

How to Build a Graph-Based Deep Learning Architecture in Traffic Domain: A Survey

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Abstract—In recent years, various deep learning architectures have been proposed to solve complex challenges (e.g., spatial dependency, temporal dependency) in traffic domain, which have achieved satisfactory performance. These architectures are composed of multiple deep learning techniques in order to tackle various challenges in traffic data. Traditionally, convolution neural networks (CNNs) are utilized to model spatial dependency by decomposing the traffic network as grids. However, many traffic networks are graph-structured in nature. In order to utilize such spatial information fully, it's more appropriate to formulate traffic networks as graphs mathematically. Recently, various novel deep learning techniques have been developed to process graph data, called graph neural networks (GNNs). More and more works combine GNNs with other deep learning techniques to construct an architecture dealing with various challenges in a complex traffic task, where GNNs are responsible for extracting spatial correlations in traffic network. These graph-based architectures have achieved state-of-the-art performance. To provide a comprehensive and clear picture of such emerging trend, this survey carefully examines various graph-based deep learning architectures in many traffic applications. We first give guidelines to formulate a traffic problem based on graph and construct graphs from various traffic data. Then we decompose these graph-based architectures to discuss their shared deep learning techniques, clarifying the utilization of each technique in traffic tasks. What's more, we summarize common traffic challenges and the corresponding graph-based deep learning solutions to each challenge. Finally, we provide benchmark datasets, open source codes and future research directions in this rapidly growing field.

Index Terms—Graph Neural Networks, GNNs, Graph Convolution Network, GCN, Graph, Deep Learning, Traffic Forecasting, Traffic Domain, ITS

I. INTRODUCTION

ALONG with the acceleration of urbanization process, mass population is quickly gathering together towards cities. In many cities, especially those in developing countries, the rapidly increasing number of private vehicles and growing demand of public transport services in these cities are putting great pressure on their current transportation systems. The traffic problems such as frequent traffic jams, serious traffic accidents and long commute have seriously degraded the travel experience of passengers and decreased the operation

efficiency of cities. To address these challenges, many cities are committed to develop an Intelligent Transportation System (ITS) which can provide efficient traffic management, accurate traffic resources allocation and high-quality transportation service. ITS also aims to reduce the possibility of accidents, relieve traffic congestion and ensure public traffic security.

To construct an Intelligent Transportation System which makes cities smart, there are mainly two indispensable components, i.e., intelligent infrastructures and advanced algorithms.

On one hand, with the increasing investment in transportation infrastructures, there are more and more traffic equipments and systems, including loop detectors, probes, road cameras on road networks, GPS in taxis or buses, smart cards on subways and buses, automatic fare collection system and online ride-hailing system. These infrastructures are heterogeneous data sources and produce traffic data around-the-clock, like numeric data (e.g., GPS trajectories, traffic measurements), image/video data (e.g., vehicle images) and textual data (e.g., incident reports). These transportation data are enormous in volume and complicated in structure, containing complex traffic patterns (e.g., spatiotemporal dependency and high nonlinear dynamics). There is an urgent need to utilize more intelligent and powerful approaches to process these data.

On the other hand, in transportation domain, researchers have witnessed the algorithms evolving from statistic methods, to machine learning models and recently deep learning approaches. In the early stage, statistic methods including ARIMA and its variants [1], [2], VAR [3], Kalman filtering [4] were prevalent for that they have solid and widely accepted mathematical foundations. However, the linear and stationarity assumptions of these methods are violated by the highly non-linearity and dynamics in traffic data, resulting in poor performance in practice. Traditional machine learning approaches such as Support Vector Machine [5], K-Nearest Neighbors [6] can model non-linearity and more complex correlations in traffic data. However, the shallow architecture, manual feature selection and separated learning in these models are considered to be unsatisfactory in big data scenarios [7].

The breakthrough of deep learning in many domains, including computer vision, natural language process has attracted attention of transportation industry and research community. Deep learning techniques overcome the handcrafted feature engineering by providing an end-to-end learning from raw traffic data. The powerful capacities of deep learning techniques to approximate any complex function in theory can model more complicated patterns in various traffic networks. In recent years, due to the increasing computing (e.g., GPU) and a sufficient amount of traffic data [7], deep learning based

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techniques have been widely employed and achieved state-of-the-art performance in multiple traffic applications. The Recurrent neural networks (RNNs) and Convolutional neural networks (CNNs) based architectures used to be popular in extracting spatiotemporal dependencies. In these architectures, RNN or its variants are employed to extract the temporal correlations in traffic data [8]. CNNs are used to capture the spatial correlations in grid-based traffic network [9]. However, many traffic networks are graph-structured in nature, e.g., road network and subway network. The spatial features learned in CNN are not optimal for representing the traffic network with graph structure. Although some previous works have analyzed traffic problems in a graph view [10], [11], [12], these traditional approaches are not powerful enough to process big data and tackle complicated correlations in traffic network.

Recently, many researches have extended deep learning approaches on graph data to exploit graph structure information [13] and proposed a new group of neural networks called graph neural networks (GNNs) [14], [15], [16], aiming to address graph-related applications. GNNs have become the state-of-the-art approaches in many domains, including natural language process [17], computer vision [18], biology [19], recommendation system [20]. Since many traffic data are graph-structured, it is natural to incorporate GNNs into the deep learning architecture to capture the spatial dependency. Many related works have been produced during the last couple of years and more are on the road. Under this circumstance, a comprehensive literature review on these graph-based deep learning architectures in transportation domain would be very timely, which is exactly our work.

To our best knowledge, we are the first to provide a comprehensive survey on graph-based deep learning works in traffic domain. Note that some works we review actually work on similar traffic problems with similar techniques. Our work can help the upcoming researchers avoid repetitive works and focus on new solutions. What's more, the practical and clear guidance in this survey enables participators to apply these new emerging approaches in real-life traffic tasks quickly.

To sum up, the main contributions of this paper are as follows:

- We systematically outline traffic problems, related research directions and challenges in traffic domain, which can help related researchers to locate or expand their researches.
- We summarize a general formulation of spatiotemporal traffic problems and provide a specific guidance to construct graphs for several typical kinds of raw traffic datasets. Such thorough summarization is quite practical and can accelerate the applications of graph-based approaches in traffic domain.
- We provide the most comprehensive review over five types of deep learning techniques widely used in graph-based traffic works. We elaborate their theoretical aspects, advantages, limitations and variants in specific traffic tasks, which can inspire the following researchers to develop more novel models.
- We discuss four challenges shared by most graph-based traffic tasks. For each challenge, we conclude multiple

deep learning-based solutions and make the necessary comparison, which can be useful suggestions for model selection in traffic tasks.

- We collect benchmark datasets, open-source codes in related papers to facilitate baseline experiments in traffic domain. Finally, we propose future research directions.

The rest of this paper is organized as follows. Section II presents other surveys in traffic domain and overviews about graph neural networks. Section III briefly outlines several traffic problems and the corresponding research directions, challenges and solutions. Section IV summarizes a general formulation about traffic problems and the graph construction from traffic datasets. Section V analyzes the core functionality, advantages and defects of GNNs and other deep learning techniques, as well as examining the tricks to create novel variants of these techniques for specific traffic tasks. Section VI discusses common challenges in traffic domain and the corresponding multiple solutions. Section VII provides hyperlinks of open codes and datasets in papers we investigate. Section VIII presents future directions. Section IX concludes the paper.

II. RELATED WORK

On one hand, there have been some surveys summarizing the development process of algorithms used in traffic tasks from different perspectives. [21] discussed differences and similarities between statistical methods and neural networks to promote the comprehension between these two communities. [22] reviewed ten challenges on short-term traffic forecasting, which stemmed from the changing needs of ITS applications. [23] conducted a comprehensive overview of approaches in urban flow forecasting. [7] provided a classification of urban big data fusion methods based on deep learning (DL): DL-output-based fusion, DL-input-based fusion and DL-double-stage-based fusion. [24], [25] discussed deep learning for popular topics including traffic network representation, traffic flow forecasting, traffic signal control, automatic vehicle detection. [26] and [27] gave a similar but more elaborate analysis on new emerging deep learning models in multiple transportation applications. [28] provided a spatio-temporal perspective to summarize the deep learning techniques in traffic domain and other domains. However, all these surveys don't take graph neural networks (GNNs) related literatures into consideration, except that [28] mentioned GNNs but in a very short subsection.

On the other hand, in recent years, there are several reviews summarizing literatures w.r.t. GNNs in different aspects. [29] is the first to overview deep learning techniques on processing data in non-Euclidean space (e.g., graph data). [30] categorized GNNs by graph types, propagation types and training types and divided related applications into structural scenarios, non-structural scenarios, and other scenarios. [31] introduced GNNs based on small graph and giant graph respectively. [32], [33] focused on reviewing related works in a specific branch of GNNs, i.e., graph convolutional network (GCN). However, they seldom introduce GNNs works related with traffic scenarios. [34] is the only survey spending a paragraph to describe GNNs in traffic domain, which is obviously not enough for anyone desired to explore this field.

In summary, there still lacks a systematic and elaborated survey to explore the rapidly developed graph-based deep learning techniques in traffic domain recently. Our work aims to fill this gap and promote the understanding of the new emerging techniques in transportation community.

III. PROBLEMS, RESEARCH DIRECTIONS AND CHALLENGES

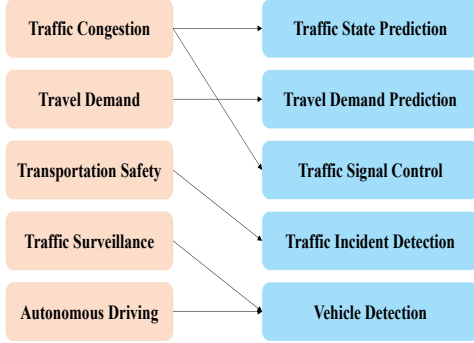


Fig. 1. Traffic problems and the corresponding research directions

In this section, we introduce background knowledge in traffic domain briefly, including some important traffic problems and research directions (as shown in Figure 1) as well as common challenges under these problems. On one hand, we believe that such a concise but systematic introduction can help readers understand this domain quickly. On the other hand, our survey shows that existing works related with graph-based deep learning techniques only cover part of these research directions, which inspires successors to transfer similar techniques to the remaining directions.

A. Traffic Problems

The goals that the transportation community aims to achieve include relieving traffic congestion, satisfying travel demand, enhancing traffic management, ensuring transportation safety and realizing automatic driving. Each problem under the corresponding traffic goal can be partitioned into several research directions and a direction can serve more than one problem.

1) **Traffic Congestion:** Traffic congestion [35] is one of the most important and urgent problems in modern cities in terms of significant time loss, air pollution and energy waste. The congestion can be solved by increasing the traffic efficiency, for example, to alleviate the traffic congestion on road network [36], [37], to control the road conditions by traffic state prediction [38], [39], to optimize vehicle flow by controlling traffic signals [40], [41].

2) **Travel Demand:** Travel demand refers to the demand of traffic services, such as taxi, bike, metro and bus. With the emerging of online ride-hailing platforms (e.g., Uber, DiDi) and rapid development of public transportation systems (e.g., metro system and bus system), travel demand prediction has become more and more important for transport authorities, business sectors and individuals. For related authorities, it can help to better allocate resources, e.g., increasing metro

frequency at rush hours, adding more buses to service hotspots. For business sector, it enables them to better manage taxi-hiring [42], carpooling [43], bike-sharing services [44], [45], and maximize their revenues. For individuals, it encourages users to consider various forms of transportation to decrease their commuting time and improve travel experience.

3) **Transportation Safety:** Transportation safety is an indispensable part of public safety. Traffic accidents can not only cause damage to victims, vehicles and road infrastructures, but also lead to traffic congestion and reduce efficiency of road network. Therefore, monitoring the traffic accidents is essential to avoid property loss and save life. Many researches focus on directions such as detecting traffic incidents [46], predicting traffic accidents from social media data [47], predicting the injury severity of traffic accidents [48], [49].

4) **Traffic Surveillance:** Nowadays, surveillance cameras have been widely deployed in city roads, generating numerous images and videos [27]. Such development has enhanced traffic surveillance, which includes traffic law enforcement, automatic toll collection [50] and traffic monitoring systems. The research directions of traffic surveillance include license plate detection [51], automatic vehicle detection [52], pedestrian detection [53].

5) **Autonomous Driving:** Along with the enhance of the vehicle's automation and development of motion-sensing technology, automatic driving vehicle has become a hot spot of technical research in transportation domain. Many tasks are related with visual recognition. The research directions of autonomous driving include lane and vehicle detection [54], pedestrian detection [55], traffic sign detection [56].

B. Research Directions

Our survey of graph-based deep learning in traffic domain shows that existing works focus mainly on two directions, i.e., traffic state prediction and passenger demand prediction. A few works focus on vehicle behavior classification [57], optimal DETC scheme [50], vehicle/human trajectory Prediction [58], [59], path availability [60], traffic signal control [61]. To our best knowledge, traffic incident detection and vehicle detection have not yet been explored based on a graph view.

1) **Traffic State Prediction:** Traffic state in literatures refers to traffic flow, traffic speed, travel time, traffic density and so on. Traffic flow prediction (TFP) [62], [63], Traffic speed prediction (TSP) [64], [65], Travel time prediction (TTP) [66], [67] are hot branches of traffic state prediction, which have attracted intensive studies.

2) **Travel Demand Prediction:** Travel demand prediction aims to estimate the future number of users who require traffic services, for example, to predict future taxi request in each area of a city [68], [69], or to predict the station-level passenger demand in subway system [70], [71], or to predict the bike hiring demand citywide [44], [45].

3) **Traffic Signal Control:** The traffic signal control is to properly control the traffic lights so as to reduce vehicle staying time at the intersections in the long run [25]. Traffic signal control [61] can optimize the traffic flow and reduce traffic congestion and emission.

4) **Traffic Incident Detection:** Major incidents can cause fatal injuries to travelers and long delays on a road network. Therefore, understanding the main cause of incidents and their impact on a traffic network is crucial for a modern transportation management system [46], [48], [49].

5) **Vehicle Detection:** Automatic vehicle detection aims to process videos or images recored by road cameras [27] to identify vehicles in possible regions [25].

C. Challenges Overview

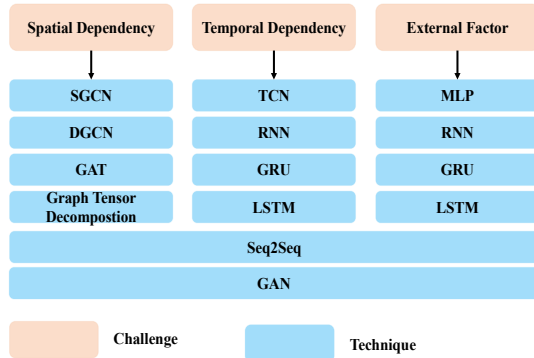


Fig. 2. Traffic challenges and the corresponding deep learning techniques

Although traffic problems and their research directions are different, they share the same challenges, e.g., spatial dependency, temporal dependency. For instance, to predict a traffic congestion in a region, its previous traffic conditions and the traffic conditions of its surrounding regions are important factors for prediction [35], [36], [37]. In vehicle trajectory prediction, the stochastic behaviors of surrounding vehicles and the historical information of self-trajectory influence the prediction performance [58]. When it comes to predict the ride-hailing demand in a region, its previous orders as well as orders in other regions with similar functionality are critical for prediction [72]. To predict the traffic signal, the geometric features of multiple intersections are taken into consideration as well as the previous traffic flow around [61]. In this paper, we summarize some common challenges as follow.

1) **Spatial Dependency:** Spatial dependency refers that the traffic condition of the target region is influenced by its surrounding regions or even distant regions. For example, the traffic speed of a road is affected by the traffic status of directly connected roads [73]. Another example is that the regions sharing similar functionality are likely to share similar pattern in traffic demand [68], [74].

2) **Temporal Dependency:** Temporal dependency refers that the traffic condition at a certain time is usually correlated with various historical observations [75]. For example, the traffic jam on a road at morning rush hours inevitably influences its flow during the following hours. Another example is that the flow of crowds in a region is affected by its own recent flow, weekly flow as well as periodical flow [76], [63], [77].

3) **External Factors:** Except the spatial data and temporal data, some types of data are highly related with traffic tasks, which are referred as external factors, such as holidays, weather conditions (e.g., rainfall, temperature, air quality),

events [78] and traffic incidents (e.g., incident time, incident type) [79]. The influence of external factors on traffic conditions can be observed in daily life. For instance, the traffic demand on holidays increases shapely compared with that at normal working days. A rainstorm absolutely decreases the traffic volume. A large-scale concert or football match results in traffic congregation, affecting traffic conditions around.

To tackle these challenges, various deep learning techniques have been proposed. For instance, convolution neural networks (CNNs) or graph neural networks (GNNs) are usually employed to model the spatial dependency on traffic network. Recurrent neural networks (RNNs) and temporal convolution network (TCN) are generally adopted to model the temporal dependency in traffic data. RNNs and MLPs are typically utilized in processing external factors. These techniques along with other tricks (e.g., gated mechanism, attention mechanism) are combined organically to form architectures which can address multiple challenges in traffic tasks. According to the way modeling spatial dependency, these deep learning architectures can be divided into grid-based architectures utilizing CNNs and graph-based architectures adopting GNNs. Recent works have shown that graph-based architectures can achieve better performance than grid-based architectures, for that most traffic networks are graph-structured and GNNs can extract such graph topology more accurately.

In this paper, we focus on graph-based deep learning architectures. We aim to provide readers guidance about how to build a graph-based deep learning architecture and we have investigated enormous existing traffic works which provide graph-based deep learning solutions. In the following sections, we first introduce a common way to formulate the traffic problem and give detailed guidelines to build a traffic graph from traffic data. Then we clarify the correlations between challenges and techniques (as shown in Figure 2) in two perspectives, i.e., the techniques perspective and the challenges perspective. In the techniques perspective, we introduce several common techniques and interpret the way how they tackle challenges in traffic tasks. In the challenges perspective, we elaborate each challenge and summarize the techniques which can tackle this challenge. In a word, we hope to provide insights into solving traffic problems with deep learning techniques based on a graph view.

IV. PROBLEM FORMULATION AND GRAPH CONSTRUCTION

Among the graph-based deep learning traffic literatures we investigate, the majority of tasks (more than 80%) focus on spatio-temporal forecasting problems, especially traffic state prediction and travel demand prediction. In this section, we first list commonly used notations. Then we summarize a general formulation of graph-based spatio-temporal prediction in traffic domain, and provide the details to construct graphs from various traffic datasets. Finally, we discuss multiple definitions of adjacency matrix, which represents the graph topology of traffic network and is the key element of graph-based solutions.

TABLE I
NOTATIONS IN THIS PAPER

Graph related elements	
\mathbf{G}	Graph
\mathbf{E}	Edges of graph \mathbf{G}
\mathbf{V}	Vertices of graph \mathbf{G}
$\mathbf{A} \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	Adjacency matrix of graph \mathbf{G}
$\mathbf{A}^T \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	The transpose matrix of \mathbf{A}
$\hat{\mathbf{A}} \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	Equal to $\mathbf{A} + \mathbf{I}_{\mathbf{N}}$, a self-looped \mathbf{A}
$\mathbf{D} \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	The degree matrix of adjacency matrix \mathbf{A}
$\mathbf{D}_I \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	The in-degree matrix of adjacency matrix \mathbf{A}
$\mathbf{D}_O \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	The out-degree matrix of adjacency matrix \mathbf{A}
$\mathbf{L} \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	Laplacian matrix of graph \mathbf{G}
$\mathbf{U} \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	The eigenvectors matrix of \mathbf{L}
$\Lambda \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	The diagonal eigenvalues matrix of \mathbf{L}
λ_{max}	The max eigenvalue of \mathbf{L}
$\mathbf{I}_{\mathbf{N}} \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$	An identity matrix
Hyper parameters	
\mathbf{N}	The number of nodes in graph \mathbf{G}
\mathbf{F}_I	The number of input features
\mathbf{F}_H	The number of hidden features
\mathbf{F}_O	The number of output features
\mathbf{P}	The number of past time slices
\mathbf{Q}	The number of future time slices
d	The dilation rate
Trainable parameters	
W, b, θ, ϕ	The trainable parameters
Θ	The kernel
Activation functions	
$\rho(\cdot)$	The activation function, e.g., tanh, sigmoid, ReLU
$\sigma(\cdot) \in [0, 1]$	The sigmoid function
$\tanh(\cdot) \in [-1, 1]$	The hyperbolic tangent function
$\text{ReLU}(\cdot) \in [0, x]$	The ReLU function
Operations	
$\ast_{\mathbf{G}}$	The convolution operator on graph
\odot	Element-wise multiplication
\cdot	Matrix multiplication
Spatial variables	
$\mathbf{X} \in \mathbb{R}^{\mathbf{N} \times \mathbf{F}_I}$	An input graph composed of \mathbf{N} nodes with \mathbf{F}_I features
$X_j \in \mathbb{R}^{\mathbf{N}}$	The j^{th} feature of an input graph
$\mathbf{X}^i \in \mathbb{R}^{\mathbf{F}_I}$	Node i in an input graph
$x \in \mathbb{R}^{\mathbf{N}}$	A simply input graph
$\mathbf{Y} \in \mathbb{R}^{\mathbf{N} \times \mathbf{F}_O}$	An output graph composed of \mathbf{N} nodes with \mathbf{F}_O features
$Y_j \in \mathbb{R}^{\mathbf{N}}$	The j^{th} feature of an output graph
$\mathbf{Y}^i \in \mathbb{R}^{\mathbf{F}_O}$	Node i in an output graph
$y \in \mathbb{R}^{\mathbf{N}}$	A simply output graph
Temporal variables	
$\mathbf{X} \in \mathbb{R}^{\mathbf{P} \times \mathbf{F}_I}$	A sequential input with \mathbf{F}_I features over \mathbf{P} time slices
$\mathbf{X}_t \in \mathbb{R}^{\mathbf{F}_I}$	The element of sequential input at time t
$\mathbf{x} \in \mathbb{R}^{\mathbf{P}}$	A simply sequential input over \mathbf{P} time slices
$\mathbf{x}_t \in \mathbb{R}$	The element of simply sequential input at time t
$\mathbf{H}_t \in \mathbb{R}^{\mathbf{F}_H}$	A hidden state with \mathbf{F}_H features at time t
$\mathbf{Y} \in \mathbb{R}^{\mathbf{P} \times \mathbf{F}_O}$	A sequential output with \mathbf{F}_O features over \mathbf{P} time slices
$\mathbf{Y}_t \in \mathbb{R}^{\mathbf{F}_O}$	The element of sequential output at time t
$\mathbf{y} \in \mathbb{R}^{\mathbf{P}}$	A simply sequential output over \mathbf{P} time slices
$\mathbf{y}_t \in \mathbb{R}$	The element of simply sequential output at time t
Spatiotemporal variables	
$\mathcal{X} \in \mathbb{R}^{\mathbf{P} \times \mathbf{N} \times \mathbf{F}_I}$	A series of input graphs composed of \mathbf{N} nodes with \mathbf{F}_I features over \mathbf{P} time slices
$\mathcal{X}_t \in \mathbb{R}^{\mathbf{N} \times \mathbf{F}_I}$	An input graph at time t
$\mathcal{X}_t^i \in \mathbb{R}^{\mathbf{F}_I}$	node i in an input graph at time t
$\mathcal{X}_{t,j} \in \mathbb{R}^{\mathbf{N}}$	the j^{th} feature of an input graph at time t
$\mathcal{X}_{t,i}^j \in \mathbb{R}$	the j^{th} feature of node i in an input graph at time t
$\mathcal{Y} \in \mathbb{R}^{\mathbf{P} \times \mathbf{N} \times \mathbf{F}_O}$	A series of output graphs composed of \mathbf{N} nodes with \mathbf{F}_O features over \mathbf{P} time slices
$\mathcal{Y}_t \in \mathbb{R}^{\mathbf{N} \times \mathbf{F}_O}$	An output graph at time t
$\mathcal{Y}_t^i \in \mathbb{R}^{\mathbf{F}_O}$	node i in an output graph at time t
$\mathcal{Y}_{t,j} \in \mathbb{R}^{\mathbf{N}}$	the j^{th} feature of an output graph at time t
$\mathcal{Y}_{t,i}^j \in \mathbb{R}$	the j^{th} feature of node i in an output graph at time t

A. Notations

In this section, we have denoted some commonly used notations, including graph related elements, variables, parameters (hyper or trainable), activation functions, and operations. The variables are comprised of input variables $\{x, X, \mathbf{x}, \mathbf{X}, \mathcal{X}\}$ and output variables $\{y, Y, \mathbf{y}, \mathbf{Y}, \mathcal{Y}\}$. These variables can be divided into three groups. The first group is composed of spatial variables which only represent spatial attributes.

The second group is composed of temporal variables only representing temporal attributes. The last group is composed of spatiotemporal variables which represent both spatial and temporal features.

B. Graph-based Spatiotemporal Forecasting

To our best knowledge, most existing graph-based deep learning traffic works are primarily about spatio-temporal forecasting. They formalize their prediction problems in a very similar way despite of different mathematical notations and representations. We summarize their works to provide a general formulation for graph-based spatio-temporal problems in traffic domain.

The traffic network is represented as a graph $\mathbf{G} = (\mathbf{V}, \mathbf{E}, \mathbf{A})$, which can be weighted [80], [66], [62] or unweighted [60], [73], [81], directed [60], [82], [83] or undirected, [63], [84], depending on specific tasks. \mathbf{V} is a set of nodes and $|\mathbf{V}| = \mathbf{N}$ refers \mathbf{N} nodes in the graph. Each node represents a traffic object, which can be a sensor [64], [63], [85], a road segment [80], [86], [87], a road intersection [66], [82], or even an GPS intersection [62]. \mathbf{E} is a set of edges referring the connectivity between nodes.

$\mathbf{A} = (\mathbf{a}_{ij})_{\mathbf{N} \times \mathbf{N}} \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$ is the adjacency matrix containing the topology information of the traffic network, which is valuable for traffic prediction. The entry \mathbf{a}_{ij} in matrix \mathbf{A} represents the node proximity and is different among various applications. It can be a binary value 0 or 1 [63], [73], [81]. Specifically, 0 indicates no edge between node i and node j while 1 indicates an edge between these two nodes. It can also be a float value representing some kind of relationship between nodes [80], [74], e.g., the road distance between two sensors [64], [76], [83].

$\mathcal{X}_t = [\mathcal{X}_t^1, \dots, \mathcal{X}_t^i, \dots, \mathcal{X}_t^{\mathbf{N}}] \in \mathbb{R}^{\mathbf{N} \times \mathbf{F}_I}$ is a feature matrix of the whole graph at time t . $\mathcal{X}_t^i \in \mathbb{R}^{\mathbf{F}_I}$ represents node i with \mathbf{F}_I features at time t . The features are usually traffic indicators, such as traffic flow [84], [83], traffic speed [64], [86], [82], or rail-hail orders [72], [74], passenger flow [70], [71]. Usually, continuous indicators are normalized during data preprocessing phase.

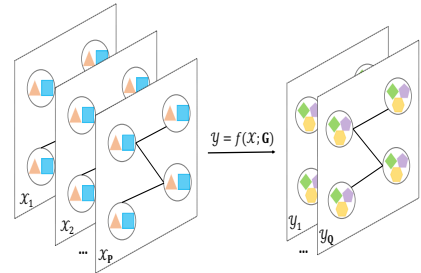


Fig. 3. The graph-based spatiotemporal problem formulation in traffic domain

Given historical indicators of the whole traffic network over past \mathbf{P} time slices, denoted as $\mathcal{X} = [\mathcal{X}_1, \dots, \mathcal{X}_i, \dots, \mathcal{X}_P] \in \mathbb{R}^{\mathbf{P} \times \mathbf{N} \times \mathbf{F}_I}$, the spatio-temporal forecasting problem in traffic domain aims to predict the future traffic indicators over the next \mathbf{Q} time slices, denoted as $\mathcal{Y} = [\mathcal{Y}_1, \dots, \mathcal{Y}_j, \dots, \mathcal{Y}_Q] \in \mathbb{R}^{\mathbf{Q} \times \mathbf{N} \times \mathbf{F}_O}$, where $\mathcal{Y}_t \in \mathbb{R}^{\mathbf{N} \times \mathbf{F}_O}$ represents output graph with

\mathbf{F}_O features at time t . The problem (as shown in Figure 3) can be formulated as follow:

$$\mathcal{Y} = f(\mathcal{X}; \mathbf{G}) \quad (1)$$

Some works predict multiple traffic indicators in the future (i.e., $\mathbf{F}_O > 1$) while other works predict one traffic indicator (i.e., $\mathbf{F}_O = 1$), such as traffic speed [86], [82], rail-hold orders [72], [74]. Some works only consider one-step prediction [88], [68], [50], i.e., forecasting traffic conditions in the next time step and $\mathbf{Q} = 1$. But models designed for one-step prediction can't be directly applied to predict multiple steps, because they are optimized by reducing error during the training stage for the next-step instead of the subsequent time steps [69]. Many works focus on multi-step forecasting (i.e., $\mathbf{Q} > 1$) [89], [39], [90]. According to our survey, there are mainly three kinds of techniques to generate a multi-step output, i.e., FC layer, Seq2Seq, dilation technique. Fully connected (FC) layer is the simplest technique as being the output layer to obtain a desired output shape [64], [63], [91], [73], [79], [92]. Some works adopt the Sequence to Sequence (Seq2Seq) architecture with a RNNs based decoder to generate output recursively through multiple steps [93], [85], [94], [89], [95], [83]. [76], [90] adopted dilation technique to get a desired output length.

In addition, some works not only consider traffic related measurements, but also take external factors (e.g., time attributes, weather) [64], [77], [79], [96] into consideration. Therefore, the problem formulation becomes:

$$\mathcal{Y} = f(\mathcal{X}, \mathcal{E}; \mathbf{G}) \quad (2)$$

Where \mathcal{E} is the external factors.

C. Graph Construction from Traffic Datasets

To model a traffic network as a graph is vital for any works that intend to utilize graph-based deep learning architectures. Although many works share a similar formulation of problem, they are different in graph construction due to the different traffic datasets they collect. We divide these datasets into four categories according to related traffic infrastructures: data collected by the sensors deployed on road network [64], [63], [65], vehicle GPS trajectories [62], [75], [82], orders of rail-hailing system [74], [69], [96], transaction records of subway [70], [71] or bus system [75]. For each category, we describe the datasets and explain the construction of nodes \mathbf{V} , edges \mathbf{E} , feature matrix \mathcal{X}_i in traffic graph \mathbf{G} .

1) **Sensors Datasets:** Traffic measurements (e.g., traffic speed) are generally collected during a short time interval by the sensors (e.g., loop detectors, probes) on a road network in metropolises like Beijing [80], California [65], Los Angeles [64], New York [86], Philadelphia [91], Seattle [81], Xiamen [85], and Washington [91]. Sensor datasets are the most prevalent datasets in existing works, specially PEMS dataset from California. Generally, a road network contains traffic objects such as sensors, road segments (shown in Figure 4). Some existing works construct a sensor graph [64], [63], [83] while others construct a road segment graph [80], [86], [91].

2) **GPS Datasets:** GPS trajectories datasets are usually generated by numbers of taxis over some period of time in a city, e.g., Beijing [62], Chengdu [62], Shenzhen [73], Cologne [82], and Chicago [87]. Each taxi produces substantial GPS records with time, location, speed information every day. Every GPS record is fitted to its nearest road on the city road map. All roads are divided into multiple road segments through road intersections. Some works extract a road segment graph [87], [73] while others extract a road intersection graph [66], [62], [82] (shown in Figure 4).

3) **Rail-hailing Datasets:** These datasets record car/taxi/bicycle demand orders over a period of time in cities like Beijing [72], [74], Chengdu [74], and Shanghai [72]. The target city with an OpenStreetMap is divided into equal-size grid-based regions. Each region is defined as a node in a graph. The feature of each node is the number of orders in its region during a given interval. [72], [74] observed that various correlations between nodes were valuable for prediction and multiple graphs were constructed (as shown in Figure 5).

4) **Transactions Datasets:** These datasets are collected by automatic fare collection (AFC) system deployed in public transit network, from which a subway graph [70], [71], [75] or a bus graph [75] can be constructed.

A subway graph: Each station in the subway system is treated as a node. If two stations of a metro line are adjacent, there is an edge between them and vice versa. The features of a station usually contain the number of passenger departing at the station and the number of passenger arriving at the station during a given time interval based on transaction records collected by AFC systems, which logs when each passenger enters and leaves a metro system.

A bus graph: Each bus stop is treated as a node. If two bus stops in a bus line are adjacent, there is an edge between them and vice versa. The features of a bus stop usually contain the number of departing passengers at the station during a given time interval, but not the number of arriving passengers, since most bus AFC systems only logs the boarding record of each passenger.

D. Adjacency Matrix

The adjacency matrix $\mathbf{A} = (\mathbf{a}_{ij})_{\mathbf{N} \times \mathbf{N}} \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}$ is the key element to extract traffic graph topology which is valuable for prediction. Element \mathbf{a}_{ij} (binary or weighted) represents heterogeneous pairwise relationship between nodes. However, based on different assumptions in traffic scenarios, the matrix can be designed in a very different way, like fixed matrix and dynamic matrix.

1) **Fixed Matrix:** Many works assume that the correlations between nodes are fixed based on some prior knowledge and don't change over time. Therefore, a fixed matrix is designed and unchanged during the whole experiment. In addition, some works extract multiple relationships between nodes, thus resulting in multiple fixed matrices [59], [45]. Generally, the pre-defined matrix represents spatial dependency in traffic network while in some works it also captures other kinds of correlations, like function similarity and transportation connectivity [72], semantic connection [74], temporal similarity [65].

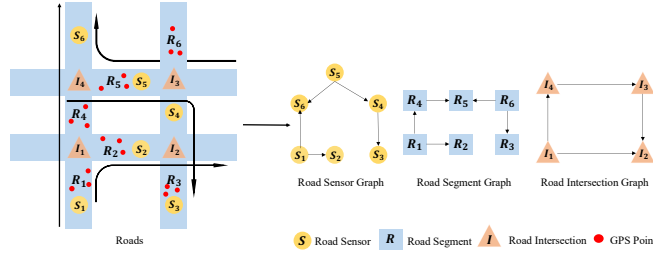


Fig. 4. Graph construction from traffic datasets: 1) In a sensor graph, sensor represents node and there is an edge between adjacent sensors on the same side of road. The features of a sensor are the traffic measurements corrected by itself. 2) In a road segment graph, road segment represents node and two connected segments have an edge. In sensors datasets, the features of a road segment are the average traffic measurements (e.g., traffic speed) recorded by all the sensors on it. In GPS datasets, the features of each road segment are the average traffic measurements recorded by all the GPS points on it. 3) In a road intersection graph, road intersection represents node and two road intersection connected by a road segment have an edge. The features of a road section are sum-up of the traffic measurements through it. Most works consider the edge direction being the traffic flow direction [64], [85], [60], [83], [62], [75], while some works ignore the direction and construct an undirected graph [63], [76], [81] [87], [82].

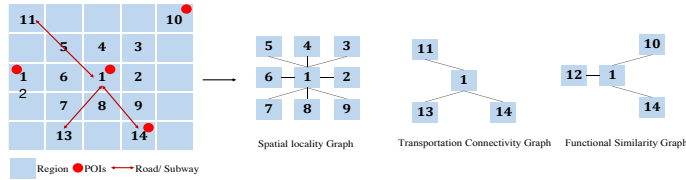


Fig. 5. Multi-relationships: 1) A spatial locality graph: This graph is based on spatial proximity and it constructs edges between a region and its 8 adjacent regions in a 3 x 3 grid. 2) A transportation connectivity graph: This graph assumes that geographically distant but conveniently reachable regions by motorway, highway or subway have strong correlations with the target region. There should be edges between them. 3) A functional similarity graph: This graph assumes that regions sharing similar functionality might have similar demand patterns. Edges are constructed between regions with similar surrounding POIs.

As to the entry value \mathbf{a}_{ij} , it is defined as 1 (connection) or 0 (disconnection) in some works [63], [91], [73], [81]. In many other works, it is defined as a function of distance between nodes [66], [62], [87], [84], [69], [82]. They used threshold Gaussian Kernel to define \mathbf{a}_{ij} as follow:

$$\mathbf{a}_{ij} = \begin{cases} \exp\left(-\frac{\mathbf{d}_{ij}^2}{\sigma^2}\right), & i \neq j \text{ and } \mathbf{d}_{ij} \geq \epsilon \\ 0, & i = j \text{ or } \mathbf{d}_{ij} < \epsilon \end{cases} \quad (3)$$

Where \mathbf{d}_{ij} is the distance between node i and node j . Hyper parameters σ^2 and ϵ are thresholds to control the distribution and sparsity of matrix \mathbf{A} .

2) **Dynamic Matrix:** Some works argue that the pre-defined matrix does not necessarily reflect the true dependency among nodes due to the defective prior knowledge or incomplete data [66]. A novel adaptive matrix is proposed and learned through node embedding. Experiments in [76], [66], [86] have proven that adaptive matrix can precisely capture the hidden spatial dependency more precisely in traffic data.

In some scenarios, the graph structure can evolve over time as some edges may become unavailable, like road congestion or closure, and become available again after alleviating congestion. An evolving topological structure [60] is incorporated into the model to capture such dynamic spatial change.

V. DEEP LEARNING TECHNIQUES PERSPECTIVE

We summarize the graph-based deep learning architectures in existing traffic literatures and find that most of them are composed of graph neural networks (GNNs) and other modules, such as recurrent neural networks (RNNs), temporal convolution network (TCN), Sequence to Sequence (Seq2Seq) model, generative adversarial network (GAN) (as shown in

Table II). It is the cooperation of GNNs and other deep learning techniques that achieves state-of-the-art performance in many traffic scenarios. This section aims to introduce their principles, advantages, defects and their variants in traffic tasks, to help participants understand how to utilize deep learning techniques in traffic domain.

A. GNNs

In the last couple of years, motivated by the huge success of deep learning approaches (e.g., CNNs, RNNs), there is an increasing interest in generalizing neural networks to arbitrarily structured graphs and such networks are classified as graph neural networks. Many works focus on extending the convolution of CNN for graph data and novel convolutions on graph have been developed rapidly. The two mainstream graph convolutions related with traffic tasks are spectral graph convolution (SGC) for undirected graph, diffusion graph convolution (DGC) for directed graph. There are also other novel convolutions [62] but the related traffic works are relatively few. Both SGC and DGC aim to generate new feature representations for each node in a graph through feature aggregation and non-linear transformation (as shown in Figure 6). Note that we refer the SGC network as SGCN and DGC network as DGCN.

1) **Spectral Graph Convolution:** In the spectral theory, a graph is represented by its corresponding normalized Laplacian matrix $\mathbf{L} = \mathbf{I}_N - \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}} \in \mathbb{R}^{N \times N}$. The real symmetric matrix \mathbf{L} can be diagonalized via eigendecomposition as $\mathbf{L} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^T$ where $\mathbf{U} \in \mathbb{R}^{N \times N}$ is the eigenvectors matrix and $\mathbf{\Lambda} \in \mathbb{R}^{N \times N}$ is the diagonal eigenvalues matrix. Since \mathbf{U} is also an orthogonal matrix, [103] adopted it as a graph

TABLE II
THE DECOMPOSITION OF GRAPH-BASED DEEP LEARNING ARCHITECTURES INVESTIGATED IN THIS PAPER

Reference	Year	Directions	Models	Modules
[59]	2018	Human Trajectory Prediction		SGCN
[50]	2019	Optimal DETC scheme		SGCN
[57]	2020	Vehicle Behaviour Classification	MR-GCN	SGCN, LSTM
[58]	2020	Vehicle Trajectory Prediction		SGCN, LSTM
[61]	2018	Traffic signal control		SGCN, Reinforcement learning
[60]	2019	Path availability	LRGCN-SAPE	SGCN, LSTM
[66]	2019	Travel time prediction		SGCN
[62]	2018	Traffic Flow Prediction	KW-GCN	SGCN, LCN
[84]	2018	Traffic Flow Prediction	Graph-CNN	CNN, Graph Matrix
[97]	2018	Traffic Flow Prediction	DST-GCNN	SGCN
[63]	2019	Traffic Flow Prediction		SGCN, CNN, Attention Mechanism
[75]	2019	Traffic Flow Prediction		SGCN, TCN, Residual
[94]	2019	Traffic Flow Prediction	GHCNN	SGCN, GRU, Seq2Seq
[89]	2019	Traffic Flow Prediction	STGSA	GAT, GRU, Seq2Seq
[83]	2019	Traffic Flow Prediction	DCRNN-RIL	DGCN, GRU, Seq2Seq
[98]	2019	Traffic Flow Prediction	MVGCN	SGCN, FNN, Gate Mechanism, Residual
[99]	2019	Traffic Flow Prediction	STGI- ResNet	SGCN, Residual
[100]	2020	Traffic Flow Prediction	FlowConvGRU	DGCN, GRU
[101]	2018	Traffic Speed Prediction		GAT, GRU, Gate Mechanism
[64]	2019	Traffic Speed Prediction	GTCN	SGCN, TCN, Residual
[65]	2019	Traffic Speed Prediction	3D-TGCN	SGCN, Gate Mechanism
[79]	2019	Traffic Speed Prediction	DIGC-Net	SGCN, LSTM
[102]	2019	Traffic Speed Prediction	MW-TGC	SGCN, LSTM
[95]	2019	Traffic Speed Prediction	AGC-Seq2Seq	SGCN, GRU, Seq2Seq, Attention Mechanism
[82]	2019	Traffic Speed Prediction	GCGA	SGCN, GAN
[92]	2019	Traffic Speed Prediction	ST-GAT	GAT, LSTM
[80]	2018	traffic state prediction	STGCN	SGCN, TCN, Gate Mechanism
[93]	2018	traffic state prediction	DCRNN	DGCN, GRU, Seq2Seq
[86]	2019	traffic state prediction		SGCN, CNN, Gate Mechanism
[77]	2019	traffic state prediction	MRes-RGNN	DGCN, GRU, Residual, Gate Mechanism
[87]	2019	traffic state prediction	GCGAN	DGCN, LSTM, GAN, Seq2Seq, Attention Mechanism
[76]	2019	traffic state prediction	Graph WaveNet	DGCN, TCN, Residual, Gate Mechanism
[73]	2019	traffic state prediction	T-GCN	SGCN, GRU
[81]	2019	traffic state prediction	TGC-LSTM	SGCN, LSTM
[38]	2019	traffic state prediction	DualGraph	Seq2Seq, MLP, Graph Matirx
[90]	2019	traffic state prediction	ST-UNet	SGCN, GRU
[85]	2020	traffic state prediction	GMAN	GAT, Gate Mechanism, Seq2Seq, Attention Mechanism
[91]	2020	traffic state prediction	OGCRNN	SGCN, GRU, Attention Mechanism
[39]	2020	traffic state prediction	MRA-BGCN	SGCN, GRU, Seq2Seq, Attention Mechanism
[44]	2018	Travel Demand-bike		SGCN, LSTM, Seq2Seq
[45]	2018	Travel Demand-bike	GCNN-DDGF	SGCN, LSTM
[70]	2020	Travel Demand-subway	PVCGN	SGCN, GRU, Seq2Seq, Attention Mechanism
[71]	2019	Travel Demand-subway	WDGTC	Tensor Completion, Graph Matrix
[72]	2019	Travel Demand-taxi	CGRNN	SGCN, RNN, Attention Mechanism, Gate Mechanism
[74]	2019	Travel Demand-taxi	GEML	SGCN, LSTM
[68]	2019	Travel Demand-taxi	MGCN	SGCN
[69]	2019	Travel Demand-taxi	STG2Seq	SGCN, Seq2Seq, Attention Mechanism, Gate Mechanism, Residual
[96]	2019	Travel Demand-taxi		SGCN, LSTM, Seq2Seq
[88]	2019	Travel Demand-taxi	ST-ED-RMGC	SGCN, LSTM, Seq2Seq, Residual

Fourier basis, defining graph Fourier transform of a graph signal $x \in \mathbb{R}^N$ as $\hat{x} = \mathbf{U}^T x$, and its inverse as $x = \mathbf{U} \hat{x}$.

[104] tried to build an analogue of CNN convolution into spectral domain and defined the spectral convolution as $y = \Theta *_{\mathcal{G}} x = \mathbf{U} \Theta \mathbf{U}^T x$, i.e., transforming x into spectral domain, adjusting its amplitude by a diagonal kernel $\Theta = \text{diag}(\theta_0, \dots, \theta_{N-1}) \in \mathbb{R}^{N \times N}$, and doing inverse Fourier transform to get the final result y in spatial domain. Although such convolution is theoretically guaranteed, it is computationally expensive as multiplication with \mathbf{U} is $\mathcal{O}(N^2)$ and the eigendecomposition of \mathbf{L} is intolerable for large scale graphs. In addition, it considers all nodes by the kernel Θ with N parameters and can't extract spatial localization.

To avoid such limitations, [105] localized the convolution and reduced its parameters by restricting the kernel Θ to be a polynomial of eigenvalues matrix Λ as $\Theta = \sum_{k=0}^{K-1} \theta_k \Lambda^k$ and K determines the maximum radius of the convolution from a central node. Thus, the convolution can be rewritten

as $\Theta *_{\mathcal{G}} x = \sum_{k=0}^{K-1} \theta_k \mathbf{U} \Lambda^k \mathbf{U}^T x = \sum_{k=0}^{K-1} \theta_k \mathbf{L}^k x$. Furthermore, [105] adopted the Chebyshev polynomials $T_k(x)$ to approximate \mathbf{L}^k , resulting in $\Theta *_{\mathcal{G}} x \approx \sum_{k=0}^{K-1} \theta_k T_k(\tilde{\mathbf{L}}) x$ with a rescaled $\tilde{\mathbf{L}} = \frac{2}{\lambda_{\max}} \mathbf{L} - \mathbf{I}_N$, λ_{\max} being the largest eigenvalue of \mathbf{L} and $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$, $T_0(x) = 1$, $T_1(x) = x$ [106]. By recursively computing $T_k(x)$, the complexity of this K -localized convolution can be reduced to $\mathcal{O}(K|\mathbf{E}|)$ with $|\mathbf{E}|$ being the number of edges.

Based on [105], [107] simplified the spectral graph convolution by limiting $K = 2$ and with $T_0(\tilde{\mathbf{L}}) = 1$, $T_1(\tilde{\mathbf{L}}) = \tilde{\mathbf{L}}$, they got $\Theta *_{\mathcal{G}} x \approx \theta_0 T_0(\tilde{\mathbf{L}}) x + \theta_1 T_1(\tilde{\mathbf{L}}) x = \theta_0 x + \theta_1 \tilde{\mathbf{L}} x$. Noticing that $\tilde{\mathbf{L}} = \frac{2}{\lambda_{\max}} \mathbf{L} - \mathbf{D}$, they set $\lambda_{\max} = 2$, resulting in $\Theta *_{\mathcal{G}} x \approx \theta_0 x + \theta_1 (\mathbf{L} - \mathbf{D}) x$. For that $\mathbf{L} = \mathbf{I}_N - \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}$ and $\mathbf{L} - \mathbf{I}_N = -\mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}$, they got $\Theta *_{\mathcal{G}} x \approx \theta_0 x - \theta_1 (\mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}) x$. Further, they reduced the number of parameters by setting $\theta = \theta_0 = -\theta_1$ to address overfitting and got $\Theta *_{\mathcal{G}} x \approx \theta (\mathbf{I}_N + \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}) x$. They further defined $\mathbf{A} = \mathbf{A} + \mathbf{I}_N$ and adopted a renormalization trick to get $y = \Theta *_{\mathcal{G}} x \approx \theta \tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \mathbf{D}^{-\frac{1}{2}} x$, where $\tilde{\mathbf{D}}$ is the

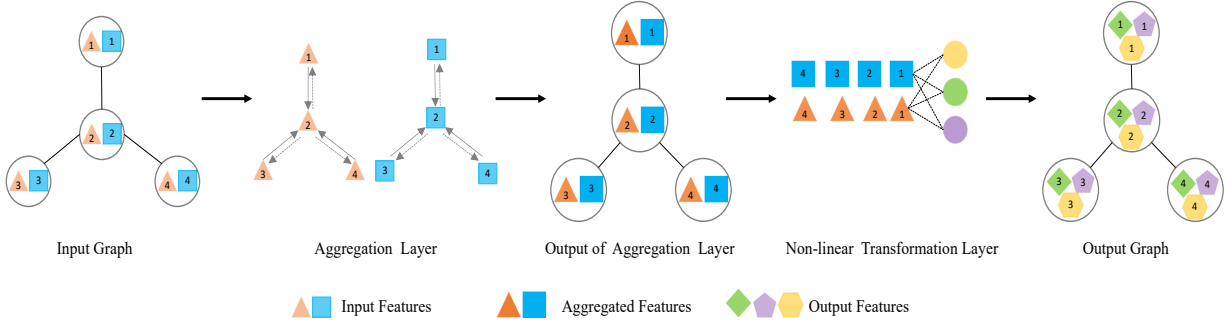


Fig. 6. A general structure of Graph Neural Networks is composed of two kind of layers: 1) Aggregation layer: On each feature dimension, the features of adjacent nodes are aggregated to the central node. Mathematically, the output of aggregation layer is the product of adjacency matrix and features matrix. 2) Non-linear transformation layer: subsequently, all the aggregated features of each node are fed into the non-linear transformation layer to create higher feature representation. All nodes share the same transformation kernel.

degree matrix of $\tilde{\mathbf{A}}$. Finally, [107] proposed a spectral graph convolution layer as:

$$Y_j = \rho(\Theta_j *_{\mathcal{G}} X) = \rho\left(\sum_{i=1}^{\mathbf{F}_I} \theta_{i,j} \tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} X_i\right), 1 \leq j \leq \mathbf{F}_O \quad (4)$$

$$Y = \rho(\tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} X W)$$

Here, $X \in \mathbb{R}^{\mathbf{N} \times \mathbf{F}_I}$ is the layer input with \mathbf{F}_I features, $X_i \in \mathbb{R}^{\mathbf{N}}$ is its i^{th} feature. $Y \in \mathbb{R}^{\mathbf{N} \times \mathbf{F}_O}$ is the layer output, $Y_j \in \mathbb{R}^{\mathbf{N}}$ is its j^{th} feature. $W \in \mathbb{R}^{\mathbf{F}_I \times \mathbf{F}_O}$ is a trainable parameter. $\rho = (\cdot)$ is the activation function. Such layer can aggregate information of 1-hop neighbors. The receptive neighborhood field can be expanded by stacking multiple graph convolution layers [39].

2) **Diffusion Graph Convolution:** Spectral graph convolution requires a symmetric Laplacian matrix to implement eigendecomposition. It becomes invalid for a directed graph with an asymmetric Laplacian matrix. Diffusion convolution originates from graph diffusion without any constraint on graph. Graph diffusion [108], [109] can be represented as a transition matrix power series giving the probability of jumping from node i to node j at each step. After many steps, such Markov process converges to a stationary distribution $\mathcal{P} = \sum_{k=0}^{\infty} \alpha(1-\alpha)^k (\mathbf{D}_O^{-1} \mathbf{A})^k$, where $\mathbf{D}_O^{-1} \mathbf{A}$ is the transition matrix and $\alpha \in [0, 1]$ is the restart probability, k is the diffusion step. In practice, a finite \mathbf{K} -step truncation of the diffusion process is adopted and each step is assigned a trainable weight θ . Based on the \mathbf{K} -step diffusion process, [93] defined diffusion graph convolution as:

$$y = \Theta *_{\mathcal{G}} x = \sum_{k=0}^{\mathbf{K}-1} (\theta_{k,1} (\mathbf{D}_O^{-1} \mathbf{A})^k + \theta_{k,2} (\mathbf{D}_I^{-1} \mathbf{A}^T)^k) x \quad (5)$$

Here, $\mathbf{D}_O^{-1} \mathbf{A}$ and $\mathbf{D}_I^{-1} \mathbf{A}^T$ represent the transition matrices and its reverse one respectively. Such bidirectional diffusion enables the operation to capture the spatial correlation on a directed graph [93]. Similar to spectral graph convolution layer, a diffusion graph convolutional layer is built as follow:

$$Y_j = \rho\left(\sum_{k=0}^{\mathbf{K}-1} \sum_{i=1}^{\mathbf{F}_I} (\theta_{k,1} (\mathbf{D}_O^{-1} \mathbf{A})^k + \theta_{k,2} (\mathbf{D}_I^{-1} \mathbf{A}^T)^k) X_i\right), 1 \leq j \leq \mathbf{F}_O$$

$$Y = \rho\left(\sum_{k=0}^{\mathbf{K}-1} (\mathbf{D}_O^{-1} \mathbf{A})^k X W_{k1} + (\mathbf{D}_I^{-1} \mathbf{A}^T)^k X W_{k2}\right) \quad (6)$$

Where parameters $W_{k1}, W_{k2} \in \mathbb{R}^{\mathbf{F}_I \times \mathbf{F}_O}$ are trainable.

3) **GNNs in Traffic Domain:** Traffic networks are graph structure naturally (See Section IV). Compared with previous studies modeling traffic network as grids [110], [111], the works modeling traffic network as graph can fully utilize spatial information.

By now, many works employ convolution operation directly on traffic graph to capture the complex spatial dependency of traffic data. Most of them adopt spectral graph convolution (SGC) while some employ diffusion graph convolution (DGC) [77], [93], [87], [76], [83], [100]. There are also some other graph neural networks such as graph attention network (GAT) [101], [92], [85], [89], tensor decomposition and completion on graph [71], but their related works are few, which might be a future research direction.

The key difference between SGC and DGC lies in their matrices which represent different assumptions on the spatial correlations of traffic network. The adjacency matrix in SGC infers that a central node in a graph has more strong correlation to its direct adjacent nodes than other distant ones, which reflects reality in many traffic scenarios [72], [64]. The state transition matrix in DGC indicates that the spatial dependency is stochastic and dynamic instead of being fixed and regular. The traffic flow is related to a diffusion process on a traffic graph to model its changing spatial correlations. In addition, the bidirectional diffusion in DGC offers the model more flexibility to capture the influence from both upstream and downstream traffic [93]. In a word, DGC is more complicated than SGC. DGC can be adopted in any traffic network graph while SGC can be only utilized to process symmetric traffic graph.

Existing graph convolution theories are mainly applied on 2-D tensor $X \in \mathbb{R}^{\mathbf{N} \times \mathbf{F}_I}$. However, the traffic data with both spatial and temporal attributes are usually 3-D tensor $\mathcal{X} \in \mathbb{R}^{\mathbf{P} \times \mathbf{N} \times \mathbf{F}_I}$. The convolution operations need to be further generalized to 3-D tensor. [80], [64], [75], [97] imposed equal convolution operation (e.g., SGC, DGC) with the same kernel on each time step of \mathcal{X} in parallel.

In order to enhance the performance of graph convolution in traffic tasks, many works develop various variants of SGC.

For instance, [63] redefined SGC with attention mechanism to adaptively capture the dynamic correlations in traffic network: $\Theta *_{\mathcal{G}} x \approx \sum_{k=0}^{\mathbf{K}-1} \theta_k (T_k(\tilde{\mathbf{L}}) \odot \mathbf{S}) x$, where $\mathbf{S} =$

$W_1 \odot \rho((XW_2)W_3(W_4X)^T + b) \in \mathbb{R}^{N \times N}$ is the spatial attention.

[65] generalized SGC on both spatial and temporal dimensions by scanning K order neighbors on graph and K_t neighbors on time-axis without padding which shortens the length of sequences by $K_t - 1$ at each step:

$$\mathcal{Y}_{t,j} = \rho\left(\sum_{t'=0}^{K_t-1} \sum_{k=0}^{K-1} \sum_{i=1}^{F_I} \theta_{j,t',k,i} \tilde{\mathbf{L}}^k \mathcal{X}_{t-t',i}\right) \quad (7)$$

Where $\mathcal{X}_{t-t',i} \in \mathbb{R}^N$ is the i^{th} feature of input \mathcal{X} at time $t-t'$, $\mathcal{Y}_{t,j} \in \mathbb{R}^N$ is the j^{th} feature of output \mathcal{Y} at time t .

[81] changed SGC as $\Theta *_{\mathcal{G}} x = (W \odot \tilde{\mathbf{A}}^K \odot \mathcal{F}\mathcal{F}\mathcal{R})x$, where $\tilde{\mathbf{A}}^K$ is the K -hop neighborhood matrix and $\mathcal{F}\mathcal{F}\mathcal{R}$ is a matrix representing physical properties of roadways. [102], [95] followed this work and redefined $\Theta *_{\mathcal{G}} x = (W \odot Bi(\mathbf{A}^K + \mathbf{I}_N))x$, where $Bi(\cdot)$ is a function clipping each nonzero element in matrix to 1.

[98] modified adjacency matrix \mathbf{A} in SGC as $\mathbf{S} = \mathbf{A} \odot \omega$ to integrate the geospatial positions information into the model and ω is a matrix calculated via a thresholded Gaussian kernel weighting function. The layer is built as $Y = \rho(\tilde{\mathbf{Q}}^{-\frac{1}{2}} \tilde{\mathbf{S}} \tilde{\mathbf{Q}}^{-\frac{1}{2}} XW)$, where $\tilde{\mathbf{Q}}$ is the degree matrix of $\tilde{\mathbf{S}} = \mathbf{S} + \mathbf{I}_N$.

[50] designed a novel edge-based SGC on road network to extract the spatiotemporal correlations of the edge features. Both the feature matrix X and adjacency matrix \mathbf{A} are defined on edges instead of nodes.

B. RNNs

Recurrent Neural Networks (RNNs) are a type of neural network architecture which is mainly used to detect patterns in a sequence of data [112]. The traffic data collected in many traffic tasks are time series data, thus RNNs are commonly utilized in these traffic literatures to capture the temporal dependency in traffic data. In this subsection, we introduce three classical models of RNNs (i.e., RNN, LSTM, GRU) and the correlations among them, which provides theoretical evidence for participators to choose appropriate model for specific traffic problem.

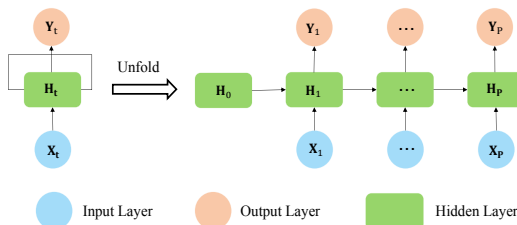


Fig. 7. The folded and unfolded structure of recurrent neural networks

1) **RNN**: Similar to a classical Feedforward Neural Network (FNN), a simple recurrent neural network (RNN) [113] contains three layers, i.e., input layer, hidden layer, output layer [114]. What differentiates RNN from FNN is the hidden layer. It passes information forward to the output layer in FNN while in RNN, it also transmits information back into itself forming a cycle [112]. For this reason, the hidden layer in RNN is called recurrent hidden layer. Such cycling trick can

retain historical information, enabling RNN to process time series data.

Suppose there are \mathbf{F}_I , \mathbf{F}_H , \mathbf{F}_O units in the input, hidden, output layer of RNN respectively. The input layer takes time series data $\mathbf{X} = [\mathbf{X}_1, \dots, \mathbf{X}_P] \in \mathbb{R}^{P \times F_I}$ in. For each element $\mathbf{X}_t \in \mathbb{R}^{F_I}$ at time t , the hidden layer transforms it to $\mathbf{H}_t \in \mathbb{R}^{F_H}$ and the output layer maps \mathbf{H}_t to $\mathbf{Y}_t \in \mathbb{R}^{F_O}$. Note that the hidden layer not only takes \mathbf{X}_t as input but also takes \mathbf{H}_{t-1} as input. Such cycling mechanism enables RNN to memorize the past information (as shown in Figure 7). The mathematical notations of hidden layer and output layer are as follow.

$$\begin{aligned} \mathbf{H}_t &= \tanh([\mathbf{H}_{t-1}, \mathbf{X}_t] \cdot W_h + b_h) \\ \mathbf{Y}_t &= \rho(\mathbf{H}_t \cdot W_y + b_y) \end{aligned} \quad (8)$$

Where $W_h \in \mathbb{R}^{(F_I+F_H) \times F_H}$, $W_y \in \mathbb{R}^{F_H \times F_O}$, $b_h \in \mathbb{R}^{F_H}$, $b_y \in \mathbb{R}^{F_O}$ are trainable parameters. $t = 1, \dots, P$ and P is the input sequence length. \mathbf{H}_0 is initialized using small non-zero elements which can improve overall performance and stability of the network [115].

In a word, RNN takes sequential data as input and generate another sequence with the same length: $[\mathbf{X}_1, \dots, \mathbf{X}_P] \xrightarrow{RNN} [\mathbf{Y}_1, \dots, \mathbf{Y}_P]$. Note that we can deepen RNN through stacking multiple recurrent hidden layers.

2) **LSTM**: Although the hidden state enables RNN to memorize the input information over past time steps, it also introduces matrix multiplication over the (potentially very long) sequence. Small values in its matrix multiplication causes the gradient decrease at each time step, resulting in the final vanish phenomenon and oppositely big values leads to exploding problem [116]. The exploding or vanishing gradients actually hinder the capacity of RNN to learn long term sequential dependencies in data [114].

To overcome this hurdle, Long Short-Term Memory (LSTM) neural networks [117] are proposed to capture long-term dependency in sequence learning. Compared with hidden layer in RNN, LSTM hidden layer has extra four parts, which are a memory cell, input gate, forget gate, and output gate. These three gates ranging in $[0,1]$ can control information flow into the memory cell and preserve the extracted features from previous time steps. These simple changes enable the memory cell to store and read as much long-term information as possible. The mathematical notations of LSTM hidden layer are as follow.

$$\begin{aligned} i_t &= \sigma([\mathbf{H}_{t-1}, \mathbf{X}_t] \cdot W_i + b_i) \\ o_t &= \sigma([\mathbf{H}_{t-1}, \mathbf{X}_t] \cdot W_o + b_o) \\ f_t &= \sigma([\mathbf{H}_{t-1}, \mathbf{X}_t] \cdot W_f + b_f) \\ \mathbf{C}_t &= f_t \odot \mathbf{C}_{t-1} + i_t \odot \tanh([\mathbf{H}_{t-1}, \mathbf{X}_t] \cdot W_c + b_c) \\ \mathbf{H}_t &= o_t \odot \tanh(\mathbf{C}_t) \end{aligned} \quad (9)$$

Where i_t , o_t , f_t is the input gate, output gate, forget gate at time t respectively. \mathbf{C}_t is the memory cell at time t .

3) **GRU**: While LSTM is a viable option for avoiding vanishing or exploding gradients, its complex structure leads to more memory requirement and longer training time. [118] proposed a simple yet powerful variant of LSTM, i.e., Gated Recurrent Units (GRU). The LSTM cell has three gates, but the GRU cell only has two gates, resulting in fewer parameters thus shorter training time. However, GRU is equally effective

as LSTM empirically [118] and is widely used in various tasks. The mathematical notations of GRU hidden layer are as follow.

$$\begin{aligned} r_t &= \sigma([\mathbf{H}_{t-1}, \mathbf{X}_t] \cdot W_r + b_r) \\ u_t &= \sigma([\mathbf{H}_{t-1}, \mathbf{X}_t] \cdot W_u + b_u) \\ \tilde{\mathbf{H}}_t &= \tanh(r_t \odot [\mathbf{H}_{t-1}, \mathbf{X}_t] \cdot W_h + b_h) \\ \mathbf{H}_t &= u_t \odot \mathbf{H}_{t-1} + (1 - u_t) \odot \tilde{\mathbf{H}}_t \end{aligned} \quad (10)$$

Where r_t is the reset gate, u_t is the update gate.

4) **RNNs in Traffic Domain:** RNNs have shown impressive stability and capability of processing time series data. Since traffic data has a distinct temporal dependency, RNNs are usually leveraged to capture temporal correlation in traffic data. Among the works we survey, only [72] utilized RNN to capture temporal dependency in traffic while more than a half adopted GRU and some employed LSTM. This can be explained that RNN survives severe gradient disappearance or gradient explosion while LSTM and GRU handle this successfully and GRU can faster the training time.

In addition, there are many tricks to augment RNNs capacity to model the complex temporal dynamics in traffic domain, such as attention mechanism, gating mechanism, residual mechanism.

For instance, [72] incorporated the contextual information (i.e., output of SGCN containing information of related regions) into an attention operation to model the correlations between observations in different timestamps: $z = F_{pool}(\mathbf{X}_t, SGCN(\mathbf{X}_t))$ and $S = \sigma(W_1 ReLU(W_2 z))$, $\mathbf{H}_t = RNN([\mathbf{H}_{t-1}, \mathbf{X}_t] \odot S)$, where $F_{pool}(\cdot)$ is a global average pooling layer, $RNN(\cdot)$ denotes the RNN hidden layer.

[77] took external factors into consideration by embedding external attributes into the input. In addition, they added the previous hidden states to the next hidden states through a residual shortcut path, which they believed can make GRU more sensitive and robust to sudden changes in traffic historical observations. The new hidden state is formulated as: $\mathbf{H}_t = GRU([\mathbf{H}_{t-1}, \mathbf{X}_t], \mathbf{E}_t) + \mathbf{H}_{t-1}W$, where \mathbf{E}_t is the external features at time t , W is linear trainable parameter, $\mathbf{H}_{t-1}W$ is the residual shortcut.

[90] inserted a dilated skip connection into GRU by changing hidden state from $\mathbf{H}_t = GRU([\mathbf{H}_{t-1}, \mathbf{X}_t])$ to $\mathbf{H}_t = GRU(\mathbf{H}_{t-s}, \mathbf{X}_t)$, where s refers to skip length or dilation rate of each layer, $GRU(\cdot)$ denotes the GRU hidden layer. Such hierarchical design of dilation brings in multiple temporal scales for recurrent units at different layers which achieves multi-timescale modeling.

Despite the tricks above, some works replace the matrix multiplication in RNNs' hidden layer with spectral graph convolution (SGC) or diffusion graph convolution (DGC), to capture spatio-temporal correlations jointly. Take GRU as example:

$$\begin{aligned} r_t &= \sigma([\mathbf{H}_{t-1}, \mathbf{X}_t] *_{\mathcal{G}} W_r + b_r) \\ u_t &= \sigma([\mathbf{H}_{t-1}, \mathbf{X}_t] *_{\mathcal{G}} W_u + b_u) \\ \tilde{\mathbf{H}}_t &= \tanh(r_t \odot [\mathbf{H}_{t-1}, \mathbf{X}_t] *_{\mathcal{G}} W_h + b_h) \\ \mathbf{H}_t &= u_t \odot \mathbf{H}_{t-1} + (1 - u_t) \odot \tilde{\mathbf{H}}_t \end{aligned} \quad (11)$$

The $*_{\mathcal{G}}$ can represent SGC, DGC or other variants. In the literatures we survey, most replacements happen in GRU and only one in LSTM [60]. Among GRU related traffic works,

[77], [93], [91], [83], [100] replaced matrix multiplication with DGC, [39], [90], [70] with SGC, [89], [101] with GAT.

Note that besides RNNs, other techniques (e.g., TCN in the next subsection) are also popular choices to extract the temporal dynamics in traffic tasks.

C. TCN

Although RNN-based models become widespread in time-series analysis, RNNs for traffic prediction still suffer from time-consuming iteration, complex gate mechanism, and slow response to dynamic changes [80]. On the contrary, 1D-CNN has the superiority of fast training, simple structures, and no dependency constraints to previous steps [119]. However, 1D-CNN is less common than RNNs in practice due to its lack of memory for a long sequence [120]. In 2016, [121] proposed a novel convolution operation integrating causal convolution and dilated convolution, which outperforms RNNs in text-to-speech tasks. The prediction of causal convolution depends on previous elements but not future elements. Dilated convolution expands the receptive field of original filter by dilating it with zeros [122]. [123] simplified the causal dilated convolution in [121] for sequence modeling problem and renamed it as temporal convolution network (TCN). Recently, more and more works employ TCN to process traffic sequential data [80], [64], [76], [75].

1) **Sequence Modeling and 1-D TCN:** Given an input sequence with length \mathbf{P} denoted as $\mathbf{x} = [\mathbf{x}_1, \dots, \mathbf{x}_{\mathbf{P}}] \in \mathbb{R}^{\mathbf{P}}$, sequence modeling aims to generate an output sequence with the same length, denoted as $\mathbf{y} = [\mathbf{y}_1, \dots, \mathbf{y}_{\mathbf{P}}] \in \mathbb{R}^{\mathbf{P}}$. The key assumption is that the output at current time \mathbf{y}_t is only related to historical data $[\mathbf{x}_1, \dots, \mathbf{x}_t]$ but not depends on any future inputs $[\mathbf{x}_{t+1}, \dots, \mathbf{x}_{\mathbf{P}}]$, i.e., $\mathbf{y}_t = f(\mathbf{x}_1, \dots, \mathbf{x}_t)$, f is the mapping function.

Obviously, RNN, LSTM and GRU can be solutions to sequence modeling tasks. However, TCN can tackle sequence modeling problem more efficient than RNNs for that it can capture long sequence properly in a non-recursive manner. The dilated causal convolution in TCN is formulated as follow:

$$\mathbf{y}_t = \Theta *_{\mathcal{T}d} \mathbf{x}_t = \sum_{k=0}^{\mathbf{K}-1} w_k \mathbf{x}_{t-dk} \quad (12)$$

Where $*_{\mathcal{T}d}$ is the dilated causal operator with dilation rate d controlling the skipping distance, $\Theta = [w_0, \dots, w_{\mathbf{K}-1}] \in \mathbb{R}^{\mathbf{K}}$ is the kernel. Zero padding strategy is utilized to keep the output length the same as the input length (as shown in Figure 8). Without padding, the output length is shortened by $(\mathbf{K} - 1)d$ [80].

To enlarge the receptive field, TCN stacks multiple dilated causal convolution layers with $d = 2^l$ as the dilation rate of l^{th} layer (as shown in Figure 8). Therefore, the receptive field in the network grows exponentially without requiring many convolutional layers or larger filter, which can handle longer sequence with less layers and save computation resources [76].

2) **TCN in Traffic Domain:** There are many traffic works related with sequence modeling, especially traffic spatio-temporal forecasting tasks. Compared with RNNs, the non-recursive calculation manner enables TCN to alleviate the

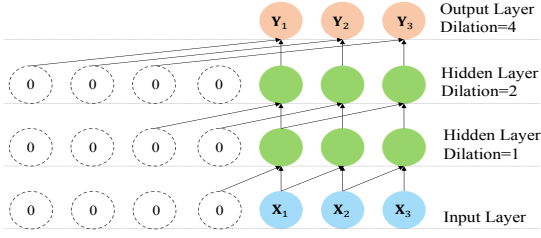


Fig. 8. Multiple dilated causal convolution layers in TCN: $[x_1, x_2, x_3]$ is the input sequence and $[y_1, y_2, y_3]$ is the output sequence with the same length. The size of kernel is 2 and the dilation rates for layers are $[1, 2, 4]$. Zero padding strategy is taken.

gradient explosion problem and facilitate the training by parallel computation. Therefore, some works adopt TCN to capture the temporal dependency in traffic data.

Most graph-based traffic data are 3-D tensors denoted as $\mathcal{X} \in \mathbb{R}^{P \times N \times F_I}$, which requires the generalization of 1-D TCN to 3-D variables. The dilated causal convolution can be adopted to produce the j^{th} output feature of node i at time t as follow [64]:

$$\mathcal{Y}_{t,j}^i = \rho(\Theta_j *_{\mathcal{T}^d} \mathcal{X}_t^i) = \rho\left(\sum_{m=1}^{F_I} \sum_{k=0}^{K-1} w_{j,m,k} \mathcal{X}_{t-dk,m}^i\right), 1 \leq j \leq F_O \quad (13)$$

Where $\mathcal{Y}_{t,j}^i \in \mathbb{R}$ is the j^{th} output feature of node i at time t . $\mathcal{X}_{t-dk,m}^i \in \mathbb{R}$ is the m^{th} input feature of node i at time $t-dk$. The kernel $\Theta_j \in \mathbb{R}^{K \times F_I}$ is trainable. F_O is the number of output features.

The same convolution kernel is applied to all nodes on the traffic network and each node produces F_O new features. The mathematical formulation of l layer is as follow [64], [75]:

$$\mathcal{Y} = \Theta *_{\mathcal{T}^d} \mathcal{X} \quad (14)$$

where $\mathcal{X} \in \mathbb{R}^{P \times N \times F_I}$ represents the historical observations of the whole traffic network over past P time slices, $\Theta \in \mathbb{R}^{K \times F_I \times F_O}$ represents the related convolution kernel, $\mathcal{Y} \in \mathbb{R}^{P \times N \times F_O}$ is the output of TCN layer.

There are some tricks to enhance the performance of TCN in specific traffic tasks. For instance, [75] stacked multiple TCN layers to extract the short-term neighboring dependencies by bottom layer and long-term temporal features by higher layer:

$$\mathcal{Y}^{(l+1)} = \sigma(\Theta^l *_{\mathcal{T}^{d^l}} \mathcal{Y}^{(l)}) \quad (15)$$

Where $\mathcal{Y}^{(l)}$ is the input of l^{th} layer, $\mathcal{Y}^{(l+1)}$ is its output and $\mathcal{Y}^{(0)} = \mathcal{X}$. $d^l = 2^l$ is the dilation rate of l^{th} layer.

To reduce the complexity of model training, [64] constructed a residual block containing two TCN layers with the same dilation rate and the block input was added to last TCN layer to get the block output:

$$\mathcal{Y}^{(l+1)} = \mathcal{Y}^{(l)} + \text{ReLU}(\Theta_1^l *_{\mathcal{T}^d} (\text{ReLU}(\Theta_0^l *_{\mathcal{T}^d} \mathcal{Y}^{(l)}))) \quad (16)$$

where Θ_1^l, Θ_0^l are the convolution kernels of the first layer and the second layer respectively. $\mathcal{Y}^{(l)}$ is the input of residual block and $\mathcal{Y}^{(l+1)}$ is its output.

[76] integrated gating mechanism [120] with TCN to learn complex temporal dependency in traffic data:

$$\mathcal{Y} = \rho(\Theta_1 *_{\mathcal{T}^d} \mathcal{X} + b_1) \odot \sigma(\Theta_2 *_{\mathcal{T}^d} \mathcal{X} + b_2) \quad (17)$$

Where $\sigma(\cdot) \in [0, 1]$ determines the ratio of information passed to the next layer.

Similarly, [80] used the Gated TCN and set the dilation rate $d = 1$ without zero padding to shorten the output length as $\mathcal{Y} = (\Theta_1 *_{\mathcal{T}^1} \mathcal{X}) \odot \sigma(\Theta_2 *_{\mathcal{T}^1} \mathcal{X})$. They argued that this can discover variances in time series traffic data.

D. Seq2Seq

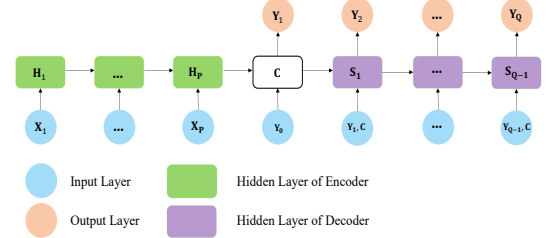


Fig. 9. Sequence to Sequence Structure without attention mechanism

1) **Seq2Seq**: Sequence to Sequence (Seq2Seq) model proposed in 2014 [124] has been widely used in sequence prediction such as machine translation [125]. Seq2Seq architecture consists of two components, i.e., an encoder in charge of converting the input sequence \mathbf{X} into a fixed latent vector \mathbf{C} , and a decoder responsible for converting \mathbf{C} into an output sequence \mathbf{Y} . Note that \mathbf{X} and \mathbf{Y} can have different lengths (as shown in Figure 9).

$$\mathbf{X} = [X_1, \dots, X_P] \xrightarrow{\text{Seq2Seq}} \mathbf{Y} = [Y_1, \dots, Y_Q] \quad (18)$$

Where P is the input length and Q is the output length.

The specific calculation of \mathbf{Y}_j is denoted as follow:

$$\begin{aligned} \mathbf{H}_i &= \text{Encoder}(X_i, \mathbf{H}_{i-1}) \\ \mathbf{C} &= \mathbf{H}_P, \mathbf{S}_0 = \mathbf{H}_P \\ \mathbf{S}_j &= \text{Decoder}(\mathbf{C}, Y_{j-1}, \mathbf{S}_{j-1}) \\ \mathbf{Y}_j &= \mathbf{S}_j W \end{aligned} \quad (19)$$

Here, \mathbf{H}_i is the hidden state related with input X_i . \mathbf{H}_0 is initialized using small non-zero elements. \mathbf{S}_j is the hidden state related with output Y_j . Y_0 is the representation of beginning sign. Note that the encoder and decoder can be any model as long as it can accept sequence (vector or matrix) and produce sequence, such as RNN, LSTM, GRU or other novel models.

A major limitation of Seq2Seq is that the latent vector \mathbf{C} is fixed for each Y_j while Y_j might have stronger correlation with X_j than other elements. To address this issue, attention mechanism is integrated into Seq2Seq, allowing the decoder to focus on task-relevant parts of the input sequence, helping the decoder make better decision.

$$\begin{aligned} \mathbf{H}_i &= \text{Encoder}(X_i, \mathbf{H}_{i-1}) \\ \mathbf{C}_j &= \sum_{i=1}^P (\theta_{ji} \mathbf{H}_i), \mathbf{S}_0 = \mathbf{H}_P \\ \mathbf{S}_j &= \text{Decoder}(\mathbf{C}_j, Y_{j-1}, \mathbf{S}_{j-1}) \\ \mathbf{Y}_j &= \mathbf{S}_j W \end{aligned} \quad (20)$$

Where $\theta_{ji} = \frac{\exp(f_{ji})}{\sum_{k=1}^P \exp(f_{jk})}$ is the normalized attention score, and $f_{ji} = f(\mathbf{H}_j, \mathbf{S}_{i-1})$ [125] is a function to measure the

correlation between i^{th} input and j^{th} output, for instance, [126] proposed three kinds of attention score calculation.

$$f_{ji} = \begin{cases} \mathbf{H}_j^T \mathbf{S}_{i-1} & \text{dot} \\ \mathbf{H}_j^T \mathbf{W}_a \mathbf{S}_{i-1} & \text{general} \\ \mathbf{v}_a^T \tanh(\mathbf{W}_a [\mathbf{H}_j, \mathbf{S}_{i-1}]) & \text{concat} \end{cases} \quad (21)$$

Another way to enhance Seq2Seq performance is the scheduled sampling technique [127]. The inputs of decoder during training and testing phases are different. Decoder during training phase is fed with true labels of training datasets while it is fed with predictions generated by itself during testing phase, which accumulates error at testing time and causes degraded performance. To mitigate this issue, scheduled sampling is integrated into the model. At j^{th} iteration during the training process, there is ϵ_j probability to feed the decoder with true label and $1-\epsilon_j$ probability with prediction at the previous step. Probability ϵ_j gradually decreases to 0, allowing the decoder to learn the testing distribution [93], keeping the training and testing as same as possible.

2) **Seq2Seq in Traffic Domain:** Since Seq2Seq can take an input sequence to generate an output sequence with different length, it is applied on multi-step prediction in many traffic works. The encoder encodes the historical traffic data into a latent space vector. Then, the latent vector is fed into a decoder to generate the future traffic conditions.

Attention mechanism is usually incorporated into Seq2Seq to model the different influence on future prediction from previous traffic observations at different time slots [87], [85], [95], [69].

The encoder and decoder in many traffic literatures are in charge of capturing spatio-temporal dependencies. For instance, [93] proposed DCGRU to be the encoder and decoder, which can capture spatial and temporal dynamics jointly. The design of encoder and decoder is usually the core contribution and novel part of relative papers. But the encoder and decoder are not necessarily the same and we have made a summarization of Seq2Seq structure in previous graph-based traffic works (as shown in Table III).

TABLE III
THE ENCODERS AND DECODERS OF SEQUENCE TO SEQUENCE ARCHITECTURE

References	Encoder	Decoder
[93]	GRU+DGCN	Same as encoder
[87]	SGCN+LSTM	LSTM+SGCN
[85]	STAtt Block	Same as encoder
[38]	MLPs	An MLP
[94]	SGCN+Pooling+GRU	GCN+Upooling+GRU
[89]	GRU with graph self-attention	Same as encoder
[39]	GRU+SGCN	Same as encoder
[95]	SGCN+ bidirectional GRU	Same as encoder
[69]	Long-term encoder (Gated SGCN)	Short-term encoder
[96]	SGCN+LSTM	LSTM
[83]	SGCN+GRU	Same as encoder
[70]	CGRM (GRU, SGCN)	Same as encoder
[88]	LSTM+RGC	RGC
[44]	LSTM	Same as encoder

Noted that the RNNs based decoder has a severe error accumulation problem during testing inference due to that each previous predicted step is the input to produce the next step prediction. [93], [89] adopted the scheduled sampling to alleviate this problem. [69] replaced the RNNs based decoder

with a short-term and long-term decoder to take in last step prediction exclusively, thus easing error accumulation. The utilization of Seq2Seq technique in traffic domain is very flexible, for instance, [87] integrated Seq2Seq into a bigger framework, being the generator and discriminator of GAN.

E. GAN

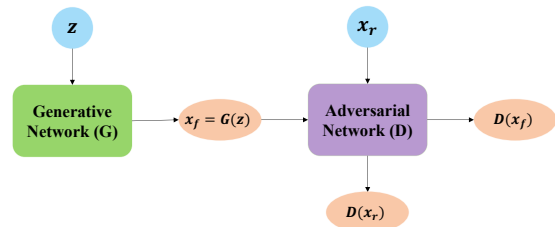


Fig. 10. Generative Adversarial Network: Generator G is in charge of producing a generated sample $x_f = G(z)$ from a random vector z , which is sampled from a prior distribution p_z . Discriminator D is in charge of discriminating between the fake sample x_f generated from G and the real sample x_r from the training data.

1) **GAN:** Generative Adversarial Network (GAN) [128] is a powerful deep generative model aiming to generate artificial samples as indistinguishable as possible from their real counterparts. GAN, inspired by game theory, is composed of two players, a generative neural network called Generator G and an adversarial network called Discriminator D (as shown in Figure 10).

Discriminator D tries to determine whether the input samples belong to the generated data or the real data while Generator G tries to cheat on Discriminator D by producing samples as true as possible. The two mutually adversarial and optimized processes are alternately trained, which strengthens the performance of both D and G . When the fake sample produced by G is very close to the ground truth and D is unable to distinguish them any more, it is considered that Generator G has learned the true distribution of the real data and the model converges. At this time, we can consider this game to reach a Nash equilibrium.

Mathematically, such process can be formulated to minimize their losses $Loss_G$ and $Loss_D$. With the loss function being cross entropy denoted as f , we can have:

$$\begin{aligned} Loss_G &= f(D(G(z)), 1) = - \sum \log D(G(z)) \\ \phi^* &= \underset{\phi}{\operatorname{argmin}}(Loss_G) = \underset{\phi}{\operatorname{argmax}}(-Loss_G) \\ &= \underset{\phi}{\operatorname{argmax}} \mathbb{E}(\log D(G(z))) \end{aligned} \quad (22)$$

$$\begin{aligned} Loss_D &= f(D(x_r), 1, D(x_f), 0) \\ &= - \sum \log D(x_r) - \sum \log(1 - D(x_f)) \\ \theta^* &= \underset{\theta}{\operatorname{argmin}}(Loss_D) = \underset{\theta}{\operatorname{argmax}}(-Loss_D) \\ &= \underset{\theta}{\operatorname{argmax}}(\mathbb{E}(\log D(x_r) + \log(1 - D(x_f)))) \end{aligned} \quad (23)$$

Where 1 is the label of true sample x_r . 0 is the label of fake sample $x_f = G(z)$. ϕ and θ are the trainable parameters of G and D respectively. Note that when G is trained, D is untrainable. Interested readers may refer to [129], [130] for survey of GAN.

2) **GAN in Traffic Domain**: When GAN is applied in traffic prediction tasks [131], [132], Generator G is usually employed to generate future traffic observations based on the historical observations. Then the generated data and the future real data are fed into Discriminator D to train it. After the training, Generator G can learn the distribution of the real traffic flow data through a large number of historical data and can be used to predict the future traffic states [87]. GAN can be also utilized to solve the sparsity problem of traffic data for its efficacy in handling data generation [82].

In addition, the generator or discriminator of GAN can be any model, such as RNNs, Seq2Seq, depending on the specific traffic tasks.

VI. CHALLENGES PERSPECTIVE

Traffic tasks are very challenging due to the complicated spatial dependency, temporal dependency in traffic data. In addition, external factors such as holiday or event can also affect the traffic conditions. In this section, we introduce four common challenges in traffic domain. We carefully examine each challenge and its corresponding solutions, making necessary comparison.

A. Spatial Dependency

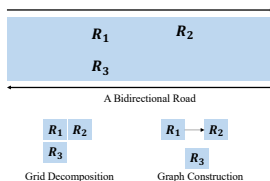


Fig. 11. The formulation of a bidirectional road: The traffic condition of road R_1 is only influenced by the same side road R_2 and has weak correlation with the opposite side road R_3 . But if this region is modeled as grids, R_3 has similar impact on R_1 as R_2 , which is against the truth. If it is model as a graph, R_1 is connected with R_2 and disconnected with R_3 , which can reflect the true relationship.

As mentioned in previous section, some literatures [110], [111], [133] extracted spatial features through decomposing the whole traffic network into grids and then employing CNNs to process the grid-based data. However, the grid-based assumption actually violates the nature topology of traffic network. Because many traffic networks are physically organized as a graph and the graph topology information is obviously valuable for traffic prediction (as shown in Figure 11). Therefore, graph neural networks can model spatial dependencies in traffic networks much better than grid based approaches. There are several kinds of GNNs combining with other deep learning techniques to model the complicated spatial dependencies, which we categorize into three spatial attributes, i.e., spatial locality, multiple relationships and global connectivity.

1) **Spatial Locality**: Spatial locality refers that adjacent regions are usually highly relevant to each other. For example, the passenger flow of a station in a subway is obviously affected by its connected stations. \mathbf{K} -localized spectral graph convolution network (SGCN) is widely adopted to aggregate the information of 0 to $\mathbf{K} - 1$ hop neighbors to the central

region. However, some works make different assumptions about the spatial locality and utilize some novel tricks.

The adjacency matrix representing the traffic topology is usually pre-defined while [63], [39] argued that neighboring locations were dynamically correlated with each other. They incorporated the attention mechanism into SGCN to adaptively capture the dynamic correlations among surrounding regions.

SGCN requires all the regions to have the same local statistics and its convolution kernel is location-independent. However, [62] clarified that the local statistics of traffic data changed from region to region and they designed location-dependent kernels for different regions automatically.

2) **Multiple Relationships**: While locality attribute focuses on spatial proximity, the target region can be correlated with distant regions through various non-Euclidean relationships (as shown in Figure 5). For instance, functional similarity refers that distant region is similar to the target region in terms of functionality, which can be characterized by the surrounding POIs [72], [64]. Transportation connectivity suggests that those geographically distant but conveniently reachable can be correlated [72]. The reachable way can be motorway, highway, subway. [72] encoded these different types of correlations using multiple graphs and leveraged multi-graph convolution to explicitly extract these correlation information. [74] adopted semantic neighbors to model the correlation between origins and destinations. The correlation is measured by the passenger flow between them.

3) **Global Connectivity**: Both spatial proximity and multi-relationship dependencies focus on parts of the network while ignore the whole structure. Global connectivity refers that traffic conditions of different regions have influenced each other in a whole network scale. There are several strategies to exploit the structure information of traffic network globally.

A popular way to capture global connectivity is to model the changing traffic conditions on the traffic network as a diffusion process that happens at the network scale, which is presented by a power series of transition matrices. Then, diffusion graph convolution network (DGCN) is adopted to extract the spatial dependency globally [77], [93], [87], [76], [83], [100].

[90] designed a novel spatial graph pooling layer with path growing algorithm to produce a coarser graph. They stacked this pooling layer before SGC layer to get multi-granularity graph convolutions, which can extract spatial features at various scopes.

[76] proposed a SGC layer with a self-adaptive adjacency matrix to capture the hidden global spatial dependency in the data. This self-adaptive adjacency matrix is learned from the data through an end-to-end supervised training.

B. Temporal Dependency

Temporal dependency refers that the prediction of a certain time is usually correlated with various historical observations [80].

As stated in Section V, many works extract the temporal dependency by RNNs based approaches. However, RNNs based approaches suffer from time-consuming iterations and confront gradient explosion/vanishing problem for capturing

long sequences. Therefore, some works adopt TCN based approaches with the superiority of simple structures, parallel computing and stable gradients [80], [64]. In addition, TCN is able to handle different temporal levels by stacking multiple layers. For instance [75], [76] stacked multiple TCN layers with the bottom layers extracting short-term neighboring dependencies and the higher layers learning long-term temporal features.

1) **Multi-timescale**: Some works extract the temporal dependency at a multi-timescale perspective [63], [98]. [63] decomposed temporal dependency into recent, daily and weekly dependencies. The recent dependency refers that the future traffic conditions are influenced by the traffic conditions recently. For instance, the traffic congestion at 9 am is inevitably influenced traffic flow at the following hours. Daily dependency describes that the repeated daily pattern in traffic data due to the regular daily routine of people, such as morning peak and evening peak. Weekly dependency considers the influence caused by the same week attributes, for instance, all Mondays share similar traffic pattern in a short-term. [63] set three parallel components with the same structure to model these three temporal attributes respectively.

2) **Different Weights**: Some works argue that the correlations between historical and future observations are varying at different previous time slices. [63] adopted a temporal attention mechanism to adaptively attach different importance to historical data.

C. Spatiotemporal Dependency

Many works capture the spatial and temporal dependency separately in a sequential manner [95], [87], [81], [57], [79], [102], [58] while the spatial and temporal dependencies are closely intertwined in traffic data. [63] argued that the historical observations of different locations at different times had varying impacts on central region in the future. Take an obvious example, a traffic accident in a critical road results in serious disruptions over related roads but at different time, due to the gradual formation and dispersion of traffic congestion.

A limitation of separately modeling is that the potential interactions between spatial features and temporal features are completely ignored, which may hurt the prediction performance. To overcome such limitation, a popular way is to incorporate the graph convolution operations (e.g., SGC, DGC) to RNNs (as stated in Section Four) to capture spatio-temporal correlations jointly [60], [77], [93], [91], [83], [100], [39], [90], [70].

D. External Factors

There are some types of data highly related with the traffic prediction tasks, such as holidays, hours/day/week/month/season/year related attributes (e.g., weekday and weekend) [64], [98], weather (e.g., rainfall, temperature, air quality) [98], special events, POIs [72] and traffic incidents (e.g., incident time, incident type) [79], which we refer as external factors or context factors. Note that [95] considered historical statistical speed information (e.g.,

average or standard deviation of traffic speed) as external factor.

Among external factors, discrete values such as day attributes, holidays and weather conditions, are usually transformed into binary vectors by one-hot encoding while continual values including temperature, wind speed are scaled by Min-Max normalization or Z-score normalization.

There are two approaches to handle external factors in the literatures we survey. The first approach is to concatenate the external factors with other features and feed them into model [77], [64]. The second approach is to design an external component in charge of processing external factors alone. The external component usually contains two FC layers, of which the first extracting important features and the second mapping low dimension features to high dimension [64], [79], [98], [44]. [96] employed multi-LSTM layers to extract representation of context factors. The output of external component is fused with other components to generate the final result.

VII. PUBLIC DATASETS AND OPEN SOURCE CODES

A. Public Datasets

We summarize some public datasets (as shown in Table IV) in our survey to help successor participate in this domain and produce more valuable works.

B. Open Source Codes

Open-source implementations are helpful for researchers to compare their approaches. We provide the hyperlinks of public source codes of the literatures reviewed in this paper (as shown in Table V) to facilitate the baseline experiments in traffic domain.

VIII. FUTURE DIRECTIONS

Table II provides an overview of the related works we carefully examine. Based on these works, we suggest some directions for researchers to further explore, which can be divided into application related, technique related, external factor related directions.

As shown in Table II, there are many works utilizing graph-based deep learning architectures to tackle traffic state prediction and traffic demand prediction, which have achieved state-of-art performances. However, there are only a handful of works analyzing traffic data on a graph perspective in other research directions, such as vehicle behavior classification [57], optimal DETC scheme [50], vehicle/human trajectory prediction [58], [59], path availability [60], traffic signal control [61]. When it comes to traffic incident detection, vehicle detection, works adopting graph-based deep learning techniques are rare. As far as we are concerned, we can't find any one of them. Therefore, the upcoming participators can explore these directions on a graph view and learn the successful experiences from the existing works.

Most existing works have employed spectral graph convolution network (SGCN) and diffusion graph convolution network (DGCN), two popular kinds of GNNs, to analyze related traffic tasks. Graph attention networks (GAT) [134] in traffic domain

TABLE IV
SOME OPEN TRAFFIC DATASETS

References	Encoder	Decoder
NYC taxi	https://www1.nyc.gov/site/tlc/about/tlc-trip-record-data.page	[86], [98], [79], [88]
NYC bike	https://www.citibikenyc.com/system-data	[98], [44], [69], [96]
San Francisco taxi	https://crawdad.org/crawdad/epfl/mobility/20090224/	[79]
Chicago bike	https://www.divvybikes.com/system-data	[44]
BikeDC (Bike Washington)	https://www.capitalbikeshare.com/system-data	[98]
California -PEMS	http://pems.dot.ca.gov/	[80], [64], [63], [86], [77], [65], [85], [76], [91], [60], [83]

TABLE V
SOME OPEN SOURCE CODES

Reference	Model	Year	Framework	Github
[93]	DCRNN	2018	tensorflow	https://github.com/liyaguang/DCRNN
[84]	GCNN	2018	keras	https://github.com/RingBDStack/GCNN-In-Traffic
[73]	T-GCN	2019	tensorflow	https://github.com/lehaifeng/T-GCN
[85]	GMAN	2019	tensorflow	https://github.com/zhengchuanpan/GMAN
[76]	Graph-WaveNet	2019	torch	https://github.com/nanzhan/Graph-WaveNet

are few [85], [89], [92], [101]. Other kinds of GNNs, such as graph auto-encoders (GAEs) [135], [136], recurrent graph neural networks (RecGNNs) [137] have achieved state-of-the-art performance on other domains, but they are seldom explored in traffic tasks up to now. Therefore, it is worth to extend these GNNs to traffic domain. In addition, most of the graph-based traffic works are regression tasks, while only [60], [57] are classification tasks. Researchers can explore the classification traffic tasks on a graph perspective.

Finally, many existing traffic models don't take external factors into consideration, for that external factors are hard to collect, quantify and have various data formats. The sparsity of external factors is still a challenge confronted by the research community. In addition, the techniques to process external factors are rather naive, for instance, a simple fully connected layer. There should be more approaches to collect and process external factors.

IX. CONCLUSION

In this survey, we conduct a comprehensive review of various graph-based deep learning architectures in traffic works. More specifically, we summarize a general graph-based formulation of traffic problem and the way to construct graphs from various traffic datasets. Further, we decompose all the investigated architectures and analyze the common modules they share, including graph neural networks (GNNs), recurrent neural networks (RNNs), temporal convolution network (TCN), Sequence to Sequence (Seq2Seq) model, generative adversarial network (GAN). We provide a thorough description of their variants in traffic tasks, hoping to provide upcoming researchers insights into how to design novel techniques for their own traffic tasks. We also summarize the common challenges in many traffic scenarios, such as spatial dependency, temporal dependency, external factors. More than that, we present multiple deep learning based solutions for each challenge. In addition, we provide some hyperlinks of public datasets and codes in related works to facilitate the upcoming researches. Finally, we suggest some future directions for participators interested in this domain.

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