Towards Prototype-Based Self-Explainable Graph Neural Network

Enyan Dai
The Pennsylvania State University
emd5759@psu.edu

Suhang Wang
The Pennsylvania State University
szw494@psu.edu

ABSTRACT

Graph Neural Networks (GNNs) have shown great ability in modeling graph-structured data for various domains. However, GNNs are known as black-box models that lack interpretability. Without understanding their inner working, we cannot fully trust them, which largely limits their adoption in high-stake scenarios. Though some initial efforts have been taken to interpret the predictions of GNNs, they mainly focus on providing post-hoc explanations using an additional explainer, which could misrepresent the true inner working mechanism of the target GNN. The works on self-explainable GNNs are rather limited. Therefore, we study a novel problem of learning prototype-based self-explainable GNNs that can simultaneously give accurate predictions and prototype-based explanations on predictions. We design a framework which can learn prototype graphs that capture representative patterns of each class as class-level explanations. The learned prototypes are also used to simultaneously make prediction for a test instance and provide instance-level explanation. Extensive experiments on real-world and synthetic datasets show the effectiveness of the proposed framework for both prediction accuracy and explanation quality.

ACM Reference Format:

Enyan Dai and Suhang Wang. 2022. Towards Prototype-Based Self-Explainable Graph Neural Network. In Proceedings of ACM Conference (Conference'17). ACM, New York, NY, USA, 9 pages. https://doi.org/10.1145/nnnnnn.nnnnnn

1 INTRODUCTION

Graph structured data such as traffic networks, social networks, and molecular graphs are very pervasive in real world. To model the graph structured data for various applications such as drug discovery [15], financial analysis [32], and recommendation system [33], various graph neural networks (GNNs) [5, 12, 17] have been proposed and made remarkable achievements. The success of GNNs relies on the message-passing mechanism, i.e., the node representations in GNNs will aggregate the information from the neighbors to capture the attribute and topology information. Many message-passing mechanisms have been investigated to learn powerful representations from graphs, facilitating various tasks such as node classification [8, 17] and graph classification [35].

Despite the great success of GNNs in modeling graphs, GNNs have the same issue of lacking explainability as other deep learning models due to the high non-linearity in the model. In addition, the message-passing mechanism of GNNs that aggregates neighborhood features to capture topology information makes it more challenging to understand the predictions. The lacking of explainability in GNNs will largely limit their adoption in critical applications pertaining to fairness, privacy and safety. For instance, a GNN model may be trained to explore the proprieties of various drugs. However, due to the black-box characteristic of GNNs, it is unknown whether the rules learned by GNN model is consistent with the chemical rules in the real-world, which raises the concern of applying predictions that may threaten the drug safety.

Extensive approaches [24, 30] have been investigated to explain trained neural networks or give self-explainable predictions on independent and identically distributed (i.i.d) data such as images. However, they fail to generalize to GNNs due to the utilization of message-passing mechanism designed for relational information preservation. Recently, some initial efforts [14, 22, 38, 41, 43] have been taken to address the explainability issue of GNNs. For example, GNNEXplainer [38] explains the prediction of an instance by identifying the crucial subgraph of the instance’s local graph. Model-level explanation is also investigated by generating graph patterns that maximize the prediction of each class by the target model [41]. However, most of existing GNN explainers focus on the post-hoc explanations, i.e., learning an additional explainer to explain the predictions of a trained GNN. Since the learned explainer cannot have perfect fidelity to the original model, the post-hoc explanations may misrepresent the true explanations of the GNNs [28]. Therefore, it is crucial to develop a self-explainable GNN, which can simultaneously give predictions and explanations.

One promising direction of self-explainable GNN is to learn prototype graphs of each class to present the key patterns of each class and simultaneously conduct prediction and give explanations with the learned prototypes. The prototypes can provide class-level and instance-level self-explanations. Figure 1 gives an illustration of the prototype-based self-explanations on a toy classification problem. As shown in the figure, the problem is to predict whether a graph is cyclic or not. Taking the class cyclic as an example, the learned prototype graphs are typical patterns of cyclic graphs of

Figure 1: An illustration of self-explanation with prototypes on classifying whether the test graph is cyclic.
various sizes. Therefore, the learned prototype graphs of class cyclic can provide class-level explanation to show representative graphs of class cyclic. For a test graph \( G_t \), we will match it with the prototype graphs of each class to give the prediction. Specifically, the instance-level explanation for predicting \( G_t \) can be: “Graph \( G_t \) is classified as cyclic, because it is most similar to the second prototype graph of class cyclic.” Though promising, learning representative graphs for self-explainable classification remains an open problem.

Therefore, in this work, we investigate a novel problem of learning prototype-based self-explainable graph neural network. However, this is a non-trivial task. There are two main challenges: (i) how to efficiently learn high-quality prototypes that are representatives of each class for class-level explanation. Though some existing works [6, 21] have studied prototype learning for self-explanations, they are mainly proposed for i.i.d data. Recently, ProtGNN [45] applies a Monte Carlo tree search to identify subgraphs from raw graph as prototypes. However, the search algorithm is very time consuming. And the prototypes are limited to the subgraphs in the dataset, which might not be that representative; and (ii) how to simultaneously give an accurate prediction and provide correct prototype-based instance-level explanation. Different from images, the matching process between the test graph and prototype graphs cannot directly use simple metric such as Euclidean distance. Moreover, the supervision of the matching result is not available. How to effectively leverage the classification supervision for prototype learning and correct explanations needs further investigation.

In an attempt to address the above challenges, we develop a novel Prototype-Based Self-Explainable GNN (PxGNN). To efficiently obtain the prototype graphs, PxGNN adopts a prototype graph generator to attain the prototype graphs from the learnable prototype embeddings. A constraint on the learnable prototype embeddings and self-supervision from graph reconstruction are utilized to guarantee the quality of learned prototype embeddings and generated prototype graphs, respectively. An encoder is deployed to match the test graph with the generated prototype graphs for self-explainable classification. Since representative prototype graphs of a certain class is supposed to be similar to the test graphs in the same class, the labels can provide implicit supervision to ensure the representativeness of the prototype graphs and guide the matching process. More specifically, a novel classification loss is proposed to simultaneously ensure the accuracy of prediction and the quality of prototype-based instance-level explanation. And the classification loss is utilized to jointly train the model and prototype embeddings to learn prototypes well represent their corresponding classes.

In summary, our main contributions are:

- We investigate a novel problem of learning prototype graphs for self-explainable classification on graph-structured data;
- We develop a new framework PxGNN, which learns an effective prototype generator with self-supervision to obtain high-quality prototype graphs for accurate predictions and explanations;
- We construct a synthetic dataset which can quantitatively evaluate the prototype-base explanation, and Extensive experiments on both real-world and synthetic datasets demonstrate the effectiveness of our PxGNN in learning representative prototypes for accurate self-explainable classification.

1Code and datasets will be released upon acceptance

2 RELATED WORK

2.1 Graph Neural Networks

Graph Neural Networks (GNNs) [4, 17, 31, 37] have shown great ability for representation learning on graphs, which facilitate various applications such as traffic analysis [46], recommendation system [37], and drug generation [4]. Generally, existing GNNs [7–9, 12, 17, 19, 31, 36] utilize a message-passing mechanism that a node’s representation is updated by aggregating and combining the features from its neighbors. For example, GCN [17] averages the representations of neighbors and the target node followed by an non-linear transformation. GAT [31] adopts an attention mechanism to better aggregate the representations of the nodes from the neighbors. Recently, various GNN models are proposed to further improve the performance of GNNs [7, 8, 16, 20, 26, 39, 47]. For instance, FastGCN [7] is proposed to alleviate the scalability issue of GCN. In addition, some methods [8, 20] focus on overcoming the oversmoothing issue of GCN and design deep GNNs to incorporate more hops of neighbors. Moreover, to facilitate the downstream tasks that are short of labels, self-supervised GNNs [16, 26, 39, 47] are investigated to learn better representations.

2.2 Explainability of Graph Neural Networks

Despite the great success of graph neural networks, the problem of lacking explainability hinders the adoption of GNNs to various high-stake domains such as credit estimation. Though extensive methods [1, 11, 13, 29, 40, 44] have been proposed to explain neural networks, they are overwhelmingly developed for i.i.d data such as images and texts and cannot be directly applied to explain GNN models. Recently, some works in explainability of GNNs are emerging [3, 10, 22, 25, 38, 41]. The majority of these GNN explainers give the explanations by extracting the crucial nodes, edges, and/or node features. For instance, GNNExplainer [38] learns soft masks for edges and node features to explain the predictions with the identified subgraphs and features. PGExplainer [22] proposes to combine the global view of GNNs to facilitate the extraction of important graphs by applying a parameterized explainer. XGNN [41] generates representative graphs for a class as model-level explanations for graph classification.

However, the aforementioned methods focus on post-hoc explanations for a trained GNN, i.e., they usually require additional explainer to explain the target GNN, which might misrepresent the decision reasons of the model. There are very few initial efforts for self-explainable GNNs [10, 45], which aims to simultaneously give predictions and explanations on the predictions. SE-GNN [10] simultaneously give the predictions and explanations of a target node by identifying the K-nearest labeled nodes. ProtGNN [45] is the most similar work to ours, which finds subgraphs from the raw graphs as prototypes to give self-explanations. However, ProtGNN only focuses on graph classification and the computational cost is very large due to the searching phase in finding the prototype subgraphs. Our proposed method is inherently different from this work: (i) we propose a novel prototype-based self-explainable GNN that is effective in both node and graph-level classification tasks; (ii) a prototype generator is deployed to efficiently learn more representative prototypes for self-explainable classification.
We denote an attributed graph by $G = (V, E, X)$, where $V = \{v_1, ..., v_N\}$ is the set of $N$ nodes, $E \subseteq V \times V$ is the set of edges, and $X = \{x_1, ..., x_N\}$ is the set of node attributes with $x_i$ being the node attributes of node $v_i$. Let $A \in \mathbb{R}^{N \times N}$ be the adjacency matrix of the graph $G$, where $A_{ij} = 1$ if nodes $v_i$ and $v_j$ are connected; otherwise $A_{ij} = 0$. In this paper, we focus on both graph classification and node classification tasks. For graph classification, a set of labeled graphs $D_L = \{G_l; y_l\}_{l=1}^{\vert D_L \vert}$ is given, where $\vert D_L \vert$ is the size of the training set and $y_l \in \{1, ..., C\}$ denotes the label of graph $G_l$. We aim to give accurate prediction on unlabeled test set $D_U = \{G_u\}_{u=1}^{\vert D_U \vert}$. As for semi-supervised node classification in a GNN with $n$ layers, the result is computed on the local graph $G_u^{(n)}$ that contains $n$ hops of the connected nodes. Thus, the node classification task can be viewed as a special case of graph classification on local graph of the center node. In this paper, we aim to develop a self-explainable GNN that can accurately predict labels and provide both class-level and instance-level explanations. First, for class-level explanation, for each class $l \in \{1, ..., C\}$, we will learn $K$ prototype graphs $P_l = \{\tilde{G}_l\}_{k=1}^K$ which are representative prototypical graph patterns of class $l$. Second, for a test graph $G_t$, we will match the test graph with the learned prototype graphs and predict the label based on prototype graphs. Then, the instance-level explanation can be: “Graph $G_t$ is predicted as class $l$, because it is similar with the prototype graphs of class $l$.” With the description above, the problem of learning prototype-based self-explainable GNN can be written as:

**Problem 1.** Given the dataset $D$, where $D = D_L$ for graph classification and $D = D_L \cup D_U$ for semi-supervised node classification, we aim to learn a self-explainable GNN $f : G \rightarrow y$, which can generate prototype graphs $\{P_l\}_{l=1}^C$ as class-level explanation and give accurate prediction to each unlabeled graph $G_u \in D_U$, along with the best matched prototype graphs $\tilde{G}_{u,\alpha}$ as the instance-level explanation.

## 4 METHODOLOGY

In this section, we present the details of the proposed framework PxGNN. In particular, PxGNN will generate prototype graphs that show the representative graph patterns of each class as class-level explanation. Meanwhile, for a test graph $G_t$, the prediction will be provided based on the similarity scores between $G_t$ and prototype graphs in different classes. Those most similar prototypes to $G_t$ also serve as instance-level explanation. In essence, we are faced with two challenges: (i) how to design the framework to effectively learn high-quality prototype graphs that capture representative patterns; and (ii) how to ensure the accuracy of the classification on the test instance and the correctness of the corresponding instance-level explanation. To address the above challenges, we propose a novel framework PxGNN, which is illustrated in Figure 2. It is composed of a prototype generator $fZ$, an encoder $fE$ and a prototype-based classifier $fC$. The prototype generator $fZ$ takes the learnable prototype embeddings as input to generate prototype graphs. The encoder $fE$ is adopted to match the test graph with the prototype graphs in feature space. Finally, based on the similarity scores between the test graph and prototype graphs in different classes, the classifier $fC$ can give the prediction with self-explanation. To generate high-quality prototype graphs, we utilize the self-supervision of the graph reconstruction to train the prototype generator and constrain the learnable prototype embedding. In addition, a novel classification loss is proposed to ensure the accuracy of predictions and the quality of explanations. Note that our PxGNN is flexible to both node classification and graph classification. The main difference between them is that the prototype graphs in node classification focus on the local graph of the test node instead of a whole graph of an instance. Next, we will use graph classification as an example to introduce each component in detail.

### 4.1 Prototype Graph Learning

Our PxGNN relies on realistic and representative prototype graphs to give accurate predictions and explanations. To obtain high-quality prototype graphs, we adopt two strategies for prototype graph generation: (i) self-supervision of reconstructing graphs from the embeddings encoded by $fE$ is utilized to train the prototype-generator $fZ$; and (ii) we propose an effective method to initialize the prototype graphs. The initialized prototype graphs are further used to guide the learning of prototype embeddings and the prototype graph generation.

#### 4.1.1 Prototype Generator and Encoder

To generate the prototype graph using the prototype generator, each prototype graph $\tilde{G}_{l, k}$ is associated with a set of learnable prototype embeddings $H_{l, k} = [\tilde{h}_1, ..., \tilde{h}_{NlK}]$, where $\tilde{h}$ denotes the embeddings of $i$-th node in $\tilde{G}_{l, k}$ and $N_{lK}$ is the number of nodes in $\tilde{G}_{l, k}$. These embeddings are learned together with other components of PxGNN and initialized using an effective strategy to facilitate the learning process, which will be discussed in Sec. 4.1.2. $N_{lK}$ can be set according to the various sizes of the initialized prototype graphs to learn prototype graphs in different sizes. The generator $fZ$ takes in $H_{l, k}$ and generates $\tilde{G}_{l, k}$. For an attributed graph, the prototype graph generator $fZ$ needs to generate both node features and graph topology. Given the node embedding $\tilde{h}_i$, the attributes of node $v_i$ is generated by a MLP as

$$\tilde{x}_i = MLP(\tilde{h}_i), \quad (1)$$

For topology prediction, we predict the link weight between node $v_i$ and $v_j$ as

$$\tilde{S}_{ij} = \sigma(W \cdot CONCAT(\tilde{x}_i, \tilde{x}_j)), \quad (2)$$

where $\sigma$ is the sigmoid function and $W$ is the learnable parameters.

To ensure that the generated prototype graph patterns are reasonable, self-supervision from the dataset $D$ is applied on prototype generator $fZ$ to generate realistic graphs that follow the distribution of $D$. Following previous graph generative model [18], graph reconstruction loss and an auxiliary encoder $fE$ are deployed to train the graph generator. Specifically, the encoder $fE$ takes the graph $G_t \in D$ as input and outputs the node embeddings $H_t$. The encoder adopts GNN to obtain node embeddings that capture both node features and graph topology information, which can be written as

$$H_t = GNN(X_t, A_t), \quad (3)$$

where $X_t$ and $A_t$ are the node attribute matrix and adjacency matrix of graph $G_t \in D$. With the embedding matrix $H_t$, we can get the
The overall reconstruction loss can be written as:

$$L_{\text{rec}} = \frac{1}{|D|} \sum_{d \in D} \sum_{i \in D} \sum_{j \in |D|} \left[ - \log(S_{j|k}) - \log(1 - S_{j|l}) \right],$$

where $S_{j|k}$ is the distribution of negative samples of node $v_j^i$, and $P_n(v_j^i)$ is the link weight between $v_j^i$ and $v_k^i$. Combining Eq.(4) and Eq.(5), the overall reconstruction loss can be written as:

$$L_{\text{rec}} = L_{\text{rec}}^X + L_{\text{rec}}^A,$$

where $\theta_X$ and $\theta_E$ are the parameters of prototype generator $f_G$ and encoder $f_E$. With Eq.(6), the prototype generator can generate realistic prototype graphs given well learned prototype embeddings.

### 4.1.2 Initialization and Constraint on Prototype Embeddings

With Eq.(6), we can get an effective prototype generator. However, to obtain useful prototype graphs, there are two requirements for prototype embeddings: (i) to make sure that the generated prototypes are realistic, the prototype embeddings should be in the same latent space as that learned by the encoder because the generator is trained to generate realistic graph when the inputs are from that space; and (ii) to make sure that the generated prototypes are representative of each class, the prototype embeddings should be centroids of the latent space learned by encoder. Therefore, we propose to firstly pretrain the encoder. Then, we initialize the prototype embeddings by identifying the representative graphs whose graph embeddings are in the center of the learned latent space. Specifically, the encoder is pretrained by the labeled graphs to learn the latent space that carries the embedding information of the graph. This label prediction of $G_i \in D_l$ with the encoder $f_E$ can be obtained by

$$h^G = \text{READOUT}(f_E(A_i, X_i)), \quad \hat{y}_l = \text{softmax}(W_C \cdot h^G),$$

where $h^G$ is the graph embedding of $G_i$, READOUT is flexible to max pooling or mean pooling, and $W_C$ is the learnable weight matrix for classification. $A_i$ and $X_i$ are the adjacency matrix and feature matrix of $G_i$. We then pretrain encoder and decoder as:

$$\min_{\theta_E, \theta_G, W_C} \frac{1}{|D_l|} \sum_{d \in D_l} l(\hat{y}_l, y_l) + \alpha L_{\text{rec}},$$

where $l(\cdot, \cdot)$ denotes the cross entropy loss, and $y_l$ is the label of $G_i$. With the pretrained encoder, we can find the representative graphs in the center of latent space. For each class $l \in \{1, \ldots, C\}$, we will apply K-Means to cluster $h^G_l : \hat{y}_l = l, G_i \in D_l$, i.e., the embeddings of graphs that are predicted as class $l$. The number of clusters/centroids of each class are pre-defined as $K$. Let $h^C_{ik}$ denote the centroid of $k$-th cluster of class $l$, we can select the graph whose graph embedding is closest to $h^C_{ik}$ by

$$G_{ik}^{\text{init}} = \arg \min_{G_i \in D_l} \|h^G_i - h^C_{ik}\|^2.$$

Then, $H_{ik}^{\text{init}}$, i.e., the initialization of prototype embedding for prototype graph $G_{ik}^{\text{init}}$, can be attained as $H_{ik}^{\text{init}} = f_E(G_{ik}^{\text{init}})$. Since the optimal prototype graphs should not differ a lot from the initialization graphs and to make the prototype embeddings remains in the desired latent space, we further add a constraint to regularize the learning process of prototype embeddings as:

$$L_R = \frac{1}{C} \sum_{l=1}^{C} \sum_{k=1}^{K} \|H_k - H_{ik}^{\text{init}}\|^2,$$

### 4.1.3 Prototype Graph Generation

With the prototype embeddings and generator, we can generate the prototype graphs. However, directly using the generated adjacency matrix would lead to a fully-connected graph which is difficult to interpret. Hence, we utilize the initialized graph $G_{ik}^{\text{init}}$ to help remove unnecessary links to obtain a realistic sparse graph. For a node pair $(v_i, v_j)$ that is not a link of $G_{ik}^{\text{init}}$, it is unlikely to be linked in the learned prototype graphs. Hence, we will set a relatively high threshold for link generation. Considering that a link $(v_i, v_j)$ in $G_{ik}^{\text{init}}$ is more likely to also appear in the learned prototype graph $G_{ik}$, a lower threshold of link elimination will be set. Let $S_{ij}$ denotes the predicted probability that node $v_i \in G_{ik}$ and $v_j \in G_{ik}$ are connected. The final adjacency
matrix \( \hat{A} \) of the prototype graph \( \hat{G}_{lk} \) can be written as:

\[
\hat{A}_{ij} = \begin{cases} 
\hat{s}_{ij} & \text{if } v_i \in \mathcal{N}^{init}(v_j) \text{ and } \hat{s}_{ij} > T_i; \\
\hat{s}_{ij} & \text{if } v_i \not\in \mathcal{N}^{init}(v_j) \text{ and } \hat{s}_{ij} > T_i; \\
0 & \text{else},
\end{cases}
\]

(11)

where \( 1 \geq T_h \geq T_i \geq 0 \) and \( \mathcal{N}^{init}(v_i) \) denotes the neighbor of \( v_i \in \mathcal{G}^{init}_{lk} \). As for the attributes of \( \mathcal{G}^{init}_{lk} \), it can be directly obtained by Eq.(1) with the learned prototype embeddings \( \hat{H}_{lk} \) as input. Note that domain specific constraints can also be incorporated in this process to generate more realistic prototype graphs.

### 4.2 Self-Explainable Prediction with Prototypes

With the prototype graph generation described in Section 4.1, we are able to conduct the prediction by finding the prototype graphs that are similar to the test graph to give predictions and instance-level explanations. Next, we will present the details of the classification, self-explanation, and the loss function that facilitate both classification accuracy and explanation quality.

#### 4.2.1 Prediction with Prototypes

Intuitively, if a test graph \( G_t \) is more similar with the prototype graphs in class \( \mathcal{C} \), the label of \( G_t \) is more likely to be class \( \mathcal{C} \). Following previous works in similarity metric learning [10], we use \( f_k \) to learn graph representation followed by a similarity function. Let \( h_t^G \) and \( \hat{h}_{lk}^G \) represent the graph embeddings of \( G_t \in \mathcal{D} \) and \( \hat{G}_{lk} \in \mathcal{P}_\mathcal{C} \) encoded by Eq.(7), the similarity score is calculated as:

\[
s(G_t, \hat{G}_{lk}) = \text{sim}(h_t^G, \hat{h}_{lk}^G),
\]

(12)

where \( \text{sim} \) is the similarity function which can be cosine similarity or distance-based similarity. With Eq.(12), we can find the prototype graphs that are similar to the test graph \( G_t \) and predict the label with weighted average of the class of the nearest prototypes. Let \( \mathcal{P}_\mathcal{C} = \{\hat{G}_{lk}^1, \ldots, \hat{G}_{lk}^M\} \) be the identified \( M \)-nearest prototype graphs. The weight \( a_{ti} \) of the \( i \)-th nearest prototype graphs is computed as:

\[
a_{ti} = \frac{\exp(s(G_t, \hat{G}_{lk}^i)/\tau)}{\sum_{i=1}^{M} \exp(s(G_t, \hat{G}_{lk}^i)/\tau)},
\]

(13)

where \( \tau \) is the temperature parameter. Let \( y_t^i \) denotes the one-hot class vector of prototype graph \( \hat{G}_{lk}^i \), the final class distribution prediction of \( G_t \) is given as:

\[
\hat{y}_t = \sum_{i=1}^{M} a_{ti} \cdot y_t^i
\]

(14)

#### 4.2.2 Explainability of PxGNN

First, the learned prototype graphs \( \mathcal{P}_\mathcal{C} \) is the class-level explanation, which shows the representative patterns of graph in class \( \mathcal{C} \). Second, for the prediction of the test graph \( G_t \), the obtained similarity scores between \( G_t \) and the prototype graphs can explain the predicted label. Moreover, we can identify the prototype graph in class \( \hat{y}_t \) that is most similar with \( G_t \) as the instance-level explanation by

\[
\hat{G}_t = \arg\max_{\hat{G}_{lk} \in \mathcal{P}_\mathcal{Y}_t} s(G_t, \hat{G}_{lk}).
\]

(15)

Since the prediction of \( G_t \) is based on several prototypes, the instance-level explanation can be flexible to be several most similar prototype graphs in class \( \hat{y}_t \).

#### 4.2.3 Classification Loss

To ensure the accuracy of the proposed PxGNN, we apply a classification loss to leverage the supervision from the labeled set \( \mathcal{D}_l \). The major idea is that a labeled graph \( G_i \in \mathcal{D}_l \) whose label is \( y_i \) should be more similar with the prototype graphs in \( \mathcal{P}_{y_i} \) than other prototype graphs that do not belong to class \( y_i \). Therefore, in the classification loss, the prototype graphs in \( \mathcal{P}_{y_i} \) is set as positive samples; while the rest prototype graphs are set as negative samples. In addition, the prototype embeddings are jointly trained with the model parameters to update the prototype graphs to be more representative. The objective function of classification loss can be formally written as:

\[
\min_{\theta, \hat{H}} \mathcal{L}_c = \frac{1}{|\mathcal{D}_l|} \sum_{G_i \in \mathcal{D}_l} -\log \frac{\sum_{\hat{G}_k \in \mathcal{P}_{y_i}} \exp(s(G_i, \hat{G}_k)/\tau)}{\sum_{\hat{G}_k \in \mathcal{P}_{\mathcal{Y}_t}} \exp(s(G_i, \hat{G}_k)/\tau)}.
\]

(16)

where \( \tau \) is the temperature hyperparameter, and \( \hat{H} \) is the set of prototype embeddings of all classes, and \( \mathcal{P} \) represents all the prototype graphs. With Eq.(16), the similarity scores of a graph with prototype graphs in different classes will be minimized, and the similarity scores between a graph and the prototype graphs share the same class will be maximized. As a result, accurate predictions can be given. Moreover, it provides supervision to guide the similarity modeling to give correct instance-level explanation.

### 4.3 Final Objective Function of PxGNN

With the reconstruction loss for prototype learning, the constraint from the initialized prototype graph embeddings, and the classification that facilitate the prediction and explanation quality, the final objective function of PxGNN is given as:

\[
\min_{\theta, \hat{H}} \mathcal{L}_c + \alpha \mathcal{L}_{rec} + \beta \mathcal{L}_b
\]

(17)

where \( \theta \) and \( \hat{H} \) denote all model parameters of PxGNN and the set of learnable prototype embeddings, respectively. \( \alpha \) and \( \beta \) are hyperparameters to control the contribution of the reconstruction loss and constraint term on prototype embeddings, respectively.

### 5 EXPERIMENTS

We conduct extensive experiments on both synthetic datasets and real-world graphs to answer the following research questions.

- **RQ1** Can our proposed PxGNN learn high-quality prototypes for accurate predictions and explanations?
- **RQ2** How the number of prototypes will affect the accuracy and quality of the learned prototypes for explanations?
- **RQ3** How does each component of our proposed method affect the prediction accuracy and prototype quality?

#### 5.1 Datasets

To evaluate our PxGNN quantitatively and qualitatively, we conduct experiments on four real-world datasets and two synthetic datasets, which include node classification and graph class tasks. The statistics of the datasets are presented in Table 1.

#### 5.1.1 Real-World Datasets

We use two datasets for node classification, i.e., Cora and Pubmed [17], and two datasets for graph classification, i.e., MUTAG [34] and Graph-SST2 [42]. **Cora** and **Pubmed** are both citation networks. We reduce the bag-of-words
5.1.2 Synthetic Datasets. We also conduct experiments on two synthetic datasets, i.e., BA-Shapes and Syn-SST, which provide the ground-truth prototype graphs for node classification and graph classification, respectively.

**BA-Shapes** [38]: It is a single graph consisting of a base Barabasi-Albert (BA) graph attached with "house"-structured motifs. Nodes in the base graph are labeled with 0. Nodes at the top/middle/bottom of the "house" are labeled with 1, 2, 3, respectively. Therefore, the "house"-structured motif is the ground-truth prototype graphs of class 1, 2, and 3. Following previous works [10, 38], random edges are added to perturb the graph. Node degrees are assigned as node features. The dataset split is the same as the cited papers.

**Syn-SST**: To obtain a dataset with ground-truth prototype graphs for graph classification, we sample graphs from Graph-SST2 as motifs to build Syn-SST. More specifically, we randomly sample five graphs for each class as the corresponding ground-truth prototypes. For each prototype graphs, we synthesize 20 perturbed versions by adding various levels of structural noises and randomly removing/injecting nodes. As a result, we obtain 100 graphs for each class in Syn-SST. For the dataset split, we randomly sample 0.5/0.25/0.25 molecules as train/validation/test set. The split sets have no overlap with each other.

5.2 Experimental Settings

5.2.1 Compared Methods. To evaluate PxGNN, we compare with the following state-of-art GNNs and self-explainable GNNs.

- **GCN** [17]: This is a spectral-based graph neural network, which aggregates the neighbor information by averaging their features.
- **GIN** [35]: To increase the ability of capturing topology information in the graph, a MLP is applied in the aggregation phase.
- **ProtGNN** [45]: It employs a search algorithm to find the subgraphs as prototypes and adopts a prototype layer [6] for self-explainable prediction. ProtGNN is designed for graph classification. We extend it to node classification by giving predictions based on the local graphs of target nodes.
- **SE-GNN** [10]: It focuses on node classification. The K-nearest labeled nodes’ local graphs for each test node are identified for self-explainable predictions. For each class, we select the mostly selected labeled node’ local graph as the prototype.

We also utilize the following post-hoc GNN explainers in extracting important subgraphs to get prototypes to compare with our proposed framework in prototype-based explanations.

- **GNExplainer** [38]: It aims to find the subgraph that results in positive predictions as the complete computation graph to give post-hoc explanations for a trained GNN.
- **PGExplainer** [22]: It adopts a MLP-based explainer to obtain the important subgraphs from a global view to reduce the computation cost and obtain better explanations.
- **SubgraphX** [42]: Instead of assuming that edges are independent to each other, SubgraphX explores different subgraphs by Monte Carlo tree search with Shapley values as importance measure.

Since they are post-hoc instance-level explainers, to generate prototypes, we first find representative graphs whose embedding lies in the center of embeddings in each class. We then obtain prototypes by extracting important subgraphs of the center graphs with the aforementioned post-hoc GNN explainers.

5.2.2 Implementation Details. For our PxGNN, a two layer GCN is applied as the encoder. A two-layer MLP is deployed for attribute generation in the prototype generator. For the similarity function in the classifier, we apply an Euclidean distance-based similarity metric. All the hyperparameters are tuned based on the performance on validation set and the quality of learned prototype graphs. We vary $\alpha$ and $\beta$ as $\{100, 10, 1, 0.1, 0.01\}$ and $\{10, 3, 1, 0.3, 0.1\}$. As for the number of prototypes per class $K$, we search from $\{2, 3, \ldots, 6\}$. We set $M$, i.e., the number of identified most similar prototypes for prediction, the same as $K$ for each dataset. For all experiments, $T_h$, $T_f$, $Q$ and $r$ are fixed as 0.8, 0.2, 50, and 1, respectively. All the experiments are conducted 5 times. The hyperparameters of baselines are also tuned with grid search for fair comparisons.

5.3 Classification and Explanation Quality

To answer RQ1, we compare PxGNN with the baselines in terms of prediction and quality of explanations with prototypes on both node classification and graph classification datasets.

5.3.1 Results on Real-World Graphs. To demonstrate the effectiveness of our proposed PxGNN in giving accurate predictions, we compare with state-of-the-art GNNs and self-explainable GNNs on real-world datasets of node classification and graph classification. We report the average results along with the standard deviations in Table 2. Note that SE-GNN is particularly designed for node classification, so experiments on graph classification datasets are not applicable for SE-GNN. From the Table 2, we can observe that:

- Our PxGNN outperforms GCN and GIN on various datasets, and achieves comparable results with SE-GNN that adopts contrastive
learning. This is because the self-supervision of graph reconstruction and supervision from the labeled dataset are leveraged in PxGNN for the encoder training and prototype generation, resulting better prediction performance.

- Compared with ProtGNN which also conducts self-explainable predictions with prototypes, the proposed PxGNN gives better prediction results especially on node classification datasets. This demonstrates that PxGNN can consistently learn high-quality prototype graphs for accurate predictions on different tasks; while simply selecting subgraphs from the figures as prototype graphs might result in sub-optimal prototypes.

We further quantitatively evaluate the quality of the learned prototypes for explanations on real-world datasets with two evaluation metrics. First, since prototype graphs should capture representative patterns of the corresponding class, the prediction confidence scores on the prototype graphs are expected to be high. Therefore, we evaluate the confidence score of the prototype graph using a trained GNN to assess the quality. Second, high-quality prototype graphs can tightly cluster the instances in the datasets. In addition, clusters corresponding to different prototype graphs should be well separated. Therefore, we use the prototypes as centers and assign each node/graph to the nearest prototype. Then, we conduct Silhouette analysis [27] to evaluate the tightness and separateness of the clusters. The Silhouette score ranges from -1 to 1. A higher Silhouette score means tighter clusters and larger distance between clusters, which indicates more representative and diverse prototypes. The Silhouette score is computed based on the embedding space learned by a graph autoencoder. For post-hoc explainers, a GCN achieves the performance in Table 2 is set as the pretrained space learned by a graph autoencoder. For post-hoc explainers, a graph autoencoder and evaluate the distance of learned prototype graphs from the ground-truth of “house” motif. And PxGNN also manage to abstract the carbon ring with represented by the bold black edges of the complete center graph. Thus, they are extracted crucial subgraph of the center graph. Thus, they are represented by the bold black edges of the complete center graph in Fig. 3. For the prototypes on BA-Shapes, we can find that our PxGNN manage to learn prototype graphs that are consistent with the ground-truth prototype graphs than the baseline prototypes. Learning prototype graphs from PxGNN match much better with the ground-truth prototype graphs than the baseline prototypes.

We compare our method with the most competitive methods in Table 3. From the table, we observe that:

- The confidence score and Silhouette score of prototype graphs learned by our PxGNN are much larger than prototypes obtained from baseline GNN explainers. This demonstrates that our method can learn representative and diverse prototype graphs.
- Compared with ProtGNN which adopts Monte Carlo tree search to find subgraphs from raw graphs as prototypes, the prototypes generated by our PxGNN are significantly better according to the quality scores. This is because the prototype generator in

### Table 3: Comparisons with baseline methods on the quality of obtained prototype graphs.

| Dataset  | Metric       | GNExplainer | PGExplainer | SubgraphX | SE-GNN | ProtGNN | Ours     |
|----------|--------------|-------------|-------------|-----------|--------|---------|----------|
| Cora     | Confidence Score (%) | 89.4 ±17.4 | 70.9 ±19.5 | 41.3 ±1.3 | 93.3 ±12.5 | 41.7 ±20.2 | 98.4 ±1.9 |
|          | Silhouette Score | 0.133       | 0.113       | 0.110     | 0.097   | 0.083   | 0.228    |
| Pubmed   | Confidence Score (%) | 93.3 ±11.2 | 89.2 ±9.4  | 72.3 ±15.3 | 94.8 ±0.8 | 66.7 ±4.9 | 99.9 ±0.1 |
|          | Silhouette Score | 0.264       | 0.205       | 0.123     | 0.210   | 0.239   | 0.423    |
| MUTAG    | Confidence Score (%) | 76.4 ±23.4 | 70.5 ±20.3 | 70.5 ±18.4 | -       | 55.9 ±14.5 | 94.5 ±4.9 |
|          | Silhouette Score | 0.579       | 0.661       | 0.660     | -       | 0.629   | 0.745    |
| Graph-SST2 | Confidence Score (%) | 87.7 ±20.3 | 90.2 ±1.0  | 89.1 ±15.1 | -       | 62.3 ±15.9 | 94.9 ±6.8 |
|          | Silhouette Score | 0.259       | 0.226       | 0.249     | -       | 0.037   | 0.309    |

### Table 4: Distance from the ground-truth prototypes.

| Dataset  | PGExplainer | SubgraphX | Ours  |
|----------|-------------|-----------|-------|
| BA-shapes| 0.606       | 0.364     | 0.105 |
| Syn-SST  | 2.884       | 2.936     | 2.231 |

**5.3.2 Results on Synthetic Datasets.** To quantitatively evaluate the class-level explanations, we conduct experiments on BA-Shapes and Syn-SST which provide ground-truth prototypes. Following previous work [2] in graph similarity measuring, we first pretrain a graph autoencoder and evaluate the distance of learned prototypes and the ground-truth prototypes in the embedding space. We compare our method with the most competitive methods in Table 3. The results are shown in Table 4. We can find that the learned prototype graphs from PxGNN match much better with the ground-truth prototype graphs than the baseline prototypes.

**5.3.3 Visualization.** To qualitatively evaluate the prototype-based explanations, we also visualize the obtained prototypes of our PxGNN and baselines on both synthetic dataset BA-Shapes and real-world dataset MUTAG. The results are shown in Fig. 3. For PxGNN, we directly present the learned prototypes of the representative class. As for PGExplainer and SubgraphX, the prototypes are extracted crucial subgraph of the center graph.

![Figure 3: Learned prototypes on BA-Shapes and MUTAG.](image)

PxGNN can learn prototypical patterns for classification with the deployed self-supervision and classification loss.

**5.4 Impacts of the Number of Prototypes**

One natural question for prototype-based explanations is how to determine the size of prototypes. Thus, to answer RQ2, we vary the number of prototypes per class as {2, 3, ..., 6} to investigate its impacts to PxGNN. The other hyperparameters are set as the
description in Section 5.2.2. The impacts are assessed from the aspects of prediction accuracy and the quality of learned prototypes. Here, the Silhouette score, which can measure the representativeness and diversity of the prototype graphs, is used for prototype quality evaluation. We only report the results on Cora, Pubmed and Graph-SST2 in Figure 4 as we have similar observations on other datasets. From Figure 4, we observe that with the increase of prototype size, the classification performance will firstly increase then maintain similar results. For the Silhouette score, it will firstly increase then decrease. This is because when the number of prototypes is too small, the prototypes cannot represent all the instances in the dataset, leading to poor performance in prediction. When the prototype size is overly large, we will obtain multiple similar prototypes for one ground-truth prototype. In this situation, the prediction performance will not increase; while silhouette score which also measures the diversity of the prototypes will decrease. The above observations also pave us a way of selecting optimal prototype size in PxGNN.

5.5 Ablation Study
To answer RQ3, we conduct ablation studies to explore the flexibility of our proposed PxGNN and the effectiveness of the self-supervision loss and constraint term in prototype generation. To show that PxGNN is flexible to various GNN backbones, we replace the GCN-based encoder to a GIN model, denoted as PxGNN\_GIN. To demonstrate the importance of the self-supervision of graph reconstruction in prototype generator training, we train a variant PxGNN\_S by setting \( \alpha \) as 0. In PxGNN, we utilize the initialization prototype graphs to constrain the prototype embeddings in the desired latent space to ensure the quality of generated prototypes. To show the effects of this constraint term, we set \( \beta \) to 0 and obtain a variant named as PxGNN\_R. Finally, to verify the necessity of updating the prototype graphs with the prototype generator, we train a variant PxGNN\_P which fixes the prototype graphs after the initialization. The hyperparameters of these variants are also tuned on the validation set. The average results on Pubmed and Graph-SST are presented in Figure 5. We can observe that:

- PxGNN\_GIN achieves similar results with PxGNN for both classification accuracy and prototype quality, which indicates the flexibility of the proposed PxGNN;
- The accuracy and prototype quality of PxGNN\_S and PxGNN\_R are significantly worse than PxGNN. This demonstrates that the self-supervision on prototype generator and the constraint on prototype embeddings are helpful for learning high-quality prototypes for the prediction and explanation;
- PxGNN outperforms PxGNN\_P by a large margin, which proves the importance of updating the prototype graphs with generator to better capture the key patterns of each class.

5.6 Parameter Sensitivity Analysis
In this subsection, we study how the hyperparameters \( \alpha \) and \( \beta \) will affect PxGNN. \( \alpha \) controls the contribution of self-supervision on encoder and prototype generator. And \( \beta \) controls the regularization applied on the learnable prototype embeddings. We alter the values of \( \alpha \) and \( \beta \) as \{10, 1, 0.1, 0.01\} and \{1, 3, 1, 0.3, 0.1\}, respectively. The setting of other hyperparameters are the same as the description in Section 5.2.2. The results are presented in Figure 5. From the figure, we observe that: (i) when \( \alpha \) is small, both the classification accuracy and prototype quality are poor. This is because little contribution of self-supervision would lead to a weak prototype generator. And a too large \( \alpha \) will also lead to the decrease of classification accuracy because the reconstruction loss dominate the whole loss function; and (ii) with the increase of \( \alpha \), the performance in both aspects will firstly increase then decrease. When \( \beta \) is overly small, the updated prototype embedding may not perfectly follow the latent space for prototype generation, leading to relatively poor prototypes. However, a too large \( \beta \) will largely restrict the updates of prototype embeddings. Combining the two figures, we can see that when \( \alpha \in [1, 10] \) and \( \beta \in [1, 3] \), PxGNN can give accurate predictions and obtain high-quality prototypes for explanations.

6 CONCLUSION AND FUTURE WORK
In this paper, we study a novel problem of learning a prototype-based self-explainable GNN. We develop a new frameworkPxGNN, which adopts a prototype generator to learn representative and realistic prototype graphs for accurate prediction and explanations. The self-supervision of graph reconstruction and the supervision from labeled instances is applied to facilitate the learning of prototypes and the performance of classification. Extensive experiments
REFERENCES

[1] David Alvarez-Melis and Tommi S Jaakkola. 2018. Towards robust interpretability with self-explainable neural networks. arXiv preprint arXiv:1806.07538 (2018).

[2] Yunshe Bui, Hao Ding, Song Bian, Ting Chen, Yizhou Sun, and Wei Wang. 2019. Simgcn: A neural network approach to fast graph similarity computation. In WSDM. 384–392.

[3] Federico Baldassarre and Hossein Askpouro. 2019. Explainability techniques for graph convolutional networks. arXiv preprint arXiv:1905.13686 (2019).

[4] Pietro Bongini, Monica Bianchini, and Franco Scarselli. 2021. Molecular generative Graph Neural Networks for Drug Discovery. Neurocomputing 450 (2021), 242–252.

[5] Josan Bruna, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. 2014. Spectral networks and locally connected networks on graphs. ICLR (2014).

[6] Chaofan Chen, Oscar Li, Daniel Tao, Alina Barnett, Cynthia Rudin, and Jonathan K Su. 2019. This looks like that: deep learning for interpretable image recognition. Advances in neural information processing systems 32 (2019).

[7] Jie Chen, Tengfei Ma, and Xia Hu. 2018. Fastgcn: fast learning with graph neural networks. In ICML. PMLR, 1725–1735.

[8] Wei-Lin Chiang, Xuanqiao Liu, Si Si, Yang Li, Samy Bengio, and Cho-Jui Hsieh. 2019. Cluster-GCN: An efficient algorithm for training deep and large graph convolutional networks. In SIGKDD. 257–266.

[9] Enyan Dai and Suhang Wang. 2021. Towards Self-Explainable Graph Neural Network. In Proceedings of the 30th ACM International Conference on Information & Knowledge Management. 302–311.

[10] Mengnan Du, Ninghao Liu, Qingquan Song, and Xia Hu. 2018. Simple and deep graph convolutional networks. In IJCAI. PMLR, 1725–1735.

[11] Peter Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. 2018. Graph attention networks. ICLR (2018).

[12] Mengnan Du, Ninghao Liu, Qingquan Song, and Xia Hu. 2018. Towards explainable graph neural networks via importance sampling. ICLR (2018).

[13] Ming Chen, Zhewei Wei, Zengfeng Huang, Bolin Ding, and Yaliang Li. 2020. Simgnn: A neural network approach to fast graph similarity computation. In NeurIPS. PMLR, 5453–5462.

[14] Chaofan Chen, Oscar Li, Daniel Tao, Alina Barnett, Cynthia Rudin, and Jonathan K Su. 2019. This looks like that: deep learning for interpretable image recognition. Advances in neural information processing systems 32 (2019).

[15] Dongsheng Luo, Wei Cheng, Dongkuan Xu, Kuanlan Wang, and Jie Tang. 2020. Gcngnn: Can gcns go as deep as cnns?. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition. 10772–10781.

[16] Zhitao Ying, Dylan Bourgeois, Jiaxuan You, Marinka Zitnik, and Jure Leskovec. 2018. Graph convolutional neural networks learn better molecular representation for drug discovery. In Advances in Neural Information Processing Systems 31. 5717–5724.

[17] Thomas Kifp and Max Welling. 2016. Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907 (2016).

[18] Thomas N Kifp and Max Welling. 2016. Variational graph auto-encoders. arXiv preprint arXiv:1612.07308 (2016).

[19] Ron Levine, Federico Monani, Xavier Bresson, and Michael M Bronstein. 2018. Cayleynets: Graph convolutional networks with complex rational spectral filters. IEEE Transactions on Signal Processing 67, 1 (2018), 97–109.

[20] Guohao Li, Matthias Muller, Ali Thabet, and Bernard Ghanem. 2019. Deep-gcns: Can gcns go as deep as cnns? In Proceedings of the IEEE/CVF International Conference on Computer Vision. 9267–9276.

[21] Oscar Li, Hao Liu, Chaofan Chen, and Cynthia Rudin. 2018. Deep learning for case-based reasoning through prototypes: A neural network that explains its predictions. In Proceedings of the AAAI Conference on Artificial Intelligence, Vol. 32.

[22] Dongsheng Luo, Wei Cheng, Dongkuan Xu, Wenchao Yu, Bo Zong, HaiFeng Chen, and Xiang Zhang. 2020. Parameterized Explaner for Graph Neural Networks. Advances in Neural Information Processing Systems 33 (2020).

[23] Thomas Mikolov, Ilya Sutskever, Kai Chen, Greg S Corrado, and Jeff Dean. 2013. Distributed representations of words and phrases and their compositionality. In NeurIPS. 3111–3119.

[24] Nicolas Papernot and Patrick McDaniel. 2018. Deep k-nearest neighbors: Towards confident, interpretable and robust deep learning. arXiv preprint arXiv:1803.04765 (2018).

[25] Philipp E Pope, Soheil Kolouri, Mohammad Rostami, Charles E Martin, and Heiko Hoffmann. 2019. Explainability methods for graph convolutional neural networks. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition. 10772–10781.

[26] Jie Chen, Tengfei Ma, and Xia Hu. 2018. Fastgcn: fast learning with graph neural networks. In ICML. PMLR, 1725–1735.

[27] Peter J Rousseveur. 1987. Silhouettes: a graphical aid to the interpretation and validation of cluster analysis. Journal of computational and applied mathematics 20 (1987), 53–65.

[28] Cynthia Rudin. 2019. Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. Nature Machine Intelligence 1, 5 (2019), 206–215.

[29] Ramprasaath R Selvaraju, Michael Cogswell, Abhishek Das, Ramakrishna Vedan-tam, Devi Parikh, and Dhruv Batra. 2017. Grad-cam: Visual explanations from deep networks via gradient-based localization. In Proceedings of the IEEE international conference on computer vision. 618–626.

[30] Kai Shu, Limeng Cui, Suhang Wang, Dongwen Lee, and Huan Liu. 2019. de-fend: Explainable fake news detection. In Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 395–405.

[31] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. 2018. Graph attention networks. ICLR (2018).

[32] Daixin Wang, Jianbin Lin, Peng Cui, Quanhui Jia, Zhen Wang, Tanny Fang, Quan Yu, Jun Zhou, Shuang Yang, and Yuan Q. 2019. A semi-supervised Graph Attention Network for Financial Fraud Detection. In ICDE. IEEE, 598–607.

[33] Hongwei Wang, Fuzheng Zhang, Mengdi Zhang, Jure Leskovec, Miao Zhao, Wenjie Li, and Zhongyang Wang. 2019. Knowledge-aware graph neural networks with label smoothness regularization for recommender systems. In SIGKDD. 968–977.

[34] Zhengbin Wu, Bharath Ramsundar, Evan N Feinberg, Joseph Gomes, Caleb Ge-neese, Anseerish S Pappu, Karl Leswing, and Vijay Pande. 2018. MolecularNet: a benchmark for molecular machine learning. Chemical science 9, 2 (2018), 513–530.

[35] Kexu Li, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. 2018. How powerful are graph neural networks? arXiv preprint arXiv:1810.00826 (2018).

[36] Kexu Li, Chenguang Li, Yonglong Tian, Tomshiro Sonobe, Ken-ichi Kawarabayashi, and Stefanie Jegelka. 2018. Representation learning on graphs with jumping knowledge networks. In International Conference on Machine Learning. PMLR, 5453–5462.

[37] Rex Ying, Ruining He, Kaifeng Chen, Pong Eksombatchai, William L Hamilton, and Jure Leskovec. 2018. Graph convolutional neural networks for web-scale recommender systems. In SIGKDD. 974–983.

[38] Zhiaoo Ying, Dylan Bourgeois, Jiaxuan You, Marinka Zitnik, and Jure Leskovec. 2019. Gnnexplainer: Generating explanations for graph neural networks. In Advances in neural information processing systems. 9244–9255.

[39] Yuning You, Tianlong Chen, Yongduo Si, Ting Chen, Zhangyang Wang, and Yang Shen. 2020. Graph contrastive learning with augmentations. Advances in Neural Information Processing Systems 33 (2020).

[40] Hao Yuan, Yonglong Tian, Tomshiro Sonobe, Ken-ichi Kawarabayashi, and Stefanie Jegelka. 2019. Interpreting deep models for text analysis via optimization and regularization methods. In Proceedings of the AAAI Conference on Artificial Intelligence, Vol. 33. 5717–5724.

[41] Hao Yuan, Jiliang Tang, Xia Hu, and Shuiwang Ji. 2020. Xgnn: Towards model-level explanations of graph neural networks. In SIGKDD. 430–438.

[42] Hao Yuan, Haiyang Yu, Shurui Gu, and Shuiwang Ji. 2020. Explainability in graph neural networks: A taxonomic survey. arXiv preprint arXiv:2012.15445 (2020).

[43] Hao Yuan, Haiyang Yu, Jie Wang, Kang Li, and Shuiwang Ji. 2021. On explainability of Graph Neural Networks via Subgraph Explorations. In Proceedings of the 38th International Conference on Machine Learning (ICML). 12241–12252.

[44] Matthew D Zeiler and Rob Fergus. 2014. Visualizing and understanding convolutional networks. In Proceedings of the IEEE conference on computer vision and pattern recognition. 1863–1872.

[45] Qizui Zhu, Bo Du, and Pingkun Yan. 2020. Self-supervised Training of Graph Convolutional Networks. arXiv preprint arXiv:2006.03380 (2020).