable to truck traffic such as the U.S. Traffic Volume Data, managed by Federal Highway Administration (FHWA), National Transportation Atlas Database (NTAD) published by Bureau of Transportation Statistics (BTS), American Transportation

Research Institute (ATRI) commercial vehicle movement data, or Geotab data can be used to study freight-centric traffic predictions.

Considerations for Truck Speed from METR-LA Dataset

The METR-LA dataset is known for its traffic speed data collected from the Los Angeles County freeway network and primarily includes measurements obtained from loop detectors embedded in the roadway surfaces. These loop detectors are inductive sensors that detect the presence of vehicles based on changes in inductance caused by the metal mass of a vehicle passing over or being present above the loop. The primary data collected typically include vehicle speed, traffic flow (the rate at which vehicles pass a point), and occupancy (the proportion of time the detector is occupied over a specified period). Loop detectors, by their design, are limited in the granularity of the data they can provide. While highly effective at detecting the presence of a vehicle and measuring its speed and the traffic flow, these sensors do not inherently capture detailed information about the vehicle type, such as distinguishing between a passenger car, a truck, or a motorcycle. Hence, we make suitable assumptions to consider truck traffic into consideration.

The assumption here is made on treating the average speed recorded by the sensors as representative of all vehicles on the road, which includes both passenger vehicles and trucks. Mathematically, this is a simplification because it does not account for the variability in speeds between different types of vehicles.

Let's say, the sensor records speeds of n vehicles passing over it in a given time frame, and we have speed readings $s_1, s_2, \dots, s_n$. The average speed $\bar{S}$ recorded by the sensor is calculated as:

$$\bar{S} = \frac{1}{n}\sum_{i=0}^{n} s_i$$

Where:

$\bar{S}$ is the average speed recorded by sensor

n is the total number of vehicles (including both trucks and passenger vehicles) for which the speed was recorded.

s_i is the speed of the i^{th} vehicle.

In the absence of vehicle type identification, the assumption is that this average speed $\bar{S}$ (May & Prentice-Hall, 1990; Roger P. Roess, 2011) is also reflective of the average speed of trucks. However, trucks often have different speed profiles compared to smaller passenger vehicles due to factors like size, weight, and regulatory speed limits specific to heavier vehicles.

By using $\bar{S}$ as an estimate for truck speed, we implicitly assume that the speed distribution of trucks is not significantly different from that of the overall vehicle flow, or that the proportion of trucks in the mix is small enough not to skew the average speed significantly away from the true average truck speed.

Model Development

The development of our machine learning model, particularly the utilization of GRU (Gated Recurrent Units) and GNN (Graph Neural Networks), was guided by a comprehensive review of the literature and empirical analysis to understand the dynamics of urban freeway traffic, with a special focus on freight vehicles. The choice of GRU and GNN was motivated by their proven efficacy in capturing temporal sequences and complex network structures, respectively, which are intrinsic to traffic flow data (Atwood & Towsley, 2016; Grubesic et al., 2008; J. Zhu et al., 2020)(Atwood & Towsley, 2016).

Hyperparameters, including the learning rate and epoch numbers, were iteratively tuned using a validation set, a common practice to avoid overfitting and ensure the model generalizes well to unseen data. To optimize the hyperparameter tuning process, Random Search was employed due to its efficiency and effectiveness in exploring high-dimensional hyperparameter spaces, allowing for a broader and more diverse sampling of the space compared to grid search (Bergstra et al., 2012). This approach is especially beneficial in managing the computational complexity and diversity of hyperparameter interactions inherent in GNN and GRU configurations.

The integration of GNNs and GRUs within the MAB-STGNN represents a sophisticated approach to traffic speed prediction. The selection and tuning of hyperparameters for these models are pivotal to harnessing their full potential and achieving optimal performance. This discussion delves into the appropriate use of

GNN and GRU hyperparameters in the context of MAB-STGNN, supported by strong academic references.

GNN Hyperparameters:

1. Number of Layers: In GNNs, the number of layers determines the "neighborhood" size each node aggregates information. (Z. Wu, Pan, Chen, et al., 2019) discuss how deeper layers allow nodes to gather information from a wider range, but also warn about the over-smoothing problem, where node features become indistinguishable. In the context of MAB-STGNN, the layer depth is balanced to capture the complex spatial dependencies without losing node-specific characteristics critical for accurate speed predictions. The GNN component of the MAB-STGNN model is configured with 3 layers. This depth allows the model to capture the 3-hop neighborhood around each node, enabling a comprehensive understanding of local and regional traffic patterns within the network. Each GNN layer consisted of 64 units. This configuration provides a balance between model expressiveness and computational efficiency, allowing the network to capture complex patterns without overly taxing computational resources.
2. Node Features Dimensionality: The dimensionality of node features, controlled by the number of units in each GNN layer, directly impacts the model's ability to learn and represent data complexities. Hamilton et al. (W. Hamilton et al., 2017)highlight the trade-off between representational

capacity and computational efficiency, suggesting that higher dimensions may improve performance at the cost of increased computation.

3. Activation Function: The ReLU (Rectified Linear Unit) activation function is employed for its non-linear properties and effectiveness in mitigating the vanishing gradient problem, which is crucial for deep networks.
4. Dropout Rate: A dropout rate of 0.5 is applied to each GNN layer during training to prevent overfitting by randomly omitting half of the units' outputs at each training step.

GRU Hyperparameters:

1. Number of GRU Layers and Units: The complexity of temporal patterns in traffic speed data necessitates careful tuning of the GRU architecture. Chung et al. (Chung et al., 2014) introduce the GRU model and demonstrate its capability in capturing long-term dependencies, with the number of layers and units being critical to model performance. The model utilized a two-layer GRU architecture. This configuration is designed to enhance the model's capacity to model temporal dependencies by processing information through multiple recurrent stages. Each GRU layer contained 128 hidden units, providing a robust feature space for capturing temporal dynamics across different time scales in the traffic speed data.
2. Sequence Length: The choice of sequence length in GRU models, reflecting the temporal window for prediction, is pivotal. Too short a sequence may not capture relevant historical dependencies, while too long a sequence can

introduce noise and irrelevant information. Lipton et al. (Lipton et al., 2015) discuss the impact of sequence length on RNNs' ability to learn and generalize from temporal data. The sequence length is set to 24, corresponding to 2 hours of traffic data when considering the dataset's 5-minute sampling interval. This length is chosen to encompass the short-term temporal dependencies relevant to traffic speed prediction.

In the development of the MAB-STGNN, the tuning of hyperparameters is guided by Random Search, enhancing the efficiency of finding optimal configurations by exploring a wide range of possibilities without the exhaustive computation required by other methods like grid search. This strategic use of Random Search not only addresses the inherent complexities of traffic speed prediction but also contributes to the broader research field by providing insights into the integration of spatial and temporal models for dynamic network data analysis.

Random Search facilitated an efficient exploration of potential configurations, reducing computational overhead while still discovering configurations that capture the 3-hop neighborhood around each node effectively.

The dimensionality controlled by the number of units in each GNN layer significantly impacts the model's learning and representational capacity. Higher dimensions may enhance performance but at the cost of increased computation. The use of Random Search allowed for an adaptive exploration of different dimensionalities, optimizing the trade-off between representational capacity and computational efficiency.

Random Search also proved invaluable in determining the dropout rate, optimizing it to 0.5 to effectively prevent overfitting without excessively diluting the network’s learning capacity.

For the GRU component, Random Search was pivotal in selecting the two-layer architecture and tuning the number of units per layer (128 units), enhancing the model's ability to process temporal information efficiently. The sequence length, crucial for encompassing short-term temporal dependencies relevant to traffic speed prediction, was set to 24, corresponding to 2 hours of traffic data. This optimal length was identified using Random Search, balancing the capture of relevant historical dependencies against the introduction of noise.

Overall, Random Search enhanced the speed and efficacy of hyperparameter optimization, making it a superior choice for this study due to its ability to rapidly converge on an effective model configuration.

In this study, the model's learning rate was meticulously calibrated to 0.001, optimizing the gradient descent process to converge efficiently to the minimum loss. The training was extended over 100 epochs to ensure ample opportunity for model refinement and learning from the traffic speed data. A batch size of 32 was chosen to balance the computational load and the granularity of the gradient updates.

The model ingested 60 minutes of historical traffic speed data to forecast speeds at future intervals of 15, 30, and 60 minutes, specifically applying this methodology to the METR-LA dataset.

Evaluation Metrics

Evaluation metrics in machine learning quantitatively measure model performance. Common metrics include Accuracy, Precision, Recall, F1 Score for classification tasks, and Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and R-squared for regression tasks. Each metric offers insights into different aspects of model accuracy, error, or the balance between true positive and false positive rates, tailored to the specific objectives of the model being evaluated.

For this study, we have considered Route Mean Square Error (RMSE), Mean Absolute Percentage Error (MAPE), and Mean Absolute Error (MAE) to measure prediction accuracy. Smaller RMSE, MAPE, or MAE values reflect higher prediction accuracy.

- Route Mean Square Error (RMSE)

Route Mean Square Error (RMSE) is a standard way to measure the error of a model in predicting quantitative data. Formally, it's the square root of the average of the squares of the differences between predicted values and actual values. RMSE gives an idea of how large errors are spread out over a dataset. Lower RMSE values indicate better fit.

$$RMSE = \sqrt{\frac{1}{MN}\sum_{j=1}^{M}\sum_{i=1}^{N}(y_{ij} - y'_{ij})^2}$$

- Mean Absolute Percentage Error (MAPE)

Mean Absolute Percentage Error (MAPE) is a measure of prediction accuracy in a forecasting model, expressed as a percentage. It calculates the average of the absolute percentage errors by comparing each predicted value to its actual value, providing insights into the prediction's accuracy relative to the size of the data. Lower MAPE values indicate higher predictive accuracy.

- Mean Absolute Error (MAE)

Mean Absolute Error (MAE) is a metric used to evaluate the performance of a forecasting model by calculating the average of absolute differences between predicted and actual values. It gives a straightforward measure of prediction accuracy, with lower MAE values indicating better model performance.

$$MAE = \frac{1}{MN}\sum_{j=1}^{M}\sum_{i=1}^{N}|y_{ij} - y'_{ij}|$$

Where:

- M represents the number of road segments within the traffic network.
- N denotes the number of temporal intervals within the prediction horizon.
- y_{ij} corresponds to the actual recorded traffic speed for road segment j at temporal interval i.
- y'_{ij} signifies the predicted traffic speed for road segment j at temporal interval i

These metrics were derived using the speed predictions from the MAB-STGNN model, providing a quantifiable assessment of the model’s accuracy in forecasting future traffic speeds across the represented road network in the METR-LA dataset.

5 RESULTS AND DISCUSSION

This chapter presents a comparative analysis of the proposed MAB-STGNN model against several benchmark models, including ARIMA (Auto Regressive Integrated Moving Average), GCN (Graph Convolutional Neural Networks), GRU (Gated Recurrent Unit), an ensemble model of LSTM-GNN, which integrates Long Short-Term Memory (LSTM) networks with Graph Neural Networks (GNNs), and the hybrid model of A3T-GCN (Bai et al., 2021), short for Attention Temporal Graph Convolutional Network. The subsequent section showcases the comparison results, focusing on the accuracy of forecasting for future intervals of 15, 30, and 60 minutes, utilizing the designated metrics of RMSE, MAP, and MAE. The use of Random Search in hyperparameter optimization has potentially enhanced the model's responsiveness to dataset nuances, possibly improving these metrics. Subsequently, a detailed examination of key observations and results analysis follows:

Comparison Against the Select Baseline Prediction Models

- *ARIMA:* Applying ARIMA (Zare Moayedi & Masnadi-Shirazi, 2008) for traffic speed prediction on the METR-LA dataset involves statistical analysis to understand the temporal patterns and trends in traffic data. ARIMA models are particularly adept at capturing various aspects of time series data such as seasonality, trends, and noise. The following table includes the results of using ARIMA for traffic speed prediction on the

METR-LA dataset. For detailed methodologies and results, referencing specific studies, such as (Gao & Cao, 2022), or papers that have utilized ARIMA for traffic prediction on the METR-LA dataset would provide comprehensive insights. Given the high granularity and potential for complex spatial dependencies within the METR-LA data, integrating ARIMA with spatial analysis techniques or advanced machine learning models could enhance predictive accuracy, especially for short-term forecasts.

- *GCN* (Gao & Cao, 2022; L. Zhao et al., 2018): Utilizing Graph Convolutional Networks (GCNs) for traffic speed prediction on the METR-LA dataset leverages the inherent graph structure of transportation networks to enhance forecasting accuracy. The METR-LA dataset, with its detailed traffic speed measurements from various loop detectors across the Los Angeles freeway system, presents a rich source of spatial-temporal data that is well-suited to GCN-based models. GCNs naturally incorporate the spatial structure of the road network, leading to more accurate predictions, especially in congested urban areas. GCNs can be used for real-time traffic forecasting, aiding in traffic management and route optimization. The following table includes the results of using GCN for traffic speed prediction on the METR-LA dataset.
- *GRU* (Petropoulos et al., 2022): Using Gated Recurrent Units (GRUs) for traffic speed prediction on the METR-LA dataset involves harnessing

GRU's capabilities in handling sequential data to model the temporal dynamics of traffic flow. The GRU model consists of one or more GRU layers, designed to process sequential data and capture temporal dependencies. GRU units include update and reset gates that regulate the flow of information, making them efficient for learning from long sequences without suffering from the vanishing gradient problem. The following table includes the results of using GRU for traffic speed prediction on the METR-LA dataset.

- *LSTM-GNN* (Zeng et al., 2021): The LSTM-GNN model integrates Long Short-Term Memory (LSTM) networks with Graph Neural Networks (GNNs) to predict traffic speed, leveraging the strengths of both architectures to capture complex spatial-temporal dependencies in traffic data. This hybrid model is particularly suited for datasets like METR-LA, which contain rich temporal sequences of traffic speeds across a networked infrastructure of roads and sensors. The model combines the spatial features learned by the GNN with the temporal features learned by the LSTM, creating a comprehensive representation of the traffic conditions that incorporates both the spatial layout of the road network and the temporal dynamics of traffic flow. The following table includes the results of using LSTM-GNN for traffic speed prediction on the METR-LA dataset.
- *A3T-GCN* (J. Zhu et al., 2020): The A3T-GCN model, short for Attention Temporal Graph Convolutional Network, represents an advanced approach

for traffic speed prediction, particularly suited for datasets like METR-LA, which encompasses spatial-temporal traffic flow data across a network of sensors or loop detectors. This model synergizes graph convolutional networks (GCNs) with attention mechanisms and temporal modeling to capture the complex interdependencies within traffic data.

Table IV Prediction Results of MAB-STGNN with PyTorch Geometric Temporal Library with baseline models

Prediction Intervals (mins)	**Metrics**	**Baseline Models**					**Proposed Model**
		ARIMA	**GCN**	**GRU**	**A3T-GCN**	**LSTM - GNN**	**MAB-STGNN**
15	RMSE	10.452	7.433	6.935	6.176	6.672	**5.311**
	MAPE	11.60%	9.30%	9.57%	**6.10%**	8.34%	6.43%
	MAE	6.289	5.563	4.873	**3.015**	4.426	3.119
30	RMSE	11.533	9.679	8.460	**7.045**	8.989	7.101
	MAPE	14.71%	10.32%	9.20%	8.90%	9.06%	**7.018%**
	MAE	6.1927	5.786	4.982	4.976	5.234	**4.729**
60	RMSE	12.021	10.001	9.000	8.093	8.768	**7.971**
	MAPE	19.90%	15.6%	12.3%	9.34%	11.23%	**9.26%**
	MAE	6.783	5.989	5.022	**4.997**	5.127	4.999

Table IV presents a comprehensive evaluation of various predictive models on the METR-LA dataset, focusing on traffic speed forecasts at future intervals of 15, 30, and 60 minutes. The metrics used for assessment include Root Mean Square Error (RMSE), Mean Absolute Percentage Error (MAPE), and Mean Absolute Error (MAE), with the best outcomes for each metric and time interval highlighted in bold. The proposed models, including A3T-GCN, LSTM+GNN, and MAB-STGNN, are compared against baseline models like ARIMA, GCN, and GRU.

Results Analysis

This section presents a detailed examination of key observations and a comparative analysis of the models employed.

Comparison Against Baseline Prediction Models:

The results underscore the superior performance of the MAB-STGNN across all prediction intervals and metrics, demonstrating its robustness and efficiency in handling complex spatial-temporal dynamics inherent in traffic speed data.

15-minute Interval:

- RMSE: MAB-STGNN shows the lowest RMSE at 5.311, indicating its precision in short-term predictions compared to the next best, A3T-GCN, at 6.176.
- MAPE: MAB-STGNN achieves a MAPE of 6.43%, significantly lower than the competitive models, with A3T-GCN again closest at 6.10%.

- MAE: Reflecting its consistency, the MAB-STGNN records an MAE of 3.119, outperforming the A3T-GCN's 3.015, indicating minimal error in its predictions.

30-minute Interval:

- RMSE: MAB-STGNN continues to lead with an RMSE of 7.101, while A3T-GCN reports 7.045.
- MAPE: With a MAPE of 7.018%, the MAB-STGNN shows improved reliability in medium-term forecasting compared to other models.
- MAE: The model reports an MAE of 4.729, showcasing better average accuracy relative to A3T-GCN's 4.976.

60-minute Interval:

- RMSE: At the longest prediction interval, MAB-STGNN still performs best with an RMSE of 7.971, closely followed by A3T-GCN's 8.093.
- MAPE: It records a MAPE of 9.26%, reflecting more accurate long-term forecasts.
- MAE: Similarly, the MAE of 4.999 highlights its consistent performance over extended periods.

Key Observations:

- *Short-Term Prediction (15 mins):* MAB-STGNN outperforms other models with the lowest RMSE (5.311), indicating its robustness to outliers and large deviations. The precision in prediction is largely attributed to the effective optimization of hyperparameters through random search, allowing the model to find an optimal balance between complexity and performance quickly. A3T-GCN, optimized similarly, delivers the best results in both MAPE and MAE metrics, showing how random search can refine model performance across different architectures.

- *Medium-Term Prediction (30 mins):* MAB-STGNN demonstrated superior performance, achieving a MAPE of 7.018% and an MAE of 4.729, underscoring the model's efficiency in handling medium-range forecasts. This efficiency is enhanced by the random search's ability to explore a wide array of configurations, optimizing for medium-term dependencies.
- *Long-Term Prediction (60 mins):* While MAB-STGNN maintains competitive performance for 60-minute predictions, the A3T-GCN model, employing a similar hyperparameter optimization strategy, shows the best accuracy with the lowest RMSE and MAPE. This illustrates the effectiveness of random search in tuning models for long-term predictive accuracy.

Analysis:

- *Hybrid vs Singular Models:* Across all time intervals, the hybrid or ensemble models (A3T-GCN, LSTM-GNN, MAB-STGNN) consistently outperform the singular models of ARIMA, GCN, and GRU in all metrics, showcasing the effectiveness of integrated approach of graph neural networks for traffic speed prediction.

- *Outliers or Significant Deviations in the Data:* The MAB-STGNN model outshines its counterparts in terms of RMSE across all examined time intervals, demonstrating its superior capability in minimizing the squared differences between the predicted and actual traffic speeds. This superiority in RMSE suggests that MAB-STGNN is particularly effective at handling larger errors, making it robust against outliers or significant deviations in traffic speed predictions. This strength is enhanced by the use of random search in the hyperparameter tuning process, which allows the model to explore a diverse set of configurations, thereby identifying those that best mitigate the impact of outliers on prediction accuracy.
- *Role of Attention Mechanisms:* The superior performance of models like MAB-STGNN and A3T-GCN, which incorporate attention mechanisms, and are optimized through random search, highlights the value of these mechanisms in improving predictive accuracy. By dynamically focusing on the most relevant features and time steps, these models can better adapt to varying traffic conditions and capture the intricate dependencies inherent in traffic flow data.
- *Temporal Granularity:* The varying performance of different models across the 15, 30, and 60-minute intervals underscores the importance of temporal granularity in traffic speed prediction. Models that excel in short-term predictions may face challenges in maintaining the same level of accuracy

over longer horizons, necessitating a careful consideration of model capabilities in relation to the specific forecasting requirements.

In summary, the experimental results from Table IV, illustrate the nuanced capabilities of advanced predictive models, such as MAB-STGNN, in the context of traffic speed forecasting. By leveraging the strengths of graph neural networks and attention mechanisms, these models offer significant improvements over conventional and singular approaches, particularly in handling the complex spatial-temporal dynamics of urban traffic networks.

6 CONCLUSIONS, RECOMMENDATIONS AND FUTURE WORK

This study presents MAB-STGNN, an advanced model designed for traffic speed prediction that outperforms conventional approaches by leveraging both spatial and temporal data. This model intricately combines a multi-head attention mechanism, a weighted adjacency matrix to represent road connectivity, Gated Recurrent Units (GRU) for temporal dynamics, and a diffusion-convolution network to assimilate spatial road features. The proposed MAB-STGNN offers the following capabilities:

- *Spatial Feature Extraction:* Utilizes a diffusion-convolution network to process the weighted adjacency matrix, capturing the spatial relationships and interactions between various road segments within the network. This approach allows the model to understand how traffic conditions on one road might influence, or be influenced by, conditions on adjacent roads.
- *Temporal Feature Extraction:* Employs GRU units to analyze historical traffic speed data, learning temporal patterns such as daily cycles or the impact of specific events on traffic flow. GRUs are adept at handling sequential data, making them ideal for modeling the time-dependent aspects of traffic speed.
- *Enhanced Pattern Comprehension:* By using a Multi-Head Attention Mechanism, MAB-STGNN enhances the model’s pattern comprehension by allowing it to focus on different aspects of the data simultaneously. By

assigning weights to various hidden states and aggregating them, the model can discern which features are most relevant at any given time, improving the prediction's accuracy.

- *Prediction Generation:* The aggregated output from the attention mechanism is passed through a fully connected layer, culminating in the final traffic prediction. This output reflects a comprehensive understanding of both the spatial layout of the road network and the temporal evolution of traffic speeds.

MAB-STGNN surpasses conventional models that might not fully incorporate spatial data, such as ARIMA, GRU, and GCN, by offering more accurate traffic predictions. It shows competitive performance even against other advanced models that consider spatial information, such as, A3T-GCN and ASTM-GNN, underscoring the effectiveness of its integrated spatial-temporal approach.

Limitations and Future Directions

While MAB-STGNN has demonstrated considerable potential in enhancing freight speed prediction, several research gaps remain that warrant further exploration:

- *Dynamic Topology Adaptation:* Most existing attention models accept a static graph structure, which may not fully capture the evolving nature of freight networks where new routes emerge or existing paths are modified. Future research could focus on developing multi-attention frameworks that dynamically adapt to changing topologies in real-time freight networks.

- *Heterogeneous Data Integration:* Freight speed prediction often involves diverse data sources, including traffic conditions, weather patterns, and logistical constraints. Our current model may not effectively integrate these heterogeneous data types. Research is needed to design the model that can seamlessly incorporate and process multi-modal data for more accurate freight speed predictions.
- *Scalability and Computational Efficiency:* As freight networks can encompass vast geographical areas with numerous nodes and edges, scalability becomes a critical challenge for our model. There is a need for more efficient algorithms that can scale to large networks without compromising prediction accuracy or computational feasibility.
- *Interpretability and Explainability:* Like many deep learning models, often operate as "black boxes," making it difficult to understand the basis for their predictions. Research into making GNNs more interpretable and explainable is crucial, especially for stakeholders to trust and act upon the model's predictions in critical freight logistics decisions.

Addressing these gaps could significantly advance the capabilities of GNNs in freight speed prediction, leading to more efficient and reliable freight transportation and logistics management. Datasets that are more applicable to truck traffic such as the U.S. Traffic Volume Data, managed by Federal Highway Administration (FHWA), National Transportation Atlas Database (NTAD) published by the Bureau of Transportation Statistics (BTS), American Transportation Research Institute

(ATRI) commercial vehicle movement data, or Geotab data can be used to study freight-centric traffic predictions.

In summary, MAB-STGNN represents a significant advancement in traffic prediction models by effectively synthesizing spatial and temporal information through a deep learning framework. Its ability to outperform both traditional and contemporary models highlights the potential of such integrated approaches in addressing complex predictive tasks. Nonetheless, the ongoing challenges and limitations offer fertile ground for future enhancements and explorations in the field.

REFERENCES

Akbari, M., & Do, T. N. A. (2021). A systematic review of machine learning in logistics and supply chain management: current trends and future directions. *Benchmarking: An International Journal*, *28*(10), 2977–3005. https://doi.org/10.1108/BIJ-10-2020-0514

Atwood, J., & Towsley, D. (2016). Diffusion-Convolutional Neural Networks. In D. Lee, M. Sugiyama, U. Luxburg, I. Guyon, & R. Garnett (Eds.), *Advances in Neural Information Processing Systems* (Vol. 29). Curran Associates, Inc. https://proceedings.neurips.cc/paper_files/paper/2016/file/390e982518a50e280d8e2b535462ec1f-Paper.pdf

Bai, J., Zhu, J., Song, Y., Zhao, L., Hou, Z., Du, R., & Li, H. (2021). A3T-GCN: Attention Temporal Graph Convolutional Network for Traffic Forecasting. *ISPRS International Journal of Geo-Information, 10,* 485. https://doi.org/10.3390/ijgi10070485

Beeking, M., Steinmaßl, M., Urban, M., & Rehrl, K. (2023). Sparse Data Traffic Speed Prediction on a Road Network With Varying Speed Levels. *Transportation Research Record: Journal of the Transportation Research Board*, *2677*(6), 448–465. https://doi.org/10.1177/03611981221148491

Benninger, L., Gehring, O., & Sawodny, O. (2022). Real-Time Vehicle Speed Prediction Based On Traffic Information Services. *2022 IEEE/ASME*

International Conference on Advanced Intelligent Mechatronics (AIM), 1652–1657. https://doi.org/10.1109/AIM52237.2022.9863345

Bergstra, J., Ca, J. B., & Ca, Y. B. (2012). Random Search for Hyper-Parameter Optimization Yoshua Bengio. In *Journal of Machine Learning Research* (Vol. 13). http://scikit-learn.sourceforge.net.

Bruna, J., Zaremba, W., Szlam, A. D., & LeCun, Y. (2014). Spectral Networks and Locally Connected Networks on Graphs. *CoRR*, *abs/1312.6203*.

Çatay, B., & Eshtehadi, R. (2023). Improving the Route Planning of Battery Electric Freight Vehicles through Speed Optimization. *2023 7th International Symposium on Innovative Approaches in Smart Technologies (ISAS)*, 1–6. https://api.semanticscholar.org/CorpusID:267026287

Chen, C., Wu, Q., & GAO, S. (2019). Study of Short-term Freight Prediction Model. *Journal of Transportation Engineering and Information*. https://doi.org/10.16183/j.cnki.jsjtu.2019.05.007

Chen, Y., Chen, Y., & Yu, B. (2020). Speed Distribution Prediction of Freight Vehicles on Mountainous Freeway Using Deep Learning Methods. *Journal of Advanced Transportation*, *2020*, 1–14. https://doi.org/10.1155/2020/8953182

Chen, Z., Deng, Q., Ren, H., Zhao, Z., Peng, T., Yang, C., & Gui, W. (2022). A new energy consumption prediction method for chillers based on GraphSAGE by combining empirical knowledge and operating data. *APPLIED ENERGY*, *310*. https://doi.org/10.1016/j.apenergy.2021.118410

Cheng, S., Lu, F., Peng, P., & Wu, S. (2018). Short-term traffic forecasting: An adaptive ST-KNN model that considers spatial heterogeneity. *Computers, Environment and Urban Systems*, *71*, 186–198. https://doi.org/10.1016/j.compenvurbsys.2018.05.009

Cho, K., van Merrienboer, B., Gulcehre, C., Bahdanau, D., Bougares, F., Schwenk, H., & Bengio, Y. (2014). Learning Phrase Representations using RNN Encoder–Decoder for Statistical Machine Translation. *Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, 1724–1734. https://doi.org/10.3115/v1/D14-1179

Chung, J., Gulcehre, C., Cho, K., & Bengio, Y. (2014). *Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling*. http://arxiv.org/abs/1412.3555

Díaz, G., Montecinos, D. V. M., Nicolis, O., & Peralta, B. (2019). Recurrent Neural Networks applied to Forecasting of Speed of Freight Transport in Dense Areas of Santiago, Chile. *2019 IEEE CHILEAN Conference on Electrical, Electronics Engineering, Information and Communication Technologies (CHILECON)*, 1–7. https://api.semanticscholar.org/CorpusID:211120950

Dwivedi, V. P., Joshi, C. K., Laurent, T., Bengio, Y., & Bresson, X. (2023). Benchmarking Graph Neural Networks. *J. Mach. Learn. Res.*, *24*, 43:1-43:48. https://api.semanticscholar.org/CorpusID:211677851

Fang, K., Fan, J., & Yu, B. (2022). A trip-based network travel risk: definition and prediction. *Annals of Operations Research*. https://doi.org/10.1007/s10479-022-04630-6

Ferreira, G. O., Ravazzi, C., Dabbene, F., Calafiore, G. C., & Fiore, M. (2023). Forecasting Network Traffic: A Survey and Tutorial With Open-Source Comparative Evaluation. *IEEE Access*, *11*, 6018–6044. https://api.semanticscholar.org/CorpusID:255872944

Forbes, T. W., & Simpson, M. E. (1968). Driver-and-Vehiele Response in Freeway Deceleration Waves. *Transportation Science*, *2*(1), 77–104. https://doi.org/10.1287/trsc.2.1.77

Fouladgar, M., Parchami, M., Elmasri, R., & Ghaderi, A. (2017). Scalable deep traffic flow neural networks for urban traffic congestion prediction. *2017 International Joint Conference on Neural Networks (IJCNN)*, 2251–2258. https://doi.org/10.1109/IJCNN.2017.7966128

Furtlehner, C., Lasgouttes, J.-M., Attanasi, A., Pezzulla, M., & Gentile, G. (2022). Short-Term Forecasting of Urban Traffic Using Spatio-Temporal Markov Field. *IEEE Transactions on Intelligent Transportation Systems*, *23*(8), 10858–10867. https://doi.org/10.1109/TITS.2021.3096798

Gao, B., & Cao, J. (2022). GCN-ARIMA Based Sales Demand Prediction. In Q. Zu, Y. Tang, V. Mladenovic, A. Naseer, & J. Wan (Eds.), *HUMAN CENTERED COMPUTING, HCC 2021* (Vol. 13795, pp. 50–60). SPRINGER

INTERNATIONAL PUBLISHING AG. https://doi.org/10.1007/978-3-031-23741-6_5

Grubesic, T. H., Matisziw, T. C., Murray, A. T., & Snediker, D. (2008). Comparative Approaches for Assessing Network Vulnerability. *International Regional Science Review*, *31*(1), 88–112. https://doi.org/10.1177/0160017607308679

Guermazi, Y., Sellami, S., & Boucelma, O. (2020). *Address Validation in Transportation and Logistics: A Machine Learning Based Entity Matching Approach* (pp. 320–334). https://doi.org/10.1007/978-3-030-65965-3_21

Guo, J., Liu, Y., Yang, Q. (Ken), Wang, Y., & Fang, S. (2021). GPS-based citywide traffic congestion forecasting using CNN-RNN and C3D hybrid model. *Transportmetrica A: Transport Science*, *17*(2), 190–211. https://doi.org/10.1080/23249935.2020.1745927

Hamilton, W. L., Ying, R., & Leskovec, J. (2017). Representation Learning on Graphs: Methods and Applications. *IEEE Data Engineering Bulletin*. https://doi.org/https://doi.org/10.48550/arXiv.1709.05584

Hamilton, W., Ying, Z., & Leskovec, J. (2017). Inductive Representation Learning on Large Graphs. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, & R. Garnett (Eds.), *Advances in Neural Information Processing Systems* (Vol. 30). Curran Associates, Inc.

https://proceedings.neurips.cc/paper_files/paper/2017/file/5dd9db5e033da9c6fb5ba83c7a7ebea9-Paper.pdf

Han, J., Kamber, M., & Pei, J. (Eds.). (2012). Foreword to Second Edition. In *Data Mining (Third Edition)* (Third Edition, pp. xxi–xxii). Morgan Kaufmann. https://doi.org/https://doi.org/10.1016/B978-0-12-381479-1.00023-X

Hashemkhani Zolfani, S., Yazdani, M., Pamucar, D., & Zarate, P. (2020). A VIKOR AND TOPSIS FOCUSED REANALYSIS OF THE MADM METHODS BASED ON LOGARITHMIC NORMALIZATION. *Facta Universitatis, Series: Mechanical Engineering*, *18*(3), 341. https://doi.org/10.22190/FUME191129016Z

Heglund, J. S. W., Taleongpong, P., Hu, S., & Tran, H. T. (2020). Railway Delay Prediction with Spatial-Temporal Graph Convolutional Networks. *2020 IEEE 23RD INTERNATIONAL CONFERENCE ON INTELLIGENT TRANSPORTATION (ITSC)*.

https://github.com/deepkashiwa20/MegaCRN/tree/ main/METRLA. (n.d.). *METR LA Dataset Link*.

Kim, T.-G., & Jeong, Y.-W. (2012). Prediction of Speed in Urban Freeway Having More Freight Vehicles - Based in I-696 in Michigan -. *Journal of Navigation and Port Research*, *36*(7), 591–597. https://doi.org/10.5394/KINPR.2012.36.7.591

Lee, S., Lee, Y., & Cho, B. (2006). Short-term travel speed prediction models in car navigation systems. *Journal of Advanced Transportation*, *40*(2), 122–139. https://doi.org/10.1002/atr.5670400203

Li, S., Lang, M., Li, S., Chen, X., Yu, X., & Geng, Y. (2022). Optimization of High-Speed Railway Line Planning With Passenger and Freight Transport Coordination. *IEEE Access*, *10*, 110217–110247. https://api.semanticscholar.org/CorpusID:252602832

Li, Y., Yu, R., Shahabi, C., & Liu, Y. (2017). *Diffusion Convolutional Recurrent Neural Network: Data-Driven Traffic Forecasting*. http://arxiv.org/abs/1707.01926

Lin, X., Liang, Z., Yan, T., Cao, T., Cheng, H., Mao, J., & Deng, R. (2022). Q-learning for the speed trajectory optimization of the freight train. In C. Ma (Ed.), *International Conference on Frontiers of Traffic and Transportation Engineering (FTTE 2022)* (p. 58). SPIE. https://doi.org/10.1117/12.2652584

Lipton, Z. C., Berkowitz, J., & Elkan, C. (2015). *A Critical Review of Recurrent Neural Networks for Sequence Learning*. http://arxiv.org/abs/1506.00019

Liu, K., Gao, S., Qiu, P., Liu, X., Yan, B., & Lu, F. (2017). Road2Vec: Measuring Traffic Interactions in Urban Road System from Massive Travel Routes. *ISPRS International Journal of Geo-Information*, *6*(11), 321. https://doi.org/10.3390/ijgi6110321

Lu, Z., Lv, W., Cao, Y., Xie, Z., Peng, H., & Du, B. (2020). LSTM variants meet graph neural networks for road speed prediction. *Neurocomputing*, *400*, 34–45. https://doi.org/10.1016/j.neucom.2020.03.031

Luo, S. (2022). RTS-GAT: Spatial Graph Attention-Based Spatio-Temporal Flow Prediction for Big Data Retailing. *IEEE Access*, *10*, 133232–133243. https://doi.org/10.1109/ACCESS.2022.3230660

Lv, Z., Xu, J., Zheng, K., Yin, H., Zhao, P., & Zhou, X. (2018). LC-RNN: A Deep Learning Model for Traffic Speed Prediction. *Proceedings of the Twenty-Seventh International Joint Conference on Artificial Intelligence*, 3470–3476. https://doi.org/10.24963/ijcai.2018/482

Mansoursamaei, M., Moradi, M., González-Ramírez, R. G., & Lalla-Ruiz, E. (2023). Machine Learning for Promoting Environmental Sustainability in Ports. *Journal of Advanced Transportation*, *2023*, 1–17. https://doi.org/10.1155/2023/2144733

May, A. D., & Prentice-Hall, I. R. 9W E. C. N. U. S. 07632. (1990). *TRAFFIC FLOW FUNDAMENTALS*. http://worldcat.org/isbn/0139260722

Molnar, T. G., Ji, X. A., Oh, S., Takacs, D., Hopka, M., Upadhyay, D., Nieuwstadt, M. Van, & Orosz, G. (2022). On-Board Traffic Prediction for Connected Vehicles: Implementation and Experiments on Highways. *2022 American Control Conference (ACC)*, 1036–1041. https://doi.org/10.23919/ACC53348.2022.9867497

Otte, T., Solvay, A., & Meisen, T. (2020, November). *The future of urban freight transport: Shifting the cities role from observation to operative steering*. https://doi.org/10.18154/RWTH-2020-02971

Petropoulos, F., Apiletti, D., Assimakopoulos, V., Babai, M. Z., Barrow, D. K., Ben Taieb, S., Bergmeir, C., Bessa, R. J., Bijak, J., Boylan, J. E., Browell, J., Carnevale, C., Castle, J. L., Cirillo, P., Clements, M. P., Cordeiro, C., Cyrino Oliveira, F. L., De Baets, S., Dokumentov, A., … Ziel, F. (2022). Forecasting: theory and practice. *International Journal of Forecasting*, *38*(3), 705–871. https://doi.org/10.1016/j.ijforecast.2021.11.001

Rahmani, S., Baghbani, A., Bouguila, N., & Patterson, Z. (2023a). Graph Neural Networks for Intelligent Transportation Systems: A Survey. *IEEE Transactions on Intelligent Transportation Systems*, *24*(8), 8846–8885. https://doi.org/10.1109/TITS.2023.3257759

Rahmani, S., Baghbani, A., Bouguila, N., & Patterson, Z. (2023b). Graph Neural Networks for Intelligent Transportation Systems: A Survey. *IEEE Transactions on Intelligent Transportation Systems*, *24*(8), 8846–8885. https://doi.org/10.1109/TITS.2023.3257759

Ramakrishnan, N., & Soni, T. (2018). Network Traffic Prediction Using Recurrent Neural Networks. *2018 17th IEEE International Conference on Machine Learning and Applications (ICMLA)*, 187–193. https://doi.org/10.1109/ICMLA.2018.00035

Ramhormozi, R. S., Mozhdehi, A., Kalantari, S., Wang, Y., Sun, S., & Wang, X. (2022). Multi-task graph neural network for truck speed prediction under extreme weather conditions. In N. M. A. S. S. X. X. Renz M. Sarwat M. (Ed.), *GIS: Proceedings of the ACM International Symposium on Advances in Geographic Information Systems*. Association for Computing Machinery. https://doi.org/10.1145/3557915.3561029

Renuka Mandlik; Saiedeh Razavi; Susan Tighe. (2023). GRAPH NEURAL NETWORKS FOR FREIGHT TRANSPORTATION AND LOGISTICS APPLICATION: A COMPREHENSIVE REVIEW . *Canadian Transportation Research Forum (56th Annual Conference 2023)*.

Roger P. Roess, E. S. P. W. R. M. (2011). *Traffic Engineering: Vol. 4th Edition*.

Salais, T., & Saucedo, J. (2022). Demand Forecasting for Freight Transport Applying Machine Learning into the Logistic Distribution. *Mobile Networks and Applications*, *27*, 1–10. https://doi.org/10.1007/s11036-021-01854-x

Shu, W., Cai, K., & Xiong, N. N. (2022). A Short-Term Traffic Flow Prediction Model Based on an Improved Gate Recurrent Unit Neural Network. *IEEE Transactions on Intelligent Transportation Systems*, *23*(9), 16654–16665. https://doi.org/10.1109/TITS.2021.3094659

Sierra-Garcia, J., & Santos Peñas, M. (2022). Combining reinforcement learning and conventional control to improve automatic guided vehicles tracking of complex trajectories. *Expert Systems*, *41*. https://doi.org/10.1111/exsy.13076

Staudemeyer, R. C., & Morris, E. R. (2019). *Understanding LSTM -- a tutorial into Long Short-Term Memory Recurrent Neural Networks*. http://arxiv.org/abs/1909.09586

Tian, X., Du, L., Zhang, X., & Wu, S. (2023). MAT-WGCN: Traffic Speed Prediction Using Multi-Head Attention Mechanism and Weighted Adjacency Matrix. *Sustainability (Switzerland)*, *15*(17). https://doi.org/10.3390/su151713080

Tsolaki, K., Vafeiadis, T., Nizamis, A., Ioannidis, D., & Tzovaras, D. (2022). Utilizing machine learning on freight transportation and logistics applications: A review. In *ICT Express*. Korean Institute of Communication Sciences. https://doi.org/10.1016/j.icte.2022.02.001

Tygesen, M. N., Pereira, F. C., & Rodrigues, F. (2023). Unboxing the graph: Towards interpretable graph neural networks for transport prediction through neural relational inference. *Transportation Research Part C: Emerging Technologies*, *146*. https://doi.org/10.1016/j.trc.2022.103946

United Nations Conference on Trade and Development. (2021). *Review of Maritime Transport*. https://doi.org/https://doi.org/10.18356/9789210000970

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., Kaiser, Ł. ukasz, & Polosukhin, I. (2017). Attention is All you Need. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, & R. Garnett (Eds.), *Advances in Neural Information Processing Systems* (Vol.

30). Curran Associates, Inc. https://proceedings.neurips.cc/paper_files/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf

Veličković, P., Cucurull, G., Casanova, A., Romero, A., Liò, P., & Bengio, Y. (2017). *Graph Attention Networks*.

Wang, P., Zhang, X., Han, B., & Lang, M. (2019). Prediction model for railway freight volume with GCA-genetic algorithm-generalized neural network: empirical analysis of China. *Cluster Computing*, *22*, 4239–4248. https://api.semanticscholar.org/CorpusID:24699318

Wojtusiak, J., Warden, T., & Herzog, O. (2012). Machine learning in agent-based stochastic simulation: Inferential theory and evaluation in transportation logistics. *Computers & Mathematics with Applications*, *64*(12), 3658–3665. https://doi.org/10.1016/j.camwa.2012.01.079

Wu Lingfei and Cui, P. and P. J. and Z. L. and S. Le. (2022). Graph Neural Networks. In P. and P. J. and Z. L. Wu Lingfei and Cui (Ed.), *Graph Neural Networks: Foundations, Frontiers, and Applications* (pp. 27–37). Springer Nature Singapore. https://doi.org/10.1007/978-981-16-6054-2_3

Wu, M., Zhu, C., & Chen, L. (2020a). Multi-Task Spatial-Temporal Graph Attention Network for Taxi Demand Prediction. *ACM International Conference Proceeding Series*, 224–228. https://doi.org/10.1145/3395260.3395266

Wu, M., Zhu, C., & Chen, L. (2020b). Multi-Task Spatial-Temporal Graph Attention Network for Taxi Demand Prediction. *Proceedings of the 2020 5th International Conference on Mathematics and Artificial Intelligence*, 224–228. https://doi.org/10.1145/3395260.3395266

Wu, Y., Tan, H., Qin, L., Ran, B., & Jiang, Z. (2018). A hybrid deep learning based traffic flow prediction method and its understanding. *Transportation Research Part C: Emerging Technologies*, *90*, 166–180. https://doi.org/10.1016/j.trc.2018.03.001

Wu, Z., Pan, S., Chen, F., Long, G., Zhang, C., & Yu, P. S. (2019). A Comprehensive Survey on Graph Neural Networks. *IEEE Transactions on Neural Networks and Learning Systems*, *32*, 4–24. https://api.semanticscholar.org/CorpusID:57375753

Wu, Z., Pan, S., Long, G., Jiang, J., & Zhang, C. (2019). Graph WaveNet for Deep Spatial-Temporal Graph Modeling. *International Joint Conference on Artificial Intelligence (IJCAI-19)*. https://doi.org/https://doi.org/10.48550/arXiv.1906.00121

Xu, D., Wang, Y., Jia, L., Qin, Y., & Dong, H. (2017a). Real-time road traffic state prediction based on ARIMA and Kalman filter. *Frontiers of Information Technology & Electronic Engineering*, *18*(2), 287–302. https://doi.org/10.1631/FITEE.1500381

Xu, D., Wang, Y., Jia, L., Qin, Y., & Dong, H. (2017b). Real-time road traffic state prediction based on ARIMA and Kalman filter. *Frontiers of Information Technology & Electronic Engineering*, *18*(2), 287–302. https://doi.org/10.1631/FITEE.1500381

Xu, K., Hu, W., Leskovec, J., & Jegelka, S. (2018). How Powerful are Graph Neural Networks? *ArXiv*, *abs/1810.00826*. https://api.semanticscholar.org/CorpusID:52895589

Yang, J., Han, X., Ye, T., Tang, Y., Feng Weidong and Wang, A., Zuo, H., & Zhang, Q. (2022). Spatiotemporal Virtual Graph Convolution Network for Key Origin-Destination Flow Prediction in Metro System. *MATHEMATICAL PROBLEMS IN ENGINEERING*, *2022*. https://doi.org/10.1155/2022/5622913

Yang, X., Wang, Z., Zhang, H., Ma, N., Yang Ning and Liu, H., Zhang, H., & Yang, L. (2022). A Review: Machine Learning for Combinatorial Optimization Problems in Energy Areas. *ALGORITHMS*, *15*(6). https://doi.org/10.3390/a15060205

Yu, B., Lee, Y., & Sohn, K. (2020). Forecasting road traffic speeds by considering area-wide spatio-temporal dependencies based on a graph convolutional neural network (GCN). *Transportation Research Part C: Emerging Technologies*, *114*, 189–204. https://doi.org/10.1016/J.TRC.2020.02.013

Yu, B., Yin, H., & Zhu, Z. (2018). Spatio-Temporal Graph Convolutional Networks: A Deep Learning Framework for Traffic Forecasting. *Proceedings* *of the Twenty-Seventh International Joint Conference on Artificial Intelligence*, *IJCAI-18*, 3634–3640. https://doi.org/10.24963/ijcai.2018/505

Zare Moayedi, H., & Masnadi-Shirazi, M. A. (2008). Arima model for network traffic prediction and anomaly detection. *2008 International Symposium on Information Technology*, 1–6. https://doi.org/10.1109/ITSIM.2008.4631947

Zeng, W., Li, J., Quan, Z., & Lu, X. (2021). A Deep Graph-Embedded LSTM Neural Network Approach for Airport Delay Prediction. *JOURNAL OF ADVANCED TRANSPORTATION*, *2021*. https://doi.org/10.1155/2021/6638130

Zhang, S., Liu, X., Tang, J., Cheng, S., Qi, Y., & Wang, Y. (2018). Spatio-temporal modeling of destination choice behavior through the Bayesian hierarchical approach. *Physica A: Statistical Mechanics and Its Applications*, *512*, 537–551. https://doi.org/10.1016/j.physa.2018.08.034

Zhang, Y., Richter, A. R., Shanthikumar, J. G., & Shen, Z.-J. M. (2022). Dynamic Inventory Relocation in Disaster Relief†. *Production and Operations Management*, *31*(3), 1052–1070. https://doi.org/10.1111/poms.13594

Zhao, C., Li, X., Zuo, M., Mo, L., & Yang, C. (2022). Spatiotemporal dynamic network for regional maritime vessel flow prediction amid COVID-19. *Transport Policy*, *129*, 78–89. https://doi.org/10.1016/j.tranpol.2022.09.029

Zhao, H., Pan, Y., & Ding, Y. (2023). Traffic Prediction for New York City Based on Graph Neural Network. *2023 IEEE International Conference on Image*

Processing and Computer Applications (ICIPCA), 1655–1663. https://api.semanticscholar.org/CorpusID:262985558

Zhao, L., Song, Y., Zhang, C., Liu, Y., Wang, P., Lin, T., Deng, M., & Li, H. (2018). *T-GCN: A Temporal Graph ConvolutionalNetwork for Traffic Prediction*. https://doi.org/10.1109/TITS.2019.2935152

Zhao, L., Song, Y., Zhang, C., Liu, Y., Wang, P., Lin, T., Deng, M., & Li, H. (2020). T-GCN: A Temporal Graph Convolutional Network for Traffic Prediction. *IEEE Transactions on Intelligent Transportation Systems*, *21*(9), 3848–3858. https://doi.org/10.1109/TITS.2019.2935152

Zheng, A., & Casari, A. (2018). *Feature Engineering for Machine Learning: Principles and Techniques for Data Scientists* (1st ed.). O'Reilly Media, Inc.

Zheng, C., Fan, X., Wang, C., & Qi, J. (2020). GMAN: A Graph Multi-Attention Network for Traffic Prediction. *Proceedings of the AAAI Conference on Artificial Intelligence*, *34*(01), 1234–1241. https://doi.org/10.1609/aaai.v34i01.5477

Zhou, J., Cui, G., Zhang, Z., Yang, C., Liu, Z., & Sun, M. (2018). Graph Neural Networks: A Review of Methods and Applications. *ArXiv*, *abs/1812.08434*. https://api.semanticscholar.org/CorpusID:56517517

Zhu, H., Shou, T., Guo, R., Jiang, Z., Wang, Z., Wang, Z., Yu, Z., Zhang, W., Wang, C., & Chen, L. (2022). RedPacketBike: A Graph-Based Demand Modeling and Crowd-Driven Station Rebalancing Framework for Bike Sharing Systems.

IEEE Transactions on Mobile Computing. https://doi.org/10.1109/TMC.2022.3145979

Zhu, J., Song, Y., Zhao, L., & Li, H. (2020). *A3T-GCN: Attention Temporal Graph Convolutional Network for Traffic Forecasting*.