Multivariate Time Series Forecasting with Transfer Entropy Graph

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Abstract: Multivariate Time Series (MTS) forecasting is an essential problem in many fields. Accurate forecasting results can effectively help in making decisions. To date, many MTS forecasting methods have been proposed and widely applied. However, these methods assume that the predicted value of a single variable is affected by all other variables, ignoring the causal relationship among variables. To address the above issue, we propose a novel end-to-end deep learning model, termed graph neural network with neural Granger causality, namely CauGNN, in this paper. To characterize the causal information among variables, we introduce the neural Granger causality graph in our model. Each variable is regarded as a graph node, and each edge represents the casual relationship between variables. In addition, convolutional neural network filters with different perception scales are used for time series feature extraction, to generate the feature of each node. Finally, the graph neural network is adopted to tackle the forecasting problem of the graph structure generated by the MTS. Three benchmark datasets from the real world are used to evaluate the proposed CauGNN, and comprehensive experiments show that the proposed method achieves state-of-the-art results in the MTS forecasting task.

Key words: Multivariate Time Series (MTS) forecasting; neural Granger causality graph; Transfer Entropy (TE)

1 Introduction

In the real world, Multivariate Time Series (MTS) data are common in various fields[1, 2], such as the sensor data in the Internet of things, traffic flows on highways, and the prices collected from stock markets (e.g., metal price)[3, 4]. In recent years, many time series forecasting methods have been widely studied and applied[5]. For univariate situations, the AutoRegressive Integrated Moving Average model (ARIMA)[6] is one of the most classic forecasting methods. However, due to the computational complexity, ARIMA is not suitable for multivariate situations. VAR[6–8] method is an extended multivariate version of the AR model, which is widely used in MTS forecasting tasks due to its simplicity. However, it cannot handle the nonlinear relationships that exist among variables, which consequently reduces its forecasting accuracy.

In addition to traditional statistical methods, deep learning methods are also applied for the MTS forecasting problem[9]. The Recurrent Neural Network (RNN)[10] and its two improved versions, namely the Long Short-Term Memory (LSTM)[11] and the Gated Recurrent Unit (GRU)[12], realize the extraction of time series dynamic information through the memory mechanism. LSTNet[13] encodes short-term local information into low-dimensional vectors using 1D convolutional neural networks, and decodes the vectors through an RNN. However, the existing deep learning methods cannot model the pairwise causal dependencies among MTS variables explicitly. For example, the future traffic flow of a specific street is easier to be influenced and predicted by the traffic information of the neighboring area. In contrast, the knowledge of
the area farther away is relatively useless\cite{14}. If such a prior causal information can be considered, it is more conducive to the interaction among variables with causality.

Granger causality analysis (G-causality)\cite{15,16} is one of the most famous studies on the quantitative characterization of time series causality. However, as a linear model, G-causality cannot handle nonlinear relationships well. Thus, Transfer Entropy (TE)\cite{17} is proposed for causal analysis, which can deal with nonlinear cases. TE has been widely used in economic\cite{18}, biological\cite{19}, and industrial\cite{20} fields.

To further address the above limitation, we propose a novel framework, called Graph Neural Network with Causality, namely CauGNN, for MTS forecasting tasks. After calculating the pairwise TE among variables, the TE matrix can be obtained, which is regarded as the adjacency matrix of the graph structure, and each variable in this matrix corresponds to one node of this graph. In addition, CNN filters with different perception scales are used for time series feature extraction to generate the feature of each node. Finally, the Graph Neural Network (GNN) is adopted to tackle the embedding and forecasting problem of the graph generated by MTS. Our major contributions are as follows:

- To the best of the authors’ knowledge, we first propose an end-to-end deep learning framework that considers MTS as a graph structure with causality.
- We use TE to extract the causality among the time series and construct the TE graph as a priori information to guide the forecasting task.
- We conduct extensive experiments on MTS benchmark datasets, and results have proved that CauGNN outperforms the state-of-the-art models.

2 Preliminary

2.1 Neural Granger causality

Neural Granger is an improved Granger causality inference method. It inherits the core idea of Granger causality, i.e., if the addition of historical information of variable \( i \) significantly improves the prediction accuracy of another variable \( j \), then variable \( i \) is the cause of variable \( j \), and vice versa. The difference is that the traditional linear Granger method uses the AR model for prediction. In contrast, the neural Granger uses deep learning and regularization to account for the nonlinearity and avoid the computational complexity caused by the pairwise calculation.

The neural Granger network structure consists of two parts: (1) the variable selection module and (2) prediction module. The variable selection module is a fully connected layer that directly accepts the historical time series as input. The neural Granger method selects key variables by adding group Lasso regularization constraints to the weight parameters of this layer. Group Lasso is an evolved version of Lasso regularization, which can divide constrained parameters into multiple subgroups. If a specific group is insignificant for prediction, the entire group of parameters will be assigned a zero value. In the variable selection module, the weights connected to an input variable are set at different time points as a group. If the weights of the subgroup are not zero under the regularization constraint, it means that the variable has a significant effect on the prediction and is thus determined as the cause of the variable to be predicted. The second part of the neural Granger is the prediction layer. This part is not significantly different from the general prediction method. Networks, such as the multilayer perceptron or LSTM, can be used. For each variable \( x_i \), a neural Granger network is established to find its cause variables.

The objective function of the network is as follows:

\[
\min_W \sum_{t=K}^T (x_{it} - g_i(x_{(t-1):(t-K)}))^2 + \lambda \sum_{j=1}^p \left\| (W^{11}_j, W^{12}_j, \ldots, W^{1K}_j) \right\|_F
\]

where \( x_{it} \) is the true value of the variable \( x_i \) at time \( t \), \( x_{(t-1):(t-K)} \) is the value of all variables in \( K \) lags, \( g_i(\cdot) \) is the function that specifies how lags from 1 to \( K \) affect the future evolution of the series, \( T \) is the observed time points, \( p \) is the number of variables, \( \lambda \) is the regularization coefficient, \( W^{11}_j, \ldots, W^{1K}_j \) represents all the weight parameters connected with the \( j \)-th variable in the variable selection module, and \( \left\| \cdot \right\|_F \) is the F-norm.

2.2 GNN

The concept of GNN was first proposed in Ref. \cite{21}, which extended existing neural networks for processing the data represented in graph domains. A wide variety of GNN models have been proposed in recent years\cite{22,23}. Most of these approaches fit within the framework of “neural message passing” proposed by Gilmer et al.\cite{24}.

In the message-passing framework, a GNN is viewed as a message-passing algorithm where node representations are iteratively computed from the features of their
neighbor nodes using a differentiable aggregation function\textsuperscript{[25–27]}. A separate line of work focuses on generalizing convolutions to graphs. The Graph Convolutional Networks (GCN)\textsuperscript{[28]} could be regarded as an approximation of the spectral-domain convolution of graph signals. GCN convolutional operation could also be viewed as the sampling and aggregating of the neighborhood information, such as GraphSAGE\textsuperscript{[29]} and FastGCN\textsuperscript{[30]}, enabling training in batches while sacrificing some time efficiency. Coming right after GCN, the Graph Isomorphism Network (GIN)\textsuperscript{[31]} and k-GNNs\textsuperscript{[32]} are developed, enabling more complex forms of aggregation. The Graph Attention Network (GAT)\textsuperscript{[33]} is another nontrivial direction to go under the topic of GNN. It incorporates attention into propagation, attending over the neighbors via self-attention. Recently, researchers have also applied GNN to the time series forecasting problem. For example, a Correlational topic of GNN. It incorporates attention into propagation, attending over the neighbors via self-attention. Recently, researchers have also applied GNN to the time series forecasting problem. For example, a Correlational

\section{Methodology}

\subsection{Problem formulation}

Given a matrix consisting of multiple observed time series $S_n = \{s_1, s_2, \ldots, s_t\}$, where $s_i \in \mathbb{R}^n$ ($i = 1, \ldots, n$) and $n$ is the number of variables, the goal of MTS forecasting is to predict $s_{t+h}$, where $h$ is the horizon ahead of the current time stamp.

\subsection{Causality graph structure with TE}

TE is a measure of causality based on information theory, which was proposed by Schreiber in 2000\textsuperscript{[34]}. Given a variable $X \in \mathbb{R}^t$, its information entropy is defined as

\begin{equation}
H(X) = - \sum p(x) \log_2 p(x)
\end{equation}

where $x$ denotes all possible values of the variable, and $p(x)$ is the corresponding probability. Information entropy is used to measure the amount of information. A larger $H(X)$ indicates that the variable $X$ contains more information. Conditional entropy is another information theory concept, given two variables $X$ and $Y$, which is defined as

\begin{equation}
H(X|Y) = - \sum p(x, y) \log_2 p(x|y)
\end{equation}

where conditional entropy $H(X|Y)$ represents the information amount of $X$ under the condition that the variable $Y$ is known. The TE of $Y$ to $X$ is defined as

\begin{equation}
T_{Y \rightarrow X} = \sum p(x_{t+1}, x^{(k)}_t, y^{(l)}_t) \log_2 p(x_{t+1}|x^{(k)}_t, y^{(l)}_t) - \sum p(x_{t+1}, x^{(k)}_t) \log_2 p(x_{t+1}|x^{(k)}_t) = \sum p(x_{t+1}, x^{(k)}_t, y^{(l)}_t) \log_2 \frac{p(x_{t+1}|y^{(l)}_t, x^{(k)}_t)}{p(x_{t+1}|x^{(k)}_t)} = H(X_{t+1}|X_t) - H(X_{t+1}|X_t, Y_t)
\end{equation}

where $x_t$ and $y_t$ represent their values at time $t$. $x^{(k)}_t = [x_t, x_{t-1}, \ldots, x_{t-k+1}]$ and $y^{(l)}_t = [y_t, y_{t-1}, \ldots, y_{t-l+1}]$. It can be found that TE is an increase in the information amount of the variable $X$ when $Y$ changes from being unknown to known. TE indicates the direction of information flow, thus characterizing causality. It is worth noting that TE is asymmetric, so the causal relationship between $X$ and $Y$ is usually further indicated in the following way:

\begin{equation}
T_{X \rightarrow Y} = T_{X \rightarrow Y} - T_{Y \rightarrow X}
\end{equation}

When $T_{X \rightarrow Y}$ is greater than 0, it means that $X$ is the cause of $Y$. Otherwise $X$ is the consequence of $Y$. In this paper, we use neural Granger to characterize the causal relationship among variables. The causality matrix $A$ of the MTS $S_n$ can be formulated with the element $a_{ij}$ corresponding to the $i$-th row and $j$-th column as

\begin{equation}
a_{ij} = \begin{cases} T_{y_i, y_j}, & T_{y_i, y_j} > c; \\ 0, & \text{otherwise} \end{cases}
\end{equation}

where $v_i$ and $v_j$ are the $i$-th and $j$-th rows of $S_n$, i.e., $i$-th and $j$-th variables of $S_n$, $c$ is the threshold to determine whether the causality is significant. $A$ can be regarded as the adjacency matrix of the MTS graph structure.

\subsection{Feature extraction of multiple receptive fields}

Time series is a special kind of data. When analyzing time series, it is necessary to consider not only its numerical value but also its trend over time. In addition, time series from the real world often has multiple meaningful periods. For example, the traffic flow of a certain street shows a similar trend every day and meaningful rules can be observed in the unit of a week. Therefore, it is reasonable to extract the features of time series in units of multiple certain periods. In this paper, we use multiple CNN filters with different receptive fields, namely kernel sizes, to extract features at multiple time scales. Given an input time series $v$ and $q$ CNN filters, denoted as $W_i$, different convolution kernel sizes $(1 \times k_i) (i = 1, 2, \ldots, q)$ are separately generated and the features $h$ are extracted as follows:

$h_i = ReLU(W_i \ast v + b_i), h = [h_1 \oplus h_2 \oplus \cdots \oplus h_q]$. "\ast" denotes the convolution operation, "$\oplus$" represents
the concatenate operation, and \( ReLU() \) is a nonlinear activation function, \( ReLU(\cdot) = \max(0, \cdot) \).

### 3.4 Node embedding based on causality matrix

After feature extraction, the input MTS is converted into a feature matrix \( H \in \mathbb{R}^{n \times d} \), where \( d \) is the number of features after the calculation introduced in Section 3.3. \( H \) can be regarded as a feature matrix of a graph with \( n \) nodes. The adjacency of nodes in the graph structure is determined by the causality matrix \( A \). For such a graph structure, GNNs can be directly applied for the embedding of nodes. Inspired by the k-GNNs model\(^{[32]}\), we propose the CauGNN model and use the following propagation mechanism for calculating the forward-pass update of a node denoted by \( v_i \):

\[
    h_i^{(l+1)} = \sigma \left( h_i^{(l)} W_1^{(l)} + \sum_{j \in N(i)} h_j^{(l)} W_2^{(l)} \right) \tag{7}
\]

where \( \sigma \) denotes the activation function (e.g., sigmoid function), \( W_1^{(l)} \) and \( W_2^{(l)} \) are parameter matrices, \( h_i^{(l)} \) is the hidden state of node \( i \) in the \( l \)-th layer, and \( N(i) \) denotes the neighbors of node \( i \). k-GNNs only perform information fusion between a certain node and its neighbors, ignoring the information of other nonneighbor nodes. This design highlights the relationship among variables, which can effectively avoid the information redundancy brought by high dimensions. By adding a priori causal information obtained by TE, the model does not need to determine the key variables for forecasting by itself. In this paper, the output dimension of the last GNN layer is 1, which is used as the prediction result.

Overall, we use \( \ell_1 \)-norm loss to measure the prediction of \( s_{t+h} \) and optimize the model via the Adam algorithm\(^{[36]}\). The schematic diagram of CauGNN is shown in Fig. 1.

### 4 Experiment

In this section, we conduct extensive experiments on three benchmark datasets for MTS forecasting tasks and compare the results of the proposed CauGNN model with the other six baselines. All the data and experiment codes are available online\(^{†}\).

#### 4.1 Data

We use three publicly available benchmark datasets.

- **Exchange-Rate\(^‡\)**: Exchange rates of eight foreign countries collected from 1990 to 2016, collected per day.
- **Energy\(^{[37]}\)**: Measurements of 26 different quantities related to the appliances’ energy consumption in a single house for 4.5 months, collected per 10 minutes.
- **Nasdaq\(^{[38]}\)**: Stock prices selected as the multivariable time series for 82 corporations, collected per minute.

#### 4.2 Methods for comparison

The methods in the comparative evaluation are as follows:

- **VAR\(^{[6–8]}\)** stands for the well-known vector regression model, which has proven to be a useful machine learning method for MTS forecasting.
- **CNN-AR\(^{[39]}\)** stands for the classical CNN. We use multilayer CNN with AR components to perform MTS forecasting.

\( † \) https://github.com/RRRussell/CauGNN.

\( ‡ \) https://github.com/laiguokun/multivariate-time-series-data.

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**Fig. 1** Schematic diagram of CauGNN. A multivariate time series consists of multiple univariate time series. CauGNN maps a multivariate time series to a graph, and each univariate time series (variable) is mapped to a node. The causality matrix is calculated to model the adjacency information of nodes, while the convolutional layer is used to catch node features. The node feature matrix and adjacency matrix are then fed into the GNN to get forecasts.
We conduct a grid search for the tunable hyper-parameters of each method in all datasets. Specifically, we set the same grid search range of input window size for each method from \(2^0, 2^1, \ldots, 2^9\) if applied. We vary hyper-parameters for each baseline method to achieve their best performance on this task. For RNN-GRU and LSTNet, the hidden dimension of the recurrent and convolutional layer is chosen from \(\{10, 20, \ldots, 100\}\). For LSTNet, the skip-length is chosen from \(\{0, 12, \ldots, 48\}\). For MLCNN, the hidden dimension of the recurrent and convolutional layer is chosen from \(\{10, 25, 50, 100\}\). We adopt the dropout layer after each layer, and set the dropout rate from \(\{0.1, 0.2\}\). We calculate the TE matrix based on the training and validation data. For CauGNN, CauGIN, CauGNN-nCau, and CauGNN-nCNN, we all set the size of the three convolutional kernels to be \(\{3, 5, 7\}\), and the number of channels of each kernel is 12 in all our models. The hidden dimension of the k-GNNs layer is chosen from \(\{10, 20, \ldots, 100\}\). For CauGIN, the hidden size is chosen from \(\{10, 20, \ldots, 100\}\). For the hyperparameter \(c\), which is the threshold to determine the significance of the causality, we search it in the range of \([0, 0.1]\), and choose it to be 0.005. The Adam algorithm is used to optimize the parameters of the proposed model. For more details, please refer to the attached code.

### 4.5 Main results

Table 1 summarizes the evaluation results of all methods on the three benchmark datasets with three metrics. Following the test settings of Ref. [13], we use each model for the time series predicting on the future moment \(\{t + 5, t + 10, t + 15\}\); thus, we set horizon= \(\{5, 10, 15\}\), which means the horizon is set from 5 to 15 days for forecasting over the exchange-rate data, from 50 to 150 minutes over the energy data, and from 5 to 15 minutes over the Nasdaq data. The best results for each metric on each dataset are set as bold in Table 1. We save the model that has the best performance on the validation set based on the MAE or RAE metric after training 1000 epochs for each method. Then we use the model to test and record the results. The results show that the proposed CauGNN model outperforms most of the baselines in most cases, indicating the effectiveness of the proposed model on MTS predicting tasks adopting the idea of using causality as the guideline for forecasting. On the other side, we observe the results of the VAR model on the Nasdaq dataset are far worse than those of other methods in some cases, partly because VAR is insensitive to the scale of input data, lowering its performance.

MLCNN shows impressive results because it can fuse near and distant future visions, and LSTNet shows
### Table 1  MTS forecasting results measured by MAE/RAE/CORR score over three datasets.

| Dataset  | Horizon | Method          | MAE  | RAE  | CORR |
|----------|---------|----------------|------|------|------|
|          |         | VAR            |      |      |      |
| Exchange-rate | 5 days  | 0.0065 0.0188 0.9619 |      |      |      |
|          | 10 days | 0.0093 0.0270 0.9470 |      |      |      |
|          | 15 days | 0.0116 0.0339 0.9318 |      |      |      |
| Energy   | 50 min  | 3.1628 0.0545 0.9106 |      |      |      |
|          | 100 min | 4.2154 0.0727 0.8482 |      |      |      |
|          | 150 min | 5.1539 0.0889 0.7919 |      |      |      |
| Nasdaq   | 5 min   | 0.1706 0.0011 0.9911 |      |      |      |
|          | 10 min  | 0.2667 0.0018 0.9273 |      |      |      |
|          | 15 min  | 0.3909 0.0026 0.5528 |      |      |      |
|          |         | CNN-AR         |      |      |      |
| Exchange-rate | 5 days  | 0.0063 0.0182 0.9638 |      |      |      |
|          | 10 days | 0.0085 0.0249 0.9490 |      |      |      |
|          | 15 days | 0.0106 0.0303 0.9372 |      |      |      |
| Energy   | 50 min  | 2.4286 0.0419 0.9159 |      |      |      |
|          | 100 min | 2.9499 0.0509 0.8618 |      |      |      |
|          | 150 min | 3.5719 0.0616 0.8150 |      |      |      |
| Nasdaq   | 5 min   | 0.2110 0.0014 0.9920 |      |      |      |
|          | 10 min  | 0.2650 0.0017 0.9199 |      |      |      |
|          | 15 min  | 0.2663 0.0017 0.9860 |      |      |      |
|          |         | RNN-GRU        |      |      |      |
| Exchange-rate | 5 days  | 0.0066 0.0192 0.9630 |      |      |      |
|          | 10 days | 0.0092 0.0268 0.9491 |      |      |      |
|          | 15 days | 0.0122 0.0355 0.9323 |      |      |      |
| Energy   | 50 min  | 2.7306 0.0471 0.9167 |      |      |      |
|          | 100 min | 3.0590 0.0528 0.8624 |      |      |      |
|          | 150 min | 3.7150 0.0641 0.8106 |      |      |      |
| Nasdaq   | 5 min   | 0.2245 0.0015 0.9930 |      |      |      |
|          | 10 min  | 0.2313 0.0015 0.9901 |      |      |      |
|          | 15 min  | 0.2700 0.0018 0.9877 |      |      |      |

comparable results by modeling periodic dependency patterns. The proposed CauGNN uses the TE matrix to collect the internal relationship between variables and analyze the topology composed of variables and relationships through the graph network. Thus, it can break through these restrictions and perform well on
general datasets.

We also fine-tune other deep learning baseline models and choose suitable hyperparameters to achieve their best performance. For the MultiHead Attention, LSTNet, and MLCNN, we set hidCNN, hidRNN, hidSkip, and window size as 50, 50, 5, and 128, respectively. For RNN-GRU, we set hidRNN as 50 and highway window as 24. As for our model CauGNN, we set hidCNN, hidGNN1, hidGNN2, and window size as 12, 30, 10, and 32, respectively. Compared with these baseline models, our proposed CauGNN model can share the same hyperparameters among various datasets and situations with robust performance, as revealed from the results.

4.6 Variant comparison

Our proposed framework has strong universality and compatibility. We replace the k-GNNs layer with the GIN layer, which also well preserves the distinctness of inputs. As shown in Table 1, the GIN layer fits into our model well and CauGIN has a similar performance with CauGNN.

For the ablation study, we also replace the TE matrix with an all-one matrix in CauGNN-nCau, assuming the value to be predicted of a single variable is related to all other variables. Thus, a completed graph is fed into the GNN layers. The experiment results show that CauGNN outperforms CauGNN-nCau, indicating the significant role that the TE matrix plays in the CauGNN model. On the other hand, we conduct experiments using the CauGNN-nCNN model, in which the CNN component is removed. The input time series data without feature extraction are fed into the GNN layer instead of the node features extracted from the CNN layer. Experiment results show that CauGNN outperforms CauGNN-nCNN, suggesting the significant role that the CNN component plays in the CauGNN model.

To test the parameter sensitivity of our model, we evaluate how the hidden size of the GNN component can affect the results. We report the MAE, RAE, and CORR metrics on the exchange-rate dataset. As seen in Fig. 2, while ranging the hidden size of GNN layers from \{10, 20, \ldots, 100\}, the model performance is steady, being relatively insensitive to the hidden dimension parameter.

To prove the superiority of multiple CNN filters, we also did an ablation study on the exchange-rate dataset when the horizon is 5 days. As shown in Fig. 3, CauGNN-RF, CauGNN-1CNN, and CauGNN represent the direct use of the raw feature (original data) as the input of the node embedding model, using one CNN filter (here, we set kernel size to 3), and the complete model CauGNN is constructed with three CNN filters. We can find that CauGNN-RF has the worst performance, indicating that the direct use of raw features will introduce too much noise, which is not conducive to the subsequent learning of the model. Meanwhile, CauGNN has the best performance, indicating that stacking multiple CNN filters can better capture multiple inherent time series period characteristics and make more accurate predictions.

5 Conclusion

In this paper, we propose a novel deep learning framework (namely CauGNN) for MTS forecasting. Using CNN with multiple receiving fields, our model introduces a priori causal information with TE features and uses a GNN for feature extraction, which effectively improves the results in the MTS forecasting. With in-depth theoretical analysis and experimental verification, we confirm that CauGNN successfully captures the causal relationship among variables and selects key variables for accurate forecasting using a GNN.

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