Learning Sparse and Continuous Graph Structures for Multivariate Time Series Forecasting

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Abstract
Accurate forecasting of multivariate time series is an extensively studied subject in finance, transportation, and computer science. Fully mining the correlation and causation between the variables in a multivariate time series exhibits noticeable results in improving the performance of a time series model. Recently, some models have explored the dependencies between variables through end-to-end graph structure learning without the need for pre-defined graphs. However, most current models do not incorporate the trade-off between effectiveness and flexibility and lack the guidance of domain knowledge in the design of graph learning algorithms. Besides, they have issues generating sparse graph structures, which pose challenges to end-to-end learning. In this paper, we propose Learning Sparse and Continuous Graphs for Forecasting (LSCGF), a novel deep learning model that joins graph learning and forecasting. Technically, LSCGF leverages the spatial information into convolutional operation and extracts temporal dynamics using the diffusion convolution recurrent network. At the same time, we propose a brand new method named Smooth Sparse Unit (SSU) to learn sparse and continuous graph adjacency matrix. Extensive experiments on three real-world datasets demonstrate that our model achieves state-of-the-art performances with minor trainable parameters.

1 Introduction
Today, our lives benefit significantly from various sensors in many fields, such as weather forecasting, transportation, hydrometry, electricity. The multivariate time series (MTS) data generated by sensors has high practical value and attracts many scholars to participate in the research. MTS forecasting is vital for a learning system that operates in an evolving environment. There is already some valuable work on this aspect [Wu et al., 2020; Li et al., 2018; Deng and Hooi, 2021].

A fundamental assumption in MTS forecasting is the correlations between variables, which means that a variable’s future information depends not only on its historical information but also on the historical information of other variables. Traditional methods, such as autoregressive integrated moving average (ARIMA) [Lee and Tong, 2011], Gaussian process model (GP) [Roberts et al., 2013], and Kalman filtering [Arnold et al., 1998], are used in many time series forecasting tasks. However, these models are neither sufficient to mine the intricate spatial-temporal dynamics nor model non-linear dependencies among MTS data, resulting in poor prediction results. Recently, some researchers have shifted to deep learning and concentrated on exploiting prominent temporal patterns shared by MTS, such as TPA-LSTM [Shih et al., 2019] and LSTNet [Lai et al., 2018]. These methods have a strong capability in modeling temporal dynamics but lack the ability to capture spatial relationships.

In the MTS forecasting tasks, effectively modeling and utilizing the correlations between variables is still an unsolved problem. Graph neural networks (GNNs) have shown high capability in handling relational dependencies due to their compositionality, local connectivity, and permutation-invariance, so some recent work [Li et al., 2018; Yu et al., 2018] has attempted to introduce them into MTS forecasting. However, these graph neural network methods require a pre-defined graph structure, and the pre-defined graph structures generally are local and static. Hence, they ignore the long-range dependencies of some nodes and fail to consider the dynamic property of MTS data. Moreover, we cannot obtain such an underlying graph structure in many cases. To solve the above questions, the method of graph structure learning (GSL) has been proposed and attracted much attention [Zhu et al., 2021]. Graph structure learning aims to learn the optimal graph structure and corresponding representation jointly. Furthermore, some literature [Franceschi et al., 2019; Fatemi et al., 2021; Shang et al., 2021] has also proved that joint graph learning and downstream tasks are better than directly using pre-defined graphs.

Recent models apply graph learning to MTS forecasting and achieve promising results. These models are MTS forecasting with GNNs (MTGNN) [Wu et al., 2020], Graph for Timeseries(GTS) [Shang et al., 2021], Adaptive Graph Convolution Recurrent Network (AGCRN) [BAI et al., 2020], Graph Deviation Network (GDN) [Deng and Hooi, 2021],
Spatial-temporal attention wavenet (STAWnet) [Tian and Chan, 2021] and Neural Relational Inference [Kipf et al., 2018]. All models can be decomposed into two building blocks: the graph structure learning and the temporal forecasting modules. Despite promising results of joint graph learning and forecasting in current models, we argue that these approaches face three major shortcomings.

First, the current models do not consider the trade-off between efficiency and flexibility. The current models either learn a graph adjacency matrix globally (shared by all time series) or construct an adjacency matrix for each batch. While the former has the advantage of being more efficient, though less flexible, since we can not adjust the graph for different inputs during testing time, the latter enjoys being more flexible yet less efficient because we need to allocate much memory to store individual adjacency matrices.

Second, there are problems with existing graph learning algorithms. Current models like GDN, MTGNN, Graph WaveNet (GWN) [Wu et al., 2019], and AGCRN essentially generate graph adjacency matrices through random initialization and learn through end-to-end. Although some other models such as GTS and STAWnet use time series for graph inferences, they do not apply substantial domain knowledge to fully mine the correlations in multivariate time series data, resulting in poor interpretability and easy overfitting.

Third, in the procedure of constructing graph structure, many models use non-differentiable functions to obtain sparse graph matrices, which poses challenges to end-to-end learning. Although some other models apply the Gumbel reparameterization technique to sample the discrete adjacency matrix from the edge probability in a differentiable way (though gradients are biased), the expressive power of the discrete matrix is limited, and the sparsity can not be controlled.

To emphasize the issues mentioned above, we propose a concise yet practical graph learning framework for multivariate time series forecasting. Our model not only considers the balance between efficiency and flexibility but also integrates the domain knowledge into the graph learning module. Moreover, we propose a new method to obtain sparse and continuous matrices. The main contributions of our works are as follows:

- We propose a model called Learning Sparse and Continuous Graphs for Forecasting (LSCGF), which follows a different route with the aim of learning continuous and sparse dependencies between variables while simultaneously training the forecasting module. Different from other models, our model can generate a specified number of graphs through the innovative graph structure learning module to balance efficiency and flexibility. Moreover, we can select the most suitable graph structure for forecasting during training and testing time by comparing the similarity of the time series with all graphs.

- Inspired by [Lee, 2013], we propose the Smooth Sparse Unit (SSU) intending to infer continuous and sparse dependencies between variables. To the best of our knowledge, this is the first method that can simultaneously sparse the learned graph structure and maintain continuity.

- We conduct extensive experiments on three real-world multivariate time series datasets, METR-LA, PEMS-BAY, Solar-Energy. As a result, the proposed model achieves state-of-the-art results with the least amount of trainable parameters.

2 Related Work

2.1 Spatial-temporal Graph Networks

The graph neural network has achieved great success in capturing the spatial relationships. The graph neural network essentially follows the neighborhood aggregation strategy, in which the node representation updates itself by iteratively aggregating the representation of the neighbors in the graph. In order to capture this spatial connection, a variety of different methods have been proposed [Kipf and Welling, 2017; Veličković et al., 2018; Hamilton et al., 2017]. Recently, to solve the complicated spatial and temporal connections in traffic prediction and skeleton-based action recognition, spatial-temporal graph networks were proposed and achieved superior results. The input of spatial-temporal graph networks is usually a multivariate time series and an additionally given adjacency matrix. They aim to predict future values or labels of multivariate time series. The objective of the spatial-temporal graph networks is to make full use of the structural information to achieve the optimal forecasting effect. Most of the recent works consider spatial and temporal modules separately. DCRNN [Li et al., 2018] uses diffusion convolution and encoder-decoder structures to capture spatial and temporal relationships, respectively. GWN [Wu et al., 2019] obtains the spatial dependency by using an adaptive adjacency matrix. STAWnet [Tian and Chan, 2021] is extended based on GWN, and it takes the method of attention to get self-learned node embedding, thereby capturing the spatial dependency. Both STAWnet and GWN use Gated-TCN as the temporal prediction module.

2.2 Graph Structure Learning

Graph representation learning is the core of many forecasting tasks, ranging from traffic forecasting to fraud detection. Many graph neural network methods are susceptible to the quality of the graph structure and require a perfect graph structure for learning embeddings. We discuss selected work about multivariate time series forecasting and refer the reader to [Zhu et al., 2021] for a complete survey. GWN generates a symmetric adjacency matrix through random initialization and learns through an end-to-end approach. MTGNN learns two embedding vectors per node and obtains the graph adjacency matrix through mathematical transformation. Similar to MTGNN, GDN infers the graph by learning a node embedding per node and builds a $k$NN graph where the similarity metric is the cosine of a pair of embeddings. LDS [Franceschi et al., 2019] approximately solves a bilevel programming...
3 Methodology

In this section, we first give a mathematical description of the problem we are addressing in this paper. Next, we describe two building blocks of our framework, the graph structure learning module, and the temporal forecasting module. They work together to capture the spatial-temporal dependencies. Finally, we outline the architecture of our framework.

3.1 Problem Formulation

In this paper, we focus on exploiting graph structure learning to improve the accuracy of multivariate time series forecasting. Let \( x_t \in \mathbb{R}^{N \times D} \) represent the value of a multivariate variable of dimension \( N \) at time step \( t \), and \( D \) denote the feature dimension, where \( x_t[i] \in \mathbb{R}^D \) denotes the \( i^{th} \) variable at time step \( t \). Given the historical \( M \) time steps observation sequence of a multivariate variable \( X = \{x_1, x_2, \ldots, x_M\} \), our goal is to predict the future \( N \)-step numerical sequence \( Y = \{x_{M+1}, x_{M+2}, \ldots, x_{M+N}\} \). Note that we do not need a pre-defined graph structure here. Specifically, let \( X_{train} \) and \( X_{valid} \) denote the training and validation sets of multivariate time series respectively, \( A \in \mathbb{R}^{K \times K} \) is the adjacent matrix of the graph representing the proximity between \( K \) time series , \( \omega \) denote the parameters used in the GNN and \( L \) and \( F \) denote the loss functions used during training and validation respectively, the use of graph structure learning methods for MTS forecasting naturally has a bilevel programming architecture as

\[
\begin{align*}
\min_{A, \omega_A} & \quad F(\omega, A, X_{valid}), \\
\text{s.t.} & \quad \omega_A \in \arg\min \omega L(\omega, A, X_{train}).
\end{align*}
\]  

(1)

Intuitively, the hierarchical relationship results from the fact that the mathematical program related to the parameters of graph learning is part of the constraint of the temporal forecasting module. However, the bilevel program problem is naturally challenging to solve. Even for the simplest example, the linear-linear bilevel programming is proved to be NP difficult [Colson et al., 2007]. Therefore, we need to make some approximations to the original bilevel problem. Inspired by [Shang et al., 2021], we consider approximating the bilevel programming to a unilevel programming problem as

\[
\min_{A(w)} F(w, A, X_{train}).
\]  

(2)

Because this approach owns the freedom to design the parameterization and can better control the number of parameters compared to an inner optimization \( w_A \). Therefore, the design of a reasonable parameterization approach is crucial for the graph structure learning module.

3.2 Graph Structure Learning Module

Graph Structure Learning is an essential operation when graph structure is missing or incomplete. LDS gives the first mathematical description of bilevel programming applying graph learning to downstream tasks. GTS approximates the bilevel optimization to the unilevel optimization and is deployed in time series forecasting. Both assume the graph adjacency matrix \( A \in \{0, 1\}^{K \times K} \) is Bernoulli distribution. This assumption is indeed conducive to the effectiveness of computation, but binary values cannot reflect the rich correlations between variables. For example, most traffic prediction models generate spatial adjacency matrix \( A \) based on a thresholded Gaussian kernel function [Shuman et al., 2013] to make \( A_{i,j} \in [0, 1] \). Therefore, in our model, instead of constructing an adjacency matrix based on Bernoulli distribution, we construct weighted adjacency matrices with each entry \( A_{i,j} \) between \( [0, 1] \), and a larger value corresponds to a higher correlation. The training time series is represented by \( X_{train} \in \mathbb{R}^{T_{train} \times N \times D} \) where \( T_{train} \) denotes the number of training time steps, \( N \) is the number of variables and \( D \) denotes the feature dimension. Given a graph adjacency matrix \( A \) and its historical \( W \) step graph signals, our problem is to learn a function \( F_A \) which is able to forecast its next \( H \) step graph signals. The overall forecasting function can be written as

\[
[X_{t-W+1:t}, A] \xrightarrow{F_A} X_{t+1:t+H}.
\]  

(3)
Period Convolution Network
In the graph structure learning module, our purpose is to extract the spatial relationships between variables from the training time series data. In this process, we assume that the difference between adjacent time steps can better reveal the spatial correlation than the original data. Take sensors that record traffic network flows as an example. Where sensors can cover the traffic network roughly, a decrease in the value of upstream sensors means that the value of downstream sensors will increase. Furthermore, the smaller the distance metric to the upstream sensor, the more sensitive the downstream sensor is to capture this change, which is reflected in the recorded time series. Therefore, we first do the “delta” operation on the training multivariate time series data:

$$
\mathcal{D}(X_{1,1}, X_{1,2}, \cdots, X_{1,T}) = \{X_{1,2} - X_{1,1}, \cdots, X_{1,T} - X_{1,T-1}\} \equiv \{\hat{X}_{1,1}, \ldots, \hat{X}_{1,T-1}\}. 
$$

Then, considering the periodicity in the time series data, we set a hyper-parameter period $P$ to segment the training time series data into $S = \lceil T_{\text{train}}/P \rceil$ segments, each containing time series $\hat{X}_{i} \in \mathbb{R}^{N \times D \times P}, i = 1, 2, \ldots, S$. After obtaining the time-series segments, we concatenate these segments to obtain a four-dimensional tensor $\mathcal{O} = [\hat{X}_1, \hat{X}_2, \ldots, \hat{X}_S] \in \mathbb{R}^{S \times N \times D \times P}$. Subsequently, we use 2D convolution and two linear layers to transform the four-dimensional tensor $\mathcal{O}$ to obtain $R$ graphs. The number of input channels is $S$, and the number of output channels is the number of graphs $R$ we aim to get. These graphs constitute the graph set $\mathcal{A}$.

Smooth Sparse Unit
In this section, we propose the Smooth Sparse Unit (SSU) to learn continuous and sparse graphs instead of using the discrete adjacency matrix produced by Gumbel softmax sampling in GTS because the continuous adjacency matrix can learn more valuable feature representation. Moreover, we also need to perform the sparsification operation for less computational cost. Inspired by Lee [2013], the mathematical principles of SSU are as follows:

**Lemma 1.** [Lee, 2013] The function $f : \mathbb{R} \rightarrow \mathbb{R}$ defined by

$$
f(x) = \begin{cases} 
  e^{-\frac{x}{2}} & (x > 0), \\
  0 & (x \leq 0),
\end{cases} 
$$

is smooth.

**Proof.** Let

$$
\varphi(x) = \frac{\alpha f(x)}{\alpha f(x) + f(1-x)} \quad (\alpha \in \mathbb{R}^+),
$$

where $f \in C^\infty(\mathbb{R})$ is defined by Equation (5). It is easy to check that $\varphi(x) \in [0, 1]$, and $\varphi(x) \equiv 0$ for $x < 0$, $\varphi(x) \equiv 1$ for $x > 1$.

**Lemma 2.** There exists a smooth function $\varphi : \mathbb{R} \rightarrow [0, 1]$ such that $\varphi(x) \equiv 0$ for $x \leq 0$; $\varphi(x) \in (0, 1)$ for $0 < x < 1$; $\varphi(x) \equiv 1$ for $x \geq 1$.

**Proof.** Let

$$
\varphi(x) = \frac{\alpha f(x)}{\alpha f(x) + f(1-x)} \quad (\alpha \in \mathbb{R}^+),
$$

where $f \in C^\infty(\mathbb{R})$ is defined by Equation (5). It is easy to check that $\varphi(x) \in [0, 1]$, and $\varphi(x) \equiv 0$ for $x \leq 0$, $\varphi(x) \equiv 1$ for $x \geq 1$.

Using the above mathematical formula, the output adjacency matrix $A$ is

$$
A = \frac{\alpha f(G)}{\alpha f(G) + f(1 - G)},
$$

where $G \in \mathbb{R}^{N \times N}$ is the output of the linear layer, $1$ denotes the all one matrix, $\alpha$ is the sparsification coefficient (hyper-parameter), $f$ is a element-wise operator defined by Lemma 1, and $A$ is the graph that we finally learned.

More details for controlling the sparsity effect of $\alpha$ and techniques of redefining gradients to accelerate convergence are presented in Appendix A.

3.3 Temporal Forecasting module
Graph Selection
After obtaining $R$ graphs through the PCN and SSU modules, what we need to do next is to select the optimal graph structure for each input time series $X_{in} \in \mathbb{R}^{B \times T_{in} \times N \times D}$, and we use the following objective function to represent:

$$
A = \arg \max_{A_i \in \mathcal{A}} \cos \langle \mathcal{X}^T \mathcal{X}, A_i \rangle,
$$

where $\cos \langle \mathcal{X}, \mathcal{Y} \rangle = \frac{\sum_{i=1}^{B} \sum_{j=1}^{D} \sum_{i,j} \sum_{k} \varphi_{ij}(x_{ik}) \varphi_{ij}(y_{jk})}{\sqrt{\sum_{i=1}^{B} \sum_{j=1}^{D} \sum_{i,j} \sum_{k} \varphi_{ij}(x_{ik})^2 \varphi_{ij}(y_{jk})}}$. $\mathcal{X} = \sum_{i=1}^{B} \sum_{j=1}^{D} X_{in[i; i]]} \in \mathbb{R}^{T_{in} \times N}$ for each batch and $B$ is the batch size.

We use the scalar product to calculate the correlation between nodes in the input data $X_{in}$, and $\cos \langle \cdot \rangle$ to measure the similarity between graphs and input data, so as to select the most suitable graph for training.

Diffusion Convolution Layer
Due to its specific design for directed graphs, we select DCRNN [Li et al., 2018] as our forecasting module to capture temporal trends. As is shown in Figure 2, our graph learning module learns the adjacency relationship between any two nodes and carries out information transfer. Besides, multi-step diffusion results in node homogeneity, which leads to node feature confusion and parametric training difficulties. For this reason, we only use one-step diffusion convolution, which is defined as

$$
W^Q_A X = (\omega^Q_0 + \omega^Q_1(D_A^{-1} A) + \omega^Q_2(D_A^{-1} A)) X,
$$

Figure 2: The left picture is the ground-truth graph or kNN graph, and the information transfer between node $i$ and node $p$ needs three-step diffusion to be realized. The right picture is the adjacency matrix produced by our graph structure learning module. It learns the associations between all nodes, so there is no need for multi-step diffusion.
with $D_O$ and $D_I$ being the out-degree and in-degree matrices and $\omega_{Q}^O$, $\omega_{Q}^I$, $\omega_{Q}^2$ being model parameters.

We leverage the recurrent neural networks (RNNs) with Gated Recurrent Units (GRU) to model the temporal dependency:

$$
\begin{align*}
    R_t &= \text{sigmoid}(W_{A}^{R}(X_t||H_{t-1}) + b_R), \\
    C_t &= \tanh(W_{A}^{C}(X_t||H_{t-1}) + b_C), \\
    U_t &= \text{sigmoid}(W_{A}^{U}(X_t||H_{t-1}) + b_U), \\
    H_t &= U_t \odot H_{t-1} + (1 - U_t) \odot C_t,
\end{align*}
$$

where $||$ is concatenation along the feature dimension and $\odot$ represents the element-wise product and $b_R$, $b_C$, $b_U$ are model parameters.

### 3.4 Framework of LSCGF

We present the framework of LSCGF in Figure 1. It consists of a graph structure learning module and a temporal forecasting module. The graph structure learning module consists of a Period Convolution Network (PCN) and a Smooth Sparse Unit (SSU). The temporal forecasting module contains the graph selection and the diffusion convolution recurrent layers. By choosing the appropriate graph during training and testing, the prediction accuracy can be significantly improved. Different from previous models like GTS, GWN, and MTGNN, our model can generate a specified number of graphs based on the training MTS data in the graph learning module. Therefore, we need to select the most appropriate graph for the temporal forecasting module. It addresses the problem of poor flexibility caused by the global graph and the issue of poor computational efficiency caused by building a graph for each batch. At the same time, we propose SSU with two major parts, the sparsification coefficient part to control the sparse degree and the gradient redefinition technique part to accelerate convergence.

### 4 Experiments

We verify LSCGF on three public multivariate time series datasets, METR-LA, PEMS-BAY, and Solar-Energy. METR-LA contains average traffic speed measured by 207 sensors on the highway of Los Angeles Country ranging from Mar 2012 to Jun 2012. PEMS-BAY records the average traffic speed measured by 325 detectors in the Bay Area ranging from Jun 2017 to May 2017. Solar-Energy contains the solar power output from 137 PV plants in Alabama State in 2007. Z-score normalization is applied to inputs. We adopt the same data pre-processing procedures as in [Li et al., 2018], and the datasets are split in chronological order with 70% for training, 10% for validation, and 20% for testing. Detailed data statistics are provided in Table 2. The source code is available at https://github.com/onceCWJ/LSCGF.

#### 4.1 Baselines

We compare LSCGF with the following models.

- VAR Vector Auto-Regression [Li et al., 2018].
- FC-LSTM Recurrent neural network with fully connected LSTM hidden units [Li et al., 2018].
- GWN Graph WaveNet. A spatial-temporal graph convolutional network, which integrates diffusion graph convolutions with 1D dilated convolutions [Wu et al., 2019].
- DCRNN Diffusion convolution recurrent neural network, which incorporates diffusion graph convolution with recurrent neural network in an encoder-decoder manner [Li et al., 2018].
### Table 3: Performance of different functions on METR-LA.

| Data       | Function         | Horizon 3 |          |          | Horizon 6 |          |          | Horizon 12 |          |          |
|------------|------------------|-----------|----------|----------|-----------|----------|----------|------------|----------|----------|
| METR-LA    | Sigmoid          | 2.68      | 5.30     | 6.94%    | 3.07      | 6.34     | 8.32%    | 3.48       | 7.41     | 9.78%    |
|            | Tanh             | 2.60      | 5.12     | 6.79%    | 2.99      | 6.18     | 8.38%    | 3.40       | 7.23     | 9.99%    |
|            | Gumbel-softmax   | 2.85      | 5.72     | 7.54%    | 3.41      | 7.02     | 9.72%    | 4.15       | 8.52     | 12.78%   |
|            | SSU              | **2.58**  | **4.99** | **6.47%**| **2.96**  | **6.01** | **7.87%**| **3.37**   | **7.06** | **9.44%**|

### Table 4: Performance of different models on Solar-Energy.

| Data       | Models          | Horizon 3 |          |          | Horizon 6 |          |          | Horizon 12 |          |          |
|------------|-----------------|-----------|----------|----------|-----------|----------|----------|------------|----------|----------|
| Solar-Energy| VAR             | 0.79      | 1.54     |          | 2.55      | 3.92     | 4.17     | 6.12       |          |          |
|            | FC-LSTM         | 0.70      | 1.88     |          | 1.17      | 2.90     | 1.98     | 4.74       |          |          |
|            | GWN             | 1.29      | 2.35     |          | 1.89      | 3.20     | 2.85     | 4.58       |          |          |
|            | DCRNN           | 0.58      | 1.60     | 0.84     | 2.24      | 1.37     | 3.64     |            |          |          |
|            | MTGNN           | 1.36      | 2.46     | 1.95     | 3.33      | 2.91     | 4.66     |            |          |          |
|            | GTS             | 0.58      | 1.66     | 0.85     | 2.33      | 1.37     | 3.67     |            |          |          |
|            | LSCGF           | **0.55**  | **1.56** | **0.80** | **2.16**  | **1.31** | **3.53** |            |          |          |

### Table 5: Trainable Parameters of different graph learning based spatial-temporal models on METR-LA.

| Data       | Models          | Number of Trainable Parameters |
|------------|-----------------|-------------------------------|
| METR-LA    | MTGNN           | 405,452                       |
|            | GWN             | 247,660                       |
|            | GTS             | 38,478,291                    |
|            | LSCGF           | **202,266**                   |

### 4.2 Experimental Setups

- **MTGNN** Multivariate time series forecasting with graph neural networks, which uses external features to generate self-adaptive graphs for downstream forecasting module [Wu et al., 2020].
- **GTS** Graph for time series, which aims to jointly learn a latent graph in the time series and use it for MTS forecasting [Shang et al., 2021].

### 4.3 Experimental Results

Table 1 and 4 compare the performances of LSCGF and baseline models for Horizon 3, 6, and 12 ahead forecasting on METR-LA, PEMS-BAY, and Solar-Energy datasets. LSCGF gets superior results on two datasets (METR-LA, Solar-Energy). Several conclusions can be made by further analysis. The performances of the proposed method outperform GTS on two datasets (METR-LA, Solar-Energy) and are slightly worse than the performances of GTS on PEMS-BAY. However, it can be seen in Table 5 that the number of parameters of our proposed model is nearly 180 times less than that of the GTS model, which saves much memory and dramatically speeds up the training and inference speed. Among all the methods, graph structure learning-based methods give the best results. It suggests that the direct application of pre-defined graph structures by conventional spatial-temporal graph networks is not necessarily the best, but instead that it is better to allow models themselves to derive adaptive graph structures. Graph structure learning frees the model from the limitations of the pre-defined graphs and improves the prediction accuracy.

### 4.4 Effect of the SSU module

Detailed proof of SSU validity is given in Appendix A. In Table 3, we replace the SSU with different functions and compare the results. The experimental results prove the correctness of our idea. Firstly, the expressive power of the continuous matrix is indeed better than that of the discrete matrix, which is why the effect obtained by continuous function significantly outweighs Gumbel-softmax. In addition, the effect of SSU is superior to other common activation functions. We also found that the training process using SSU is more stable and effective during the training process.

### 5 Conclusion

In this paper, we have proposed a novel model that joins graph structure learning and forecasting. Our model captures spatial-temporal dependencies efficiently and flexibly by combining the graph structure learning module and temporal forecasting module. We propose an effective method to learn latent spatial dependencies adaptively from the data and overcome the defects of the previous graph structure learning methods. It also provides guidance for the design
of graph structure learning algorithms in various fields. On three public datasets, LSCGF achieves state-of-the-art results. In future work, we will study the efficient design of graph structure algorithms in multiple areas so that more models can get rid of the limitations of the pre-defined graph structure and improve the effect.

A Description of SSU module

A.1 Sparsification coefficient

As we defined in context, let

\[ f(x) = \begin{cases} e^{-\frac{x}{\alpha}} & (x > 0), \\ 0 & (x \leq 0), \end{cases} \]

\[ \varphi(x) = \frac{\alpha f(x)}{\alpha f(x) + f(1-x)} (\alpha \in \mathbb{R}_+), \]

where parameter \( \alpha \) is called sparsification coefficient. Because it can determine the shape of curve \( \varphi \) and the sparse degree of adjacency matrix generated by SSU. The sparsification effect of SSU is described below.

It is easy to say that \( \varphi(x) \equiv 0, \varphi'(x) \equiv 0 \) for \( x \leq 0 \); \( \varphi(x) \equiv 1, \varphi'(x) \equiv 0 \) for \( x \geq 1 \). So we just consider \( 0 < x < 1 \), and let \( t = \frac{f(1-x)}{f(1-x) + \alpha} = e^{\frac{x}{\alpha} - \frac{1}{\alpha}} := g(x) \). For \( g'(x) = e^{\frac{1}{\alpha} - \frac{1}{x}} \left[-\frac{1}{\alpha x^2} - \frac{1}{\alpha x^2}\right] < 0 \), \( g(x) \) decreases strictly monotonically on \((0,1)\), and is a bijection. Thus \( g(x) \) has an inverse function \( g^{-1}(x) \).

For \( \varphi(x) < \epsilon \), i.e. \( \frac{\alpha}{\alpha + t} < \epsilon \),

\[ t > \alpha \left(\frac{1}{\epsilon} - 1\right) \iff x < g^{-1}(\alpha \left(\frac{1}{\epsilon} - 1\right)) \equiv \sup \]

For \( \varphi(x) > 1 - \epsilon \), i.e. \( \frac{\alpha}{\alpha + t} > 1 - \epsilon \),

\[ t < \alpha \left(\frac{1}{1 - \epsilon} - 1\right) \iff x > g^{-1}(\alpha \left(\frac{1}{1 - \epsilon} - 1\right)) \equiv \inf \]

In Figure 4, fixing \( \epsilon \), as \( \alpha \) decreases, \( \sup, \inf \) increase and the length of interval \( \varphi^{-1}((0,\epsilon)) = (0,\sup) \) increase, and vice versa. If we consider the adjacency matrix \( A = (A_{ij})_{n \times n} \) is the element-wise uniform distribution in \([0,1]\), then as \( \alpha \) decreases, the probability of \( A_{ij} \) falling into \((0,\sup)\) and \( A \) being sparse increases. Therefore, we get the conclusion that \( \alpha \) can control the sparsification effect of SSU.

A.2 Gradient redefinition

In our experiments, as \( x \) approaches 0 and 1, the gradient approaches 0 rapidly, which leads to the vanishing gradient problem. So in fact, it is extensively difficult to really train the adjacency matrix values to zero and achieve the sparsification effect. Therefore, we redefine the gradient as 1 in intervals \((0,\sup)\) and \((\inf,1)\) to accelerate convergence making the activation value fall into \((0,1)\) or \((\varphi(\sup),\varphi(\inf))\) faster.

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