

Balanced Spatial-Temporal Graph Structure Learning for Multivariate Time Series Forecasting: A Trade-off between Efficiency and Flexibility

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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 predefined graphs. However, current models do not incorporate the trade-off between efficiency and flexibility and make insufficient use of the information contained in time series in the design of graph structure learning algorithms. This paper alleviates the above issues by proposing Balanced Graph Structure Learning for Forecasting (BGSLF), a novel and effective deep learning model that joins graph structure learning and forecasting. Technically, BGSLF leverages the spatial information into convolutional operations and extracts temporal dynamics using the diffusion convolutional recurrent network. The proposed framework emphasizes the trade-off between efficiency and flexibility by introducing Multi-Graph Generation Network (MGN) and Graph Selection Module. In addition, a method named Smooth Sparse Unit (SSU) is designed to sparse the learned graph structures, which conforms to the sparse spatial correlations in the real world. Extensive experiments on four real-world datasets demonstrate that our model achieves state-of-the-art performances with minor trainable parameters. Our code is publicly available at <https://github.com/onceCWJ/BGSLF>.

Keywords: Graph Structure Learning, Multivariate Time Series Forecasting, Sparse Learning

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1. Introduction

Today, our lives benefit significantly from various sensors in many fields, such as weather forecasting, transportation, hydrology, and 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.

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)] and vector auto-regression (VAR) [Zivot and Wang (2006)], are used in many time series forecasting tasks. However, these models are insufficient to mine intricate spatial-temporal dynamics or model nonlinear dependencies between MTS data. Recently, some researchers [Sutskever et al. (2014); Lai et al. (2018); Shih et al. (2019)] have shifted to deep learning and concentrated on exploiting prominent temporal patterns shared by MTS. These methods have a strong capability in modeling temporal dynamics but lack the ability to capture dynamic spatial relationships.

In the MTS forecasting tasks, effectively modeling and utilizing the correlations between variables is still a challenging problem. Graph neural networks (GNNs) have shown high capability in handling relational dependencies due to their compositionality, local connectivity, and permutation-invariance, so some early work [Li et al. (2018); Chen et al. (2020); Yu et al. (2018)] has attempted to introduce them into MTS forecasting. However, these graph neural network methods require a predefined graph structure, and the predefined 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. Moreover, we cannot obtain such an underlying graph structure in many cases. The method of graph structure learning (GSL) has been proposed to solve the above questions 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 [Fatemi et al. (2021); Franceschi et al. (2019); Shang et al. (2021)] has revealed that joint graph learning and downstream tasks are better than directly using predefined graphs, partly due to the noise in the predefined graph structure.

Recent models apply graph structure learning to MTS forecasting and achieve promising results. These representative models are MTS forecasting with GNNs (MTGNN) [Wu et al. (2020)], Graph for Timeseries (GTS) [Shang et al. (2021)], Adaptive Graph Convolutional Recurrent Network (AGCRN) [BAI et al. (2020)], Graph WaveNet (GWN) [Wu et al. (2019)], Spatial-temporal attention wavenet (STAWnet) [Tian and Chan (2021)], Graph Deviation Network (GDN) and Neural Relational Inference (NRI) [Kipf et al. (2018)]. Despite promising results of joint graph structure learning and forecasting in current models, we argue that these approaches face three major shortcomings.

First, the current models do not emphasize the trade-off between efficiency and flexibility. The current models either learn a graph adjacency matrix globally (shared by all time series) or infer an adjacency matrix for each batch. The former can be more efficient but less flexible as we cannot adjust the graph for different inputs during training and inference.

On the other hand, the latter enjoys more flexibility but less efficiency as we need to allocate much memory to store the individual adjacency matrices.

Second, current models like GDN, MTGNN, GWN, and AGCRN essentially generate graph adjacency matrices through random initialization and refine the graph structure through end-to-end learning. Although some other models such as GTS and STAWnet apply training sets of MTS for graph inference, they do not apply substantial domain knowledge (e.g., periodicity) to fully mine the correlations in multivariate time series, resulting in poor interpretability and easy overfitting.

Third, some models [Wu et al. (2020); Deng and Hooi (2021)] apply non-differentiable functions to get sparse graph matrices, which are of high gradient variance bringing increased end-to-end training difficulty.

To circumvent the issues mentioned above, we propose a concise yet practical graph structure learning framework for multivariate time series forecasting. Our model strikes a good balance between efficiency and flexibility, and employs more detailed operations in graph generation. Moreover, we propose a new method to obtain sparse and continuous graph matrices. The main contributions of our works are as follows:

- We propose a model called *Balanced Graph Structure Learning for Forecasting* (BGS LF), which follows a different route with the aim of learning smooth 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 graph structure learning module to balance efficiency and flexibility. Furthermore, we can select the best graph structure for forecasting during training and inference by measuring the cosine similarity between the time series variables and all graphs.
- In Graph Structure Learning Module, in order to infer graphs that are more adaptable to prediction, we introduce some concise yet effective operations to preprocess training MTS. Through our method, we save lots of parameters and improve forecasting performances.
- Inspired by Lee (2013), we propose the Smooth Sparse Unit (SSU) intending to infer continuous and sparse dependencies between variables. With the aid of SSU, the use of non-differentiable functions (e.g., Top- K operation) or regularization in inferring sparse graph structures can be avoided.
- We conduct extensive experiments on four real-world multivariate time series datasets, PEMS04, PEMS08, METR-LA, Solar-Energy. As a result, the proposed model achieves state-of-the-art results with minor trainable parameters.

2. Related Work

2.1. Spatial-temporal Graph Networks

The graph neural network has achieved great success in capturing spatial relationships. In order to capture this spatial connection, a variety of methods have been proposed [Kipf and Welling (2017); Veličković et al. (2018)]. Most of these methods essentially follow the neighborhood aggregation strategy, in which the node representation updates itself by iteratively aggregating the representation of the neighbors in the graph. Recently, to solve the

complicated spatial and temporal connections in traffic prediction and skeleton-based action recognition [Shi et al. (2019)], 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. DCRNN [Li et al. (2018)] uses diffusion convolution and encoder-decoder structures to capture spatial and temporal relationships, respectively. ASTGCN [Guo et al. (2019)] adopts the spatial-temporal attention mechanism to model dynamic spatial-temporal correlations in traffic data. More recent works such as MRA-BGCN [Chen et al. (2020)] and GMAN [Zheng et al. (2020)] further add more complicated spatial and temporal attention mechanisms with GCN [Kipf and Welling (2017)] to capture the dynamic spatial and temporal correlations. The above methods were successful in traffic prediction at the time. However, these models are limited by the predefined graph structure, so these methods' performance and generalization ability can be improved.

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. Most of the recent works on MTS forecasting consider spatial and temporal modules separately. GWN [Wu et al. (2019)] captures the spatial dependency by training an adaptive adjacency matrix. STAWnet [Tian and Chan (2021)] takes the method of attention to get self-learned node embedding so as to capture the spatial dependency. Both STAWnet and GWN use dilated casual convolutions [Bai et al. (2018)] as the temporal forecasting module. 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 [Van Lint and Van Hinsbergen (2012)] where the similarity metric is the cosine of a pair of embeddings. AGCRN [BAI et al. (2020)] proposes two adaptive modules for enhancing graph convolutional networks to infer dynamic spatial dependencies among different traffic series. LDS [Franceschi et al. (2019)] approximately solves a bilevel programming problem to jointly learn the Bernoulli distribution of the adjacency matrices and the parameters of graph convolutional networks. In order to reduce expensive computation in LDS, GTS no longer regards the graph structure as hyperparameters for optimization but transforms the problem into unilevel programming. Other works [Wang et al. (2022); Wang and Feng (2017)] consider generating and sparsifying graphs from spectral methods. Moreover, some studies [Fatemi et al. (2021); Zügner et al. (2021)] have revealed that there does not exist a golden standard for evaluating the quality of the learned graph structure except for forecasting accuracy.

3. Methodology

In this section, we first give a mathematical description of the problem addressed in this paper. Next, we describe two building blocks of our framework, the graph structure learning

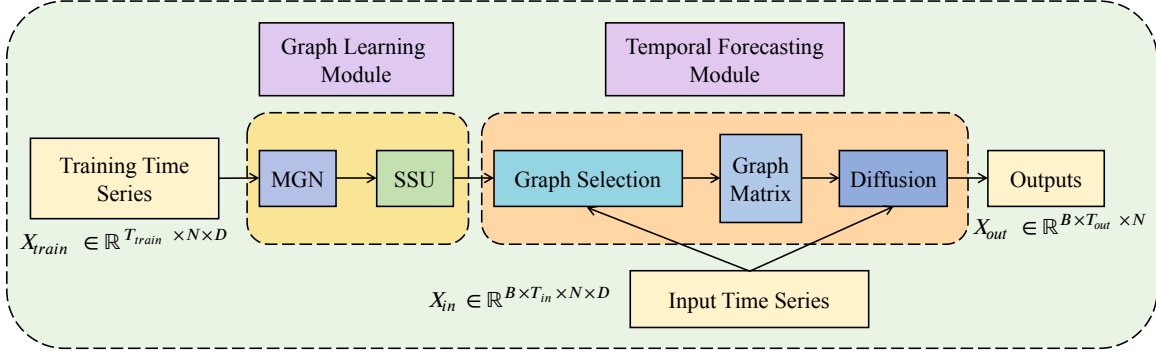


Figure 1: The framework of BGSFLF. The training time series are passed through the graph learning module to generate the graph set \mathbb{A} , containing two components, Multi-Graph Generation Network (MGN) and Smooth Sparse Unit (SSU). Graph selection is performed in the temporal forecasting module by measuring the similarity between the input time series and the graphs in \mathbb{A} . Finally, the selected graph matrix and the input data are fed into the diffusion convolutional network to produce the output.

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 MTS of N variables at time step t , and D denotes 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 $\mathbf{X} = \{\mathbf{x}_{t_1}, \mathbf{x}_{t_2}, \dots, \mathbf{x}_{t_M}\}$, our goal is to predict the future E -step numerical sequence $\mathbf{Y} = \{\mathbf{x}_{t_{M+1}}, \mathbf{x}_{t_{M+2}}, \dots, \mathbf{x}_{t_{M+E}}\}$. Note that we do not need a predefined 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, ω denotes 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 for MTS forecasting has a bilevel programming architecture as

$$\begin{aligned} \min_{A, \omega_A} F(\omega_A, A, X_{valid}), \\ \text{s.t. } \omega_A \in \arg \min_{\omega} L(\omega, A, X_{train}). \end{aligned} \quad (1)$$

Intuitively, the hierarchical relationship results from the fact that the mathematical program related to the parameters of graph structure learning is part of the constraint of the temporal forecasting module. However, the bilevel program problem is naturally difficult 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. Similar to Shang et al. (2021), we consider approximating the bilevel programming to a unilevel programming problem as

$$\min_{A(w)} F(w, A, X_{\text{train}}). \quad (2)$$

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. The construction of adjacency matrix is crucial in graph structure learning. Current methods [Deng and Hooi (2021); Wu et al. (2020); Shang et al. (2021)] focus on learning discrete adjacency matrix $A \in \{0, 1\}^{K \times K}$. However, binary values can not represent the rich correlations between variables. Therefore, instead of constructing discrete adjacency matrices based on Bernoulli sampling or some non-differentiable functions (e.g., Top- K operation), we construct continuous adjacency matrices $A_{i,j} \in [0, 1]$ with the aid of SSU in our model. The training set of MTS is represented by $X_{\text{train}} \in \mathbb{R}^{T_{\text{train}} \times N \times D}$ where T_{train} denotes the number of training time samples, N is the number of road sensors 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 \mathcal{F}_A which is able to forecast its next H step graph signals. The overall forecasting function can be written as

$$[\mathbf{X}_{t-W+1:t}, A] \xrightarrow{\mathcal{F}_A} \mathbf{X}_{t+1:t+H}. \quad (3)$$

3.2.1. MULTI-GRAPH GENERATION NETWORK

In the graph structure learning module, our purpose is to extract dynamic spatial relationships between variables from the training MTS. Changes in the values of different variables at cross-time can better reflect the spatial relationships between variables. In the transportation domain, for example, the numerical changes of the sensors over time offer insights into how traffic dynamics propagate along with the network. Therefore, we first do the difference operation on the training MTS in order to reveal more moderate correlations:

$$\begin{aligned} \text{Diff}(\mathbf{X}_{:,1}, \mathbf{X}_{:,2}, \mathbf{X}_{:,3}, \dots, \mathbf{X}_{:,T}) &= \{\mathbf{X}_{:,1}, \mathbf{X}_{:,2} - \mathbf{X}_{:,1}, \mathbf{X}_{:,3} - \mathbf{X}_{:,2}, \dots, \mathbf{X}_{:,T} - \mathbf{X}_{:,T-1}\}, \\ &\triangleq \{\hat{\mathbf{X}}_{:,1}, \hat{\mathbf{X}}_{:,2}, \dots, \hat{\mathbf{X}}_{:,T}\} = \hat{\mathbf{X}} \in \mathbb{R}^{T_{\text{train}} \times N \times D}. \end{aligned} \quad (4)$$

Then, considering the periodicity of the time series, we set a hyper-parameter period P to segment $\hat{\mathbf{X}}$ into $S = \lfloor T_{\text{train}}/P \rfloor$ segments, each containing time series $\hat{\mathbf{X}}_i \in \mathbb{R}^{P \times N \times D}$, $i = 1, 2, \dots, S$. After obtaining the time-series segments, we concatenate these segments to obtain a four-dimensional tensor $\mathcal{O} = [\hat{\mathbf{X}}_1, \hat{\mathbf{X}}_2, \dots, \hat{\mathbf{X}}_S] \in \mathbb{R}^{S \times P \times N \times D}$:

$$\mathcal{O} = \text{Concat}(\text{Segment}_{\text{period}=P}(\hat{\mathbf{X}})). \quad (5)$$

For the parameterization of \mathbb{A} , we use a feature extractor to yield a feature representation for each graph in \mathbb{A} . First, reshape the four-dimensional tensor $\mathcal{O} \in \mathbb{R}^{S \times P \times N \times D}$ to a three-dimensional tensor $\mathcal{Q} \in \mathbb{R}^{N \times S \cdot D \times P}$, in order to save computational consumption for subsequent calculations and make the dimensions match the subsequent convolutional operations. Finally, we use 1D convolution and three fully connected layers to transform the three-dimensional tensor \mathcal{Q} to obtain R graphs:

$$\mathbb{A}'' = \sigma(\delta(\delta(\delta(\text{Conv}(\mathcal{Q})W_1 + b_1))W_2 + b_2)W_3 + b_3) \in \mathbb{R}^{N \times R \times N}, \quad (6)$$

$$\mathbb{A}' = \text{reshape}(\mathbb{A}'') \in \mathbb{R}^{R \times N \times N}. \quad (7)$$

Here δ represents the ReLU activation function, and σ represents the Sigmoid activation function, $W_1, W_2, W_3, b_1, b_2, b_3$ are trainable parameters of the fully connected layers. We adopt a form similar to Squeeze-and-Excitation [Hu et al. (2018)] in the design of the three-layer fully connected networks, which saves lots of training parameters. The graphs in the graph set \mathbb{A}' are then passed through SSU to get the final graph representation \mathbb{A} for downstream prediction tasks.

3.2.2. 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 [Jang et al. (2016)] in GTS. 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*

$$f(x) = \begin{cases} e^{-\frac{1}{x}} & (x > 0), \\ 0 & (x \leq 0), \end{cases} \quad (8)$$

is smooth.

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

$$\varphi(x) = \frac{\alpha f(x)}{\alpha f(x) + f(1-x)} \quad (\alpha \in \mathbb{R}_+), \quad (9)$$

where $f \in C^\infty(\mathbb{R})$ is defined by Equation (8). It is easy to check that $\varphi(x) \in [0, 1]$, and $\varphi(x)$ is 0 for $x \leq 0$, 1 for $x \geq 1$. ■

Using the above mathematical formula, the output adjacency matrices \mathbb{A} are

$$\mathbb{A} = \frac{\alpha f(\mathbb{A}')}{\alpha f(\mathbb{A}') + f(\mathbf{1} - \mathbb{A}')} \in \mathbb{R}^{R \times N \times N},$$

where $\mathbf{1}$ denotes the all one matrix, α is the sparsification coefficient (hyper-parameter), f is an element-wise operator defined by Lemma 1, and \mathbb{A} is the graph set that we finally learned for downstream prediction tasks.

More details for controlling the sparsity effect of α and techniques of redefining gradients to accelerate convergence are presented in supplementary material.

3.3. Temporal Forecasting module

3.3.1. GRAPH SELECTION

After obtaining R graphs through the MGN and SSU, the optimal graph structure should be selected for each input time series $X_{\text{in}} \in \mathbb{R}^{B \times T_{\text{in}} \times N \times D}$, and we use the following objective function to represent:

$$A = \arg \max_{A_i \in \mathbb{A}} \cos \langle \mathcal{X}^T \mathcal{X}, A_i \rangle, \quad (10)$$

where $\cos \langle \mathcal{X}, \mathcal{Y} \rangle = \frac{\sum_{i,j} x_{ij} y_{ij}}{\sqrt{\sum_{i,j} x_{ij}^2 \cdot \sum_{i,j} y_{ij}^2}}$, $\mathcal{X} = \sum_{i=1}^B \sum_{j=1}^D X_{\text{in}[i, :, :, j]} \in \mathbb{R}^{T_{\text{in}} \times N}$ 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 and inference.

3.3.2. DIFFUSION CONVOLUTIONAL RECURRENT NETWORK

Due to its specific design for directed graphs, we adopt DCRNN [Li et al. (2018)] as our forecasting module to capture temporal trends. Considering that multi-step diffusion may lead to node homogeneity and bring difficulty to parameter training, we only use one-step diffusion convolutional operation, which is defined as

$$W_A^Q X = \left(\omega_0^Q + \omega_1^Q (D_O^{-1} A) + \omega_2^Q (D_I^{-1} A) \right) X, \quad (11)$$

with D_O and D_I being the out-degree and in-degree matrices and $\omega_0^Q, \omega_1^Q, \omega_2^Q$ being model parameters.

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

$$\begin{aligned} R_t &= \text{sigmoid} (W_A^R (X_t || H_{t-1}) + b_R), \\ C_t &= \text{tanh} (W_A^C (X_t || R_t \odot H_{t-1}) + b_C), \\ U_t &= \text{sigmoid} (W_A^U (X_t || H_{t-1}) + b_U), \\ H_t &= U_t \odot H_{t-1} + (1 - U_t) \odot C_t, \end{aligned} \quad (12)$$

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 BGSLF

We present the framework of BGSLF in Figure 1. It consists of a graph structure learning module and a temporal forecasting module. The graph structure learning module consists of Multi-Graph Generation Network (MGN) and Smooth Sparse Unit (SSU). The temporal forecasting module contains the Graph Selection Module and the Diffusion Convolutional Recurrent Network. By choosing the appropriate graph during training and testing, the forecasting accuracy can be significantly improved. Different from previous models like

Table 1: Dataset statistics.

Datasets	# Samples	# Nodes	Sample Rate	Input Length	Output Length
PEMS04	16,969	307	5 minutes	12	12
PEMS08	17,833	170	5 minutes	12	12
METR-LA	34,272	207	5 minutes	12	12
Solar-Energy	52,560	137	10 minutes	12	12

GTS, AGCRN, and MTGNN, our model can generate a specified number of graphs based on the training MTS data in the graph structure learning module. Therefore, we need to select the most appropriate graph for the temporal forecasting module. Furthermore, it addresses the problem of poor flexibility caused by the global graph and the issue of poor computational efficiency caused by building one 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 BGSFL on four public multivariate time series datasets, PEMS04, PEMS08, METR-LA, and Solar-Energy. PEMS04 is collected by Caltrans Performance Measurement System (PEMS) and released in ASTGCN [Guo et al. (2019)] consisting of average speed, traffic volume in San Francisco Bay Area. The period is from January to February 2018. Similar as PeMS04, PEMS08 consists of average speed, traffic volume collected by PeMS in San Bernardino from July to August in 2016. METR-LA contains average traffic speed measured by 207 sensors on the highway of Los Angeles Country ranging from Mar 2012 to Jun 2012. 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. We tune the hyperparameters on the validation data by grid search for BGSFL. We adopt the Adam optimizer, and the number of training epochs is set as 300. Detailed data statistics are provided in Table 1.

4.1. Baselines

Select the traditional and leading performance models. We compare BGSFL with the following models.

- HA Historical average, which models the traffic flow as a periodic process and uses the weighted average of previous periods as the prediction.
- VAR Vector Auto-Regression [Zivot and Wang (2006)].
- FC-LSTM Recurrent neural network with fully connected LSTM hidden units [Sutskever et al. (2014)].

- ASTGCN Attention-based spatio-temporal graph convolutional network, which further integrates spatial and temporal attention mechanisms to STGCN for capturing dynamic spatial and temporal patterns. We take its recent components to ensure the fairness of comparison [Guo et al. (2019)].
- AGCRN Adaptive Graph Convolutional Recurrent Network. An adaptive graph convolutional network, which designs two adaptive modules for enhancing graph convolutional network with new capabilities [BAI et al. (2020)].
- DCRNN Diffusion convolutional recurrent neural network, which incorporates diffusion graph convolution with recurrent neural network in an encoder-decoder manner [Li et al. (2018)].
- 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)].

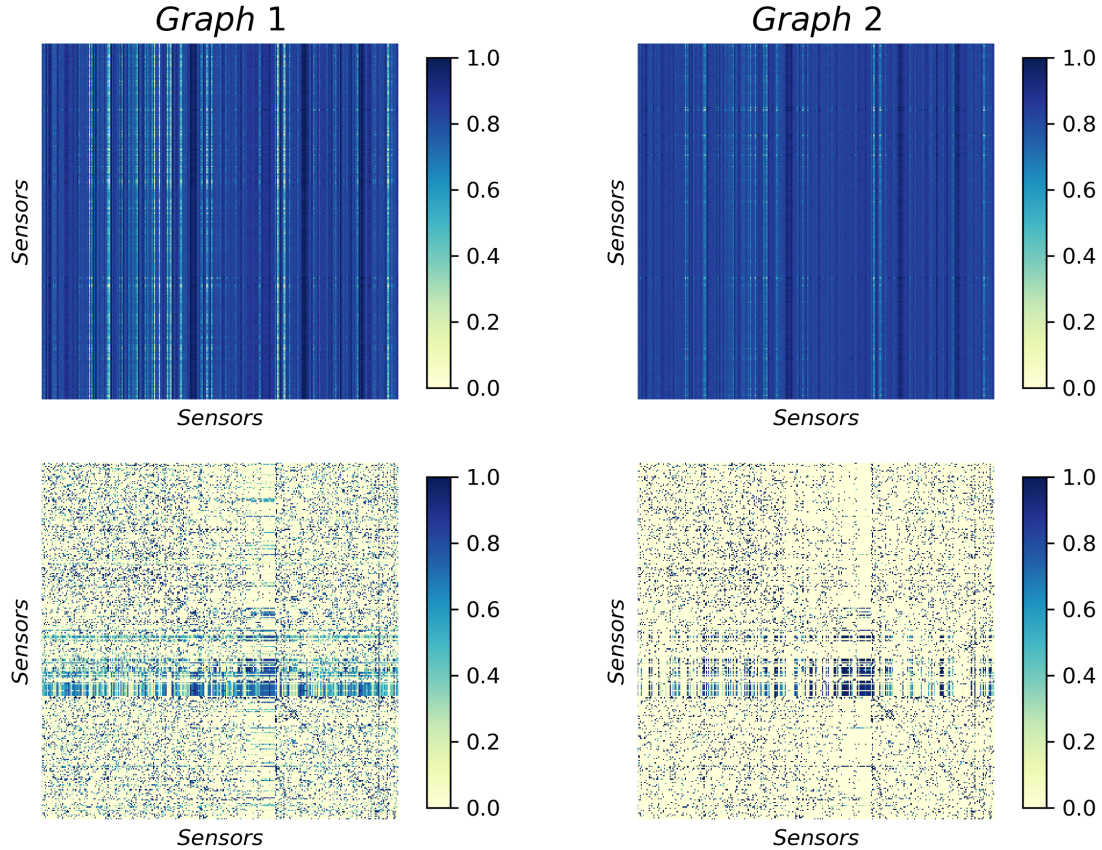
4.2. Experimental Setups

We implement our experiments on the platform PyTorch using 4 NVIDIA GeForce RTX 3090 GPUs. The hyperparameter period P is set to $12 \times 12 \times 2 = 288$, which is equivalent to using the daily-periodic segment method. We recommend that the hyperparameter R for the number of generated graphs be set to 2-4, generating too many graphs will lead to insufficient graph training, and only one graph cannot adequately capture the complex spatial patterns in the time series. Both will lead to a decrease in the final result. All of these methods are evaluated with three common metrics: mean absolute error (MAE), root mean square error (RMSE) and mean absolute percentage error (MAPE). Due to the non-uniform distribution of the solar power output of PV plants in spatial and temporal domains, there are many zeros in Solar-Energy. Hence, we only adopt MAE and RMSE in this dataset. We choose to use mean absolute error (MAE) as the training objective of BGSLF. Missing values are excluded both from training and testing. All the tests use 12 observed data points to forecast multivariate time series in the next 3, 6, and 12 steps. The initial learning rate is $3e-3$ with decay rate 0.1 per 10 epochs, and the minimum learning rate is $3e-5$. DCRNN and ASTGCN require a predefined graph, but the Solar-Energy dataset does not have one. Therefore, we apply the training multivariate time series to construct a k NN graph as the predefined graph structure.

BGSLF

Table 2: Performance of BGSLF and baselines on four real-world datasets.

Data	Models	Horizon 3			Horizon 6			Horizon 12		
		MAE	RMSE	MAPE	MAE	RMSE	MAPE	MAE	RMSE	MAPE
PEMS04	HA	24.50	39.83	16.58%	24.50	39.83	16.58%	24.50	39.83	16.58%
	VAR	20.85	32.54	15.03%	22.33	34.46	16.24%	25.16	38.11	18.79%
	FC-LSTM	22.33	34.09	18.91%	25.87	39.27	19.94%	34.09	50.27	25.08%
	ASTGCN	19.74	31.50	12.95%	21.49	34.32	13.88%	25.74	40.73	16.22%
	DCRNN	18.58	29.78	13.56%	19.84	31.76	14.71%	22.14	34.61	17.46%
	MTGNN	23.40	33.25	31.75%	24.15	34.53	32.47%	25.99	37.58	32.34%
	AGCRN	18.84	30.74	12.43%	19.53	31.92	12.92%	21.00	34.28	13.73%
	GTS	18.90	29.81	12.80%	19.58	31.22	13.48%	20.96	33.30	14.61%
	BGSLF (ours)	18.53	29.40	12.73%	19.25	30.85	13.34%	20.49	32.66	14.32%
PEMS08	HA	21.19	36.64	13.79%	21.19	36.64	13.79%	21.19	36.64	13.79%
	VAR	16.56	24.91	10.62%	19.16	28.58	12.34%	23.22	33.93	15.68%
	FC-LSTM	17.43	26.87	13.64%	20.82	32.28	12.59%	27.61	41.52	17.75%
	ASTGCN	16.03	24.75	10.26%	17.83	27.58	11.20%	21.58	32.80	12.97%
	DCRNN	14.50	22.48	9.76%	15.55	24.38	10.45%	17.58	27.30	11.62%
	MTGNN	16.48	24.13	22.84%	17.86	26.22	24.32%	20.41	29.39	28.33%
	AGCRN	15.33	24.06	9.72%	16.51	26.11	10.31%	19.01	29.94	11.71%
	GTS	14.94	23.09	9.77%	15.66	24.33	10.53%	17.07	27.03	11.71%
	BGSLF (ours)	14.40	22.62	9.26%	15.04	23.98	9.82%	16.45	26.26	10.76%
METR-LA	HA	4.15	7.77	12.90%	4.15	7.77	12.90%	4.15	7.77	12.90%
	VAR	4.42	7.89	10.20%	5.41	9.13	12.70%	6.52	10.11	15.80%
	FC-LSTM	3.44	6.30	9.60%	3.77	7.23	10.90%	4.37	8.69	13.20%
	ASTGCN	3.01	5.85	8.16%	3.53	7.14	10.16%	4.25	8.60	12.80%
	DCRNN	2.77	5.38	7.30%	3.15	6.45	8.80%	3.60	7.60	10.50%
	MTGNN	2.69	5.18	6.86%	3.05	6.17	8.19%	3.49	7.23	9.87%
	AGCRN	3.60	9.30	7.97%	4.62	11.89	9.73%	5.95	14.80	11.78%
	GTS	2.64	4.95	6.80%	3.01	5.85	8.20%	3.41	6.74	9.90%
	BGSLF (ours)	2.59	5.09	6.68%	2.97	6.11	8.02%	3.38	7.16	9.44%
Solar-Energy	HA	6.11	8.74	-	6.11	8.74	-	6.11	8.74	-
	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	-
	ASTGCN	0.65	1.70	-	0.95	2.47	-	1.69	4.12	-
	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	-
	AGCRN	0.58	1.60	-	0.84	2.24	-	1.40	3.67	-
	GTS	0.58	1.66	-	0.85	2.33	-	1.37	3.67	-
	BGSLF (ours)	0.55	1.56	-	0.80	2.16	-	1.31	3.53	-



(a) The initial and final states of the first graph adjacency matrix.

(b) The initial and final states of the second graph adjacency matrix.

Figure 2: The adjacent matrices obtained from the graph structure learning module on the PEMS04 dataset.

Table 3: Trainable Parameters of different graph structure learning based spatial-temporal models on METR-LA and PEMS04 when achieving the best results.

Data	Models	Parameters	Data	Models	Parameters
METR-LA	MTGNN	405,452	PEMS-04	MTGNN	549,100
	AGCRN	747,810		AGCRN	748,810
	GTS	38,478,291		GTS	19,125,459
	BGSLF	156,698		BGSLF	159,934

4.3. Experimental Results

Table 2 compares the performances of BGSLF and baseline models for Horizon 3, 6, and 12 ahead forecasting on PEMS04, PEMS08, METR-LA, and Solar-Energy datasets. Ta-

Table 4: Performance of different functions on METR-LA.

Data	Function	Horizon 3			Horizon 6			Horizon 12		
		MAE	RMSE	MAPE	MAE	RMSE	MAPE	MAE	RMSE	MAPE
METR-LA	Sigmoid	2.68	5.30	6.94%	3.07	6.34	8.32%	3.48	7.41	9.78%
	ReLU	2.59	5.11	6.66%	2.98	6.19	8.10%	3.41	7.29	9.71%
	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	2.59	5.09	6.68%	2.97	6.11	8.02%	3.38	7.16	9.44%

ble 2 shows the following: **(1)** On all four datasets collected at multiple locations and with different sampling rates, our proposed model achieves the start-of-the-art performance whether long-term or short-term, which demonstrates the effectiveness of our proposed models. **(2)** It is necessary to carefully design the graph structure learning module. Methods like AGCRN and MTGNN apply random initialization to initialize graph structures that lack latent spatial associations among multivariate time series and may fail to capture critical dependencies between nodes, resulting in performance degradation. **(3)** With respect to the second-best model GTS, we can observe that BGS LF achieves small improvement on METR-LA. However, it can be seen in Table 3 that the number of parameters of our proposed model is nearly 240 times less than that of the GTS model, which saves much memory and dramatically speeds up the training and inference speed. **(4)** The careful design of multi-graph generation network and graph selection module help our model dynamically capture the spatial correlation between nodes and balance efficiency and flexibility.

4.4. Effect of the SSU module

Detailed proof of SSU validity is given in supplementary material. In Table 4, 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 better than that of the discrete matrix, which is why the effect obtained by continuous function significantly outweighs Gumbel-softmax. In addition, due to the unique smoothness design and gradient redefinition method, the effect of SSU is better than other common activation functions in this task. The dependencies among different sensors learned by the graph structure learning module are visualized in Figure 2, where we set the number of learned graphs to 2. The upper heat maps in Figure 2 show the initial graphs obtained when the model starts training, and the lower represent the graph structure obtained when the model finishes training. It can be seen that our model successfully learned the sparse relationship between sensors. At the same time, the final states of the two graphs share similar patterns, indicating that some nodes are strongly related.

5. Conclusion

In this paper, we propose a novel model that joins graph structure learning and forecasting. It highlights three critical issues with previous models and provides concise and practical solutions. Our research emphasizes that the training multivariate time series can be applied to generate a specified number of valid graph structures, and the optimal spatial structure

can be selected by computing the similarity of each input multivariate time series. With a unique design of multi-graph generation network and graph selection module, the model is well balanced between efficiency and flexibility. Experiments were conducted on four real-world datasets to demonstrate the superiority of our proposed model. The well-trained embeddings and learned graphs could also be potentially applied to other tasks. Moreover, the model can also be used as a component in more complex time series forecasting models due to its concise design and superior performance.

6. Future Work

The scalability of spatial-temporal graph neural networks is still a challenging problem. BGSLF can perform well on datasets with a small number of nodes, but the performance on large-scale nodes is unknown. Nevertheless, so far, few spatial-temporal graph neural networks take into account scalability issues. In the future, the problem of scalability can be tentatively solved from the matrix factorization [BAI et al. (2020); Han et al. (2021)] or from spectral methods [Wang (2021)]. Due to the wide application of big data, the trade-off between scalability and accuracy will be an essential research direction for spatial-temporal data mining in the future.

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