Explaining Dynamic Graph Neural Networks via Relevance Back-propagation

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Abstract—Graph Neural Networks (GNNs) have shown remarkable effectiveness in capturing abundant information in graph-structured data. However, the black-box nature of GNNs hinders users from understanding and trusting the models, thus leading to difficulties in their applications. While recent years witness the prosperity of the studies on explaining GNNs, most of them focus on static graphs, leaving the explanation of dynamic GNNs nearly unexplored. It is challenging to explain dynamic GNNs, due to their unique characteristic of time-varying graph structures. Directly using existing models designed for static graphs on dynamic graphs is not feasible because they ignore temporal dependencies among the snapshots. In this work, we propose DGExplainer to provide reliable explanation on dynamic GNNs. DGExplainer redistributes the output activation score of a dynamic GNN to the relevances of the neurons of its previous layer, which iterates until the relevance scores of the input neuron are obtained. We conduct quantitative and qualitative experiments on real-world datasets to demonstrate the effectiveness of the proposed framework for identifying important nodes for link prediction and node regression for dynamic GNNs.

Index Terms—Explainable AI, Dynamics, Graph Neural Networks, Layer-wise Relevance Propagation

I. INTRODUCTION

A graph is a ubiquitous data structure that models the pairwise interactions of entities. For example, in social, information, chemical, and biological domains, the data can be naturally modeled as graphs. Graph Neural Networks (GNNs) have emerged as state-of-the-art for tackling graph data [1]. [2]. While many real-world graphs are dynamic and evolving over time, various GNN models are proposed to deal with those dynamic graph structures [3]–[5]. Though GNNs make useful predictions, the black-box nature hinders users from understanding and trusting their predictions.

The studies on explainability for static GNNs have attracted great interest in recent years. Some methods are approximation-based, which use gradient or surrogate functions to approximate the target instance output from a local model [6]–[8]. However, a good approximation does not guarantee a good explanation in the sense of fidelity, due to the fact that the surrogate which approximates the target model possibly uses distinct features [9]. And some other methods are perturbation-based [10]–[12] via masking features, thus will generate an artificial impact on the model prediction and may trigger the adversarial property of deep neural networks [13]. Additionally, gradient-based methods rest on an additive assumption of feature values or the gradients to measure the importance of the input features towards the output. In summary, existing methods suffer from the adversarial triggering issue, fidelity issue, as well as additive assumption.

Though urgently needed, it is a challenging task to design such an algorithm without the above issues. Dynamic graphs are represented as a sequence of graph snapshots from different timesteps, so how to model this temporal evolutionary pattern is a crucial problem. To this end, we propose a framework DGExplainer (Dynamic Graph neural network Explainer) to provide a faithful explanation for dynamic GNNs. DGExplainer uses a backward propagation manner to compute the relevance of the output corresponding to each input feature in the dynamic GNN model. Similar to many recent backward-based methods [14]–[17], the basic idea is to compute a small subset of node features that are most important to the prediction as an explanation. First, it decomposes the prediction of a dynamic GNN and computes the relevances in a time-related module by employing Layer-wise relevance propagation (LRP). Then it further computes the relevances of the input features by back-propagating the relevances of the graph-related modules in the graph at each timestamp. Finally, by aggregating the obtained relevances from the above two steps, we can get the final relevances of node features as the measurement of the importance of the prediction. Here we list our main contributions:

- We formally define the problem of explainability of dynamic graph neural networks. As far as we know, it is one of the first few attempts to study this problem.
- We propose a novel framework (DGExplainer) to generate explanations for dynamic GNNs, from the perspective of decomposition. DGExplainer can effectively calculate the relevance scores which represent the contributions of each component for a dynamic graph.
- We demonstrate the effectiveness of the DGExplainer on six real-world datasets. The quantitative experiments indicate that the proposed method could provide faithful explanations. The qualitative experiments show that the proposed method can encode time dependency in relevance scores at different timesteps.

II. METHODOLOGY

In this section, we elaborate on the proposed methods in detail. First, we introduce the notations and problem definition. Then, we elucidate the general setting of dynamic graph neural network models. Finally, we develop the proposed method for explaining dynamic GNNs.
Figure 1: The network structure of the GCN-GRU model. Note that the GRUs and GCNs share the same parameters. \{H_l\}_{l=0}^{T}, \{X_l\}_{l=1}^{T}, \{A_l\}_{l=1}^{T} denote hidden features in GRU, node features, transformed features by GCN, adjacency matrices in different time slots, respectively.

A. Problem Definition
Given a dynamic graph as a sequence of snapshots \(G = \{G_t\}_{t=1}^{T}\), where \(T\) is the length of the sequence. \(G_t = \{V_t, E_t\}\) represents the graph at time \(t\) and \(V_t, E_t\) represents the node set, the edge set, respectively. The adjacency matrix at timestamp \(t\) is represented as \(A_t \in \mathbb{R}^{N \times N}\), where \(N = |V_t|\) is the number of nodes. The feature matrix is denoted as \(X_t \in \mathbb{R}^{N \times D}\), where \(D\) is the feature dimension, and \(x_i^t\) is the attribute vector for node \(i\) at timestamp \(t\), i.e. the \(i\)th row of \(X_t\). Without loss of generality, here we exploit \(A^{(i,j)}\) to denote the entry at \(i\)-th row, \(j\)-th column of adjacency matrix \(A\), and use \(x^{(i)}\) to denote the \(i\)-th entry of vector \(x\). We leverage \(R_k\) to denote the relevance of \(k\), where \(k\) can represent a node, an edge, a feature, etc. Also, we use \(R_{k_1 \rightarrow k_2}\) to denote the relevance of \(k_1\) is distributed from \(k_2\). The goal of explaining dynamic GNNs is to find the subgraph in \(G\) that is the most important at timestamp \(t\), given a dynamic GNN model \(f(G)\).

B. Relevance-Propagation Based Explanation
Layer-wise relevance propagation (LRP) is first proposed in [15], which aims to compute the contribution (relevance) of each pixel for the prediction of an instance given the image classifier. It assumes that the relevance is proportional to the weighted activation value this neuron produces, which follows the intuition that the larger the output activation, the more information this neuron carries, and the more contribution it has to the result. The relevance score of the output neuron is defined as the prediction score. To compute the relevance of an individual neuron, the proposed framework operates by back-propagating the relevance scores from high-level neurons recursively to low-level neurons layer by layer, finally reach to the input neurons. The propagation rule can be summarized as follow:

\[
R_{k_1 \rightarrow k_2}^{(l)} = \sum_{k_2} \frac{W_{k_1 k_2} a_{k_1}^{(l)}}{\epsilon + \sum_k W_{k k_2} a_k^{(l)}} R_{k_2}^{(l+1)},
\]

where \(W_{k_1 k_2}\) is the connection weight of neuron \(k_1\) and \(k_2\), \(R_{k_2}^{(l+1)}\) and \(R_{k_2}^{(l)}\) are relevances for the neuron \(k_2\) at layer \(l+1\) and the relevance of \(k_1\) from \(k_2\) at layer \(l\), \(a_{k_1}^{(l)}\) is the activation of neuron \(k_1\) at layer \(l\), and \(\epsilon\) is a predefined stabilizer that prevent the denominator to be zero. The main challenge for layer-wise relevance propagation is to design a proper propagation rule for the relevance redistribution of each layer.

C. Dynamic graph neural network model
A dynamic graph neural network (DGNN) takes a dynamic graph as input and outputs a graph with updated topology, node, and/or edge information. In this work, we exploit the GCN-GRU as our basic model. We summarize our model structure in Fig. 1. Specifically, the graph convolution is defined as follows:

\[
F_t^{(l+1)} = \sigma(V_l F_t^{(l)} W_t^{(l)}),
\]

where \(V_l := D_l^{-\frac{1}{2}} A_l D_l^{-\frac{1}{2}}\) is the normalized adjacency matrix, and \(D_l\) is the degree matrix with \(D_l^{(i,i)} = \sum_j A_l^{(i,j)}\). \(A_t := A_t + I_N\), \(D_t := D_t + I_N\), \(I_N\) is an identity matrix with size \(N\). \(F_t^{(l)}\) is the output at the \(l\)th layer, and \(F_t^{(0)} = X_t\). Here we assume the GCN has \(M\) layers, thus the final representation contains graph structural information is \(\hat{X}_t = F_t^{(M)}\).

Then the representation \(\{X_t\}_{t=1}^{T}\) obtained from GCN, is fed into GRU. A GRU cell is a basic unit in GRU, where the input is \(\hat{x}_t = (X_t^{(i-1)})\), the hidden state is \(h_t = (H_t^{(i-1)})\). Then the update rule of a GRU cell is shown below:

\[
\begin{align*}
\tau &= \sigma(W_{ir} \hat{x}_t + b_{ir} + W_{hr} h_{t-1} + b_{hr}) \\
\zeta &= \sigma(W_{iz} \hat{x}_t + b_{iz} + W_{hz} h_{t-1} + b_{hz}) \\
n &= \tanh(W_{in} \hat{x}_t + b_{in} + r \circ (W_{hn} h_{t-1} + b_{hn})) \\
h_t &= (1 - r) \circ h_{t-1} + r \circ n,
\end{align*}
\]

where \(r, \zeta, \tau, h, h_{hr}, h_{rz}, h_{zr}, h_{iz}, h_{iz}, h_{iz}, h_{iz}\) are learnable parameters in GRU, \(\sigma(\cdot)\) denotes an activation function, and \(\circ\) stands for an element-wise product operation.

III. EXPLANATION FOR DYNAMIC GNNs
Here, we introduce how to back-propagate the relevance through the GCN-GRU model for dynamic graphs. Fig. 2 demonstrates the layer-wise back-propagation process for calculating the relevance of the input features. Given an input dynamic graph \(G = \{G_t\}_{t=1}^{T}\) and a dynamic GNN model \(f(\cdot)\), for a graph snapshot \(G_t\), LRP aims to find out, which nodes contribute to what extent to a (positive or negative) classification or regression result by redistributing the prediction to the relevance of each neuron, such that the relevance of the neuron at the last layer is defined as \(R_{h_T} := f(G_t)_t\), where the task can be a classification (assuming the results from the classifier are thresholded at zero) or regression. For a single node, our method is a mapping: \(\mathbb{R}^N \rightarrow \mathbb{R}^3\), such that the relevance denotes the extent of the contribution to the result.
A. Compute the relevances in GRU

Given $R_{kh}$ at $t = T$, the goal is to compute $R_{hn-1}$ and $R_{xh-1}$ from $R_{h}$. As described in Sec. II-B, relevance back-propagation redistributes the activation of a descendant neuron to its predecessor neurons. And the relevance is proportional to the weighted activation value. Eqn. 3d shows the relation of different components in the last step of GRU. Note that, neurons $r$ and $z$ only have a message from neuron $h_{t-1}$, as shown in Eqn. 3a and Eqn. 3b, so their message (contribution) to $h_{t}$ could be merged into the message from neuron $h_{t-1}$ and their relevance scores can be regarded as constants, so we do not have to consider their relevances. Thus, based on Eqn. 3d, the relevance of components $h_{t}$, $n$, $h_{t-1}$ satisfy:

$$R_{h_{t}} = R_{h_{t-1} \rightarrow h_{t}} + R_{n \rightarrow h_{t}}.$$  

(4)

Notice that $h_{t-1}$ is used to compute $n$ in Eqn. 3d and $h_{t}$ in Eqn. 3d, which reveals that $R_{hn-1}$ have two sources, $n$ and $h_{t}$. Therefore, we can define $R_{hn}$ based on $R_{hn-1}$ and $R_{h_{t-1} \rightarrow n}$ as:

$$R_{hn} = R_{h_{t-1} \rightarrow h_{t}} + R_{n \rightarrow h_{t}},$$  

(5)

It can be concluded that, if we can derive $R_{h_{t-1} \rightarrow h_{t}}$ and $R_{hn}$, we will be able to get $R_{hn}$. Thus, we formulate this problem into three steps, computing $R_{h_{t-1} \rightarrow h_{t}}$, $R_{hn}$, and $R_{hn}$, as below:

(a) Computing $R_{h_{t-1} \rightarrow h_{t}}$: First, from Eqn. 3d, we can obtain:

$$\frac{R_{n \rightarrow h_{t}}}{R_{h_{t-1} \rightarrow h_{t}}} = \frac{z \circ n}{(1 - z) \circ h_{t-1}}.$$  

(6)

Solving for 4 and 6, we obtain:

$$R_{n \rightarrow h_{t}} = \frac{z \circ n}{h_{t-1} + \epsilon} \circ R_{h_{t}} = R_{n},$$  

(7)

$$R_{h_{t-1} \rightarrow h_{t}} = \frac{(1 - z) \circ h_{t-1}}{h_{t-1} + \epsilon} \circ R_{h_{t}},$$  

(8)

where $\epsilon > 0$ is a constant introduced to keep the denominator non-zero.

Notice that the only ancestor neuron of $n$ is $h_{t}$, so here $R_{n \rightarrow h_{t}}$ is actually $R_{n}$, so in the following left section, we use $R_{n}$ for simplicity.

(b) Computing $R_{hn}$: Denote different components in Eqn. 3c as:

$$n_{1} := W_{ln} \hat{x}_{t},$$  

(9a)

$$n_{2} := r \circ (W_{hn} h_{t-1}) = W_{rn} h_{t-1},$$  

(9b)

$$b_{n} := b_{in} \circ r \circ b_{hn}.$$  

(9c)

Then their relevance satisfies:

$$R_{n_{1}} = R_{n_{1}} + R_{n_{2}} + R_{b_{n}},$$  

(10)

$$R_{n_{1}} : R_{n_{1}} : R_{b_{n}} = n_{1} : n_{2} : b_{n},$$  

(11)

hence $R_{n_{1}}$ and $R_{n_{2}}$ can be obtained as:

$$R_{n_{1}} = \frac{W_{ln} \hat{x}_{t}}{\epsilon + (W_{ln} \hat{x}_{t} + b_{n} \circ r \circ (W_{hn} h_{t-1} + b_{hn}))} \circ R_{n_{1}},$$  

(12)

$$R_{n_{2}} = \frac{r \circ (W_{hn} h_{t-1})}{\epsilon + (W_{ln} \hat{x}_{t} + b_{n} \circ r \circ (W_{hn} h_{t-1} + b_{hn}))} \circ R_{n_{2}}.$$  

(13)

Let $n_{1}^{(k)}$ denote the $k$-th entry of $n_{1}$, according to (9a), we have $n_{1}^{(k)} = \sum_{j} W_{ln}^{(k,j)} \hat{x}_{t}^{(j)}$. The relevance $R_{n_{1}}$ is redistributed in proportion to the contribution for $n_{1}$ and hence $R_{xn}$, which equals to $R_{xn \rightarrow n_{1}}$ because $n_{1}$ is the only source of the relevance to $\hat{x}_{t}$, by using LRP-$\epsilon$ rule [13].

$$R_{xn \rightarrow n_{1}} = \sum_{k} \frac{W_{ln}^{(k,j)} \hat{x}_{t}^{(j)}}{\epsilon + \sum_{l} W_{ln}^{(k,l)} \hat{x}_{t}^{(l)}} R_{n_{1}}.$$  

(14)

Since $h_{t-1}$ only influences $n_{2}$ among the three parts of $n$, we obtain $R_{hn}$ using $\epsilon$-rule for Eqn. 9b:

$$R_{hn}^{(j)} = \frac{W_{rn}^{(k,j)} h_{t-1} \hat{x}_{t}^{(j)}}{\epsilon + \sum_{l} W_{rn}^{(k,l)} h_{t-1} \hat{x}_{t}^{(l)}} R_{n_{2}}.$$  

(15)

(c) Compute $R_{h_{t-1} \rightarrow n}$: Upon obtaining $R_{n \rightarrow h_{t}}$ and $R_{hn}$, in [7] and [8] based on Eqn. 5, $R_{h_{t-1} \rightarrow n}$ can be computed by adding Eqn. 8 and Eqn. 15 together:

$$R_{h_{t-1} \rightarrow n} = R_{h_{t-1} \rightarrow h_{t}} + \sum_{j} R_{hn}^{(j)}.$$  

(16)

Notice that $R_{xh}$ is the relevance of a sample $\hat{x}_{t}$, which is a row in $X_{t}$. By computing $\{R_{xh}^{(1)}\}_{i=1}^{N}$, we can get $R_{xh}^{(1)} = [R_{xh}^{(1)}; R_{xh}^{(2)}; \ldots; R_{xh}^{(N)}]$.

B. Back-propagate the relevances in GCN

Then we backprop in the GCN to get $R_{x}$ from $R_{xh}$. Note that the $R_{xh}$ is the relevance of the output $\hat{X}$ of the GCN at the time step $t$ and $R_{xh} = R_{F_{m}}$. We can rewrite Eqn. 2 as:

$$F_{t}^{(l+1)} = \sigma(P_{l}^{(l)}W_{l}^{(l)}),$$  

(17)

$$P_{l}^{(l)} := V_{l}^{(l)}.$$  

(18)

Let $F_{t}^{(l+1)}(k,:), (P_{l}^{(l)})(k,:), (P_{l}^{(l)})(c,k)$, $(F_{l}^{(l)})(c,k)$ denote the $k$-th row of $F_{t}^{(l+1)}$, the $k$-th row of $P_{l}^{(l)}$, the $k$-th column of $F_{l}^{(l)}$, the $k$-th column of $F_{l}^{(l)}$, respectively. We have

$$(F_{t}^{(l+1)})(k,:) = \sigma((P_{l}^{(l)})(k,:))W_{l}^{(l)}),$$  

(19)

$$(P_{l}^{(l)})(c,k) := V_{l}^{(l)}(F_{l}^{(l)})(c,k).$$  

(20)

Leveraging the $\epsilon$ rule, we assign the relevance by:

$$R_{F_{l}^{(l)}(c,k)} = \sum_{b} \frac{(P_{l}^{(l)}(b,k))W_{l}^{(l)}(b,k)}{\epsilon + \sum_{b} (P_{l}^{(l)}(b,k))W_{l}^{(l)}(b,k)} R_{F_{l}^{(l+1)}(k,:)};$$  

(21)

$$R_{F_{l}^{(l)}(c,k)} = \sum_{b} \frac{V_{l}^{(l)}(b,a)F_{l}^{(l)}(a,c)}{\epsilon + \sum_{a} V_{l}^{(l)}(b,a)F_{l}^{(l)}(a,c)} R_{F_{l}^{(l+1)}(c,k)},$$  

(22)

where $(W_{l}^{(l)}(b,k))$ represents the entry at $j$-th row and $k$-th column of $W_{l}^{(l)},$ and $V_{l}^{(l)}(b,a)$ denotes the entry at $b$-th row and $j$-th column of $V_{l}^{(l)}$. $R_{F_{l}^{(l+1)}}$ can henceforth be obtained from $R_{F_{l}^{(l+1)}}$ via Eqn. 21 and Eqn. 22, and finally $R_{F_{l}^{(l)}}$ can be obtained. Notice that $F_{l}^{(0)} = X_{t}$, so we have $R_{F_{l}^{(0)}} = R_{xh}$ and hence the backward process for obtaining relevance in the GCN is completed. To further identify important nodes at a specific time-slot, we transform the relevances into absolute values sum up all the relevances along the feature dimension to get the relevance of a node at time $t$: $R_{xh}^{(1)} = \sum_{j=1}^{N} (R_{xh}^{(1)}(j))$. The entire algorithm is summarized in Algorithm 1.
Algorithm 1 DGExplainer

Input: The input \( \{X_t\}_{t=1}^T \) and \( \{A_t\}_{t=1}^T \), the final relevance \( \{R_{h_t}\}_{t=1}^T \), the pre-trained model \( f(\cdot) \).

Output: The relevances \( \{RX_t\}_{t=1}^T \).

1: // Forward process:
2: for each \( t \in [1, T] \) do
3:     Compute \( \hat{X}_t \) via \( F^{(t)} = \sigma(V_t F^{(t)} W^{(f)}) \) with \( F^{(0)} = X_t \).
4:     for each \( j \in [1, N] \) do
5:         Compute the hidden state \( h_t \) for the \( j \)-th sample \( X_{t}^{(j)} \) via Eqn. (3) with \( h_{t-1} \).
6:     end for
7: end for
8: // Backward process:
9: for each \( t = T, T-1, \ldots, 1 \) do
10:     for each \( j \in [1, N] \) do
11:         Compute \( R_{h_t} \) via Eqn. (7, 12, 13), and \( R_{h_t} \) for the \( j \)-th sample \( X_{t}^{(j)} \) via Eqn. (14) and hence obtain \( R_{h_t}^{(j)} \).
12:     end for
13: end for
14: Stack \( \{R_{h_t}^{(j)}\}_{j=1}^N \) to get \( R_{h_t} \).
15: Calculate \( RX_t \) by iteratively applying Eqn. (21, 22) with \( RX_t = R_{h_t}^{(j)} \) and \( R_{X_t} \).
16: end for
17: return \( \{RX_t\}_{t=1}^T \).

IV. EXPERIMENTS

In this section, we conduct extensive experiments on six real datasets in terms of three evaluation metrics to evaluate the performance of the proposed approach.

A. Datasets

We evaluate our proposed method with other representative methods on real-world datasets. As described in Table I the datasets are split into the training and test sets according to the temporal dimension. For each dynamic graph \( G_t \), given partially observed snapshots \( \{G_1, G_2, \ldots, G_T\} \) with node attributes \( X = \{X_1, \ldots, X_T\} \) and adjacency matrices \( A = \{A_1, \ldots, A_T\} \), our goal is to predict the behavior of \( G_{T+1} \) for node attribution regression or dynamic link prediction. More details about the datasets can be found below.

| Dataset      | RH | PeMS04 | PeMS08 | Enron | FB | COLAB |
|--------------|----|--------|--------|-------|----|-------|
| # Nodes      | 55,863 | 307 | 170 | 184 | 663 | 315 |
| # Edges      | 858,990 | 680 | 340 | 266 | 1068 | 308 |
| # Train/Test | 122/34 | 45/14 | 50/12 | 8/3 | 6/3 | 7/3 |
| # Time Step  | 6 | 4 | 4 | 4 | 4 | 4 |

- Reddit Hyperlink [18] (Reddit): it is a directed network extracted from posts that generate hyperlinks connecting one subreddit to another. We use this dataset for link prediction.
- PeMS04 and PeMS08 [19]: they are real-time traffic datasets, and are aggregated into every 5-minute interval from the raw data, so each detector contains 288 data points per day. The data are transformed by zero-mean normalization to let the average be 0. The task is node regression.
- Enron [20], FB [21], COLAB [22]: they are dynamic graphs constructed from email messages exchanged between employees, co-authorship relationships among authors, and the Facebook wall posts, correspondingly. We collect and tackle the three datasets following the previous work [23].

B. Tasks

Following the setting in a previous work [5], we conduct experiments on two tasks, including link prediction and node classification. The output embedding of a node \( u \) produced by the GCN-GRU model at time \( t \) is represented by \( h_T^u \).

Link prediction: For implementation, we concatenate the feature embeddings of \( u \) and \( v \) as \( [h_T^u; h_T^v] \) and apply an MLP to predict the link probability by optimizing the cross-entropy loss. Reddit Hyperlink, Enron, FB, and COLAB are used for experimentation for this task. We leverage Area Under Curve (AUC) as the evaluation metric.

Node regression: To get a prediction value for a node \( u \) at time \( t \), we exploit a softmax activation function for the last layer of GCN, outputting the provability vector \( h_T^u \). Two datasets are used for the experiments of this task, including PeMS04 and PeMS08. The evaluation metric is mean absolute error (MAE).

C. Compared methods and evaluation indexes

1) Compared methods

We compare the performance of our algorithm with two explainability methods:

- Sensitivity Analysis (SA) [7]: It assumes that the norm of the gradient over input variables demonstrates their relative importance. Then the saliency map \( M_{Grad} \) for the input \( x \) is computed by \( M_{Grad} = \frac{\partial y^c}{\partial x} \), where \( y^c \) is the score for class \( c \) before a softmax layer.
- Grad×Input [24]: Grad×Input corresponds to the element-wise product of the input with the gradient. The result \( M_{GI} \) for Grad×Input is obtained by \( M_{GI} = \frac{\partial y^c}{\partial x} \odot x \).

2) Evaluation indexes

Next, we also report quantitative metrics that capture desirable aspects of explanations: sparsity, stability, and fidelity. Following these metrics, we compare the quality of each explanation baseline and demonstrate the trade-offs.

- Sparsity: Sparsity measures the fraction of nodes that are selected for an explanation [8, 25]. It evaluates whether the model could efficiently mark the most contributive part in the dataset. High Sparsity scores mean that fewer numbers of NOEs are identified as important. In our experiment, we compute sparsity by calculating the ratio of nodes with saliency values or relevances lower than a certain pre-defined threshold on a scale of 0 to 1.
- Fidelity: Fidelity is used to characterize whether the explanations are faithfully important to the model predictions [26]. In the experiment, we obtain fidelity by calculating the difference in classification accuracy or regression errors obtained by occluding all nodes with importance values greater than a threshold, on a scale of 0 to 1. And we averaged the fidelity scores across classes for each method.
- Stability: Stability measures the explanation when small changes are applied to the input [26]. Good explanations should be stable, which means that the explanations remain the same when there are small changes. To evaluate the stability of methods under input perturbations, we add 20% more edges randomly and evaluate the change of relevances/importances produced by the model.
D. Experimental settings
We run all of our experiments on an NVIDIA RTX A4000 Ti GPU with 16GB of RAM. For all datasets, we consider a two-layer GCN. We train the model on the training set for 100 epochs with the Adam optimizer [27] and with the initial learning rate of 0.01. When necessary, we employ a two-layer MLP with 64 hidden units. For the proposed model, we fix the \( \epsilon = 0.0001 \). Note that the model performance results are obtained on average analysis. Our evaluation metrics include sparsity, fidelity and stability.

E. Quantitative Evaluation
In this section, we show the effectiveness of our framework in capturing those important nodes in terms of fidelity, sparsity, and stability.

Results on Fidelity. Fidelity reflects whether an explanation method is capable of capturing important nodes. A good explanation method should have high fidelity. To measure fidelity, we first sort the nodes from high to low according to their importance, and then we occlude several top nodes and keep other nodes reserved (e.g. remained 90%, 80%, 70%, 60%, 50%). As illustrated in Fig. (3), the proposed method achieves the best performance on most datasets and obtains comparable results on the remaining datasets.

Results on Sparsity. According to different thresholds, we plot the sparsity measurements as illustrated in Fig. (4). We can see the proposed method achieves the highest sparsity.

Results on Stability. A stable explanation method should give close explanations when the inputs have small perturbations. Hence, for stability indexes, the lower, the better. As illustrated in Table (II), the proposed method is better than Grad⊙Input but not as satisfactory as SA.

F. Qualitative Results
In addition to the quantitative experiments, we also visualize the explanation of PeMS04 and demonstrate the effectiveness of our proposed framework in Fig. (5).

Table II: The stability performance on the datasets.

| Dataset | RH | PeMS04 | PeMS08 | Enron | FB | COLAB |
|---------|----|--------|--------|-------|----|-------|
| SA      | 0.172 | 0.183  | 0.151  | 0.130 | 0.130 | 0.177 |
| Grad⊙Input | 0.286 | 0.221  | 0.157  | 0.148 | 0.151 | 0.245 |
| DGExplainer | 0.211 | 0.201  | 0.160  | 0.146 | 0.149 | 0.248 |

Figure 5: The illustration of the proposed method on PeMS04 dataset. The warm color shows positive effects and the cold color shows negative effects. The depth of the color reflexes the degree of the effect.

In this example, we show three graphs from time stamp \( t = 1 \) to \( t = 3 \) from PeMS04 dataset. Our model successfully identifies node 7 has the largest positive effect on the prediction. And at \( t = 2 \), node 7 begins to have traffic to node 1, and node 8 is identified as the most contributive node that positively affects the prediction at this time.

V. Conclusion
In this paper, we study the explainability of DGGNs and propose a practical framework, named DGExplainer, that relies on the backward relevance to yield explanations for the prediction of DGGNs. We systematically evaluate the performance of representative explainability methods for DGGNs using the metrics of sparsity, fidelity and stability, meanwhile conducting qualitative experiments to illustrate the effectiveness of the proposed model. The results demonstrate that DGExplainer has a satisfactory performance. We hope this framework can benefit the machine learning community in dynamic graph neural networks.
Figure 4: Comparison of sparsity measurement on different datasets.

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