

# Exploiting Neighbor Effect: Conv-Agnostic GNNs Framework for Graphs with Heterophily

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**Abstract**—Due to the homophily assumption in graph convolution networks, a common consensus is that graph neural networks (GNNs) perform well on homophilic graphs but may fail on the heterophilic graphs with many inter-class edges. In this work, we re-examine the heterophily problem of GNNs and investigate the feature aggregation of inter-class neighbors. Instead of treating the inter-class edges as harmful, under some conditions, we argue that they may provide helpful information for node classification from an entire neighbor’s perspective. To better evaluate whether the neighbor is helpful for the downstream tasks, we present the concept of the neighbor effect of each node and use the von Neumann entropy to measure the randomness/identifiability of the neighbor distribution for each class. Moreover, we propose a Conv-Agnostic GNNs framework (CAGNNs) to enhance the performance of GNNs on heterophily datasets by learning the neighbor effect for each node. Specifically, we first decouple the feature of each node into the discriminative feature for downstream tasks and the aggregation feature for graph convolution. Then, we propose a shared mixer module for all layers to adaptively evaluate the neighbor effect of each node to incorporate the neighbor information. Experiments are performed on nine well-known benchmark datasets for the node classification task. The results indicate that our framework is able to improve the average prediction performance by 9.81%, 25.81%, and 20.61% for GIN, GAT, and GCN, respectively. Extensive ablation studies and robustness analysis further verify the effectiveness, robustness, and interpretability of our framework.

**Index Terms**—Graph neural networks, Node classification, Representation learning, Heterophily, Homophily

## I. INTRODUCTION

Recently, emerging graph neural networks (GNNs) have demonstrated remarkable ability for semi-supervised node classification tasks. Most GNNs learn node representation by recursively aggregating neighbor information [1], [2]. Under the homophily assumption, i.e., connected nodes on edges tend to be the same class, the graph convolution, which is often regarded as a Laplacian smoother [3], smooths each node representation by its intra-class neighbor representations through the aggregation process to make the classification task profitable. However, the applications of GNNs in heterophilic graphs whose connected nodes often have different labels are usually problematic [4]–[7].

Heterophily is observed in a wide range of real-world graphs, including dating, molecular, and transaction networks [7], [8]. Most existing literature agrees that the massive inter-class edges in heterophilic graphs are harmful for feature aggregation since they may blur the classification boundary and thus decrease the performance for subsequent

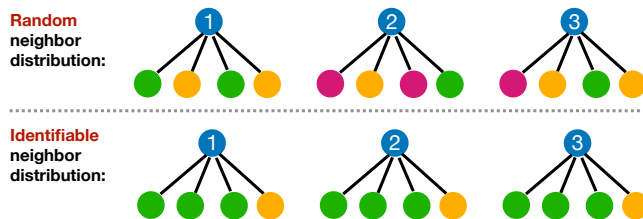


Fig. 1: The identifiability of neighbors. Nodes with the same colors share the same class labels. The above neighbor distribution for the blue class is random and the bottom is not random. Although many inter-class edges exist, the identifiable patterns from the non-random distribution of dissimilar neighbors may also help graph convolution classify the center node’s label.

node classification tasks [9]–[12]. To evaluate the application performance of GNNs on different graphs and to guide the model design, the homo-ratio metrics based on the proportion of inter-class edges are introduced in [8], [9]. Although consistent with the homophily assumption, they fail to explain the completely different node classification performance with a similar homo-ratio, as reported in [8]. Therefore, it compels us to re-examine the heterophily problem of GNNs and to answer the following two questions: (1) Is inter-class neighborhood aggregation truly harmful or unnecessary in all cases? (2) How to improve the traditional GNNs’ performance on heterophilic graphs.

As shown in Fig. 1, we first note that the inter-class edges may be beneficial to improve the node classification task if their neighbor distribution is identifiable instead of random. The critical point is to treat the neighbor as an entirety and measure the identifiability of each class neighbor distribution rather than considering the proportion of inter-class edges. A class with random neighbor distribution is considered to have lower identifiability, whereas a specific neighbor-connected pattern is considered to have higher identifiability. An extreme example is the bipartite graph. Although the graph is highly heterophilic (each edge connected two nodes of the opposite class), node features are still distinguishable after a simple mean aggregation operator since their neighbor’s distribution is identifiable [13], [14].

Therefore, we present a novel metric to quantify the identifiability of the neighbor’s distribution, which can indicate the class/graph-level neighbor effect. Motivated by this metric, we propose a Conv-Agnostic GNNs Framework (CAGNNs) to improve traditional GNNs’ performance on heterophilic graphs

by learning the node-level neighbor effect. We summarize the main contribution as follows.

(1) *We present a novel concept of the neighbor effect and quantify it with Von Neumann entropy.* Instead of considering the inter-class edges perspective, we extract the neighbors' label distribution matrix at the class-level to evaluate the identifiability of neighbors for the entire graph. Specifically, we extend the Von Neumann entropy [15] as a new metric to measure the identifiability of neighbors for the graph. This metric can explain the performance difference under the same node/edge-homo ratio of some datasets and show that the neighbor effect is vital to understanding and improving the GNN performance. This motivates us to consider the neighbor effect explicitly when performing aggregation for GNNs.

(2) *We propose CAGNNs as a framework to improve traditional GNNs by learning the neighbor effect for each node.* During the training stage, since the labels may be insufficient to identify the neighbor effect and the neighbor effect for each node may be different when aggregating, we measure the neighbor effect for each node based on the feature and local structures to improve the traditional GNNs. Concretely, we propose a general framework CAGNNs to decouple the features of a node into discriminative features for downstream tasks and the aggregating features from neighbors. Furthermore, we propose a mixer module to adaptively combine these two kinds of features for each node. It learns to determine the neighbor effect and decides whether to absorb or discard the neighbors' information.

(3) *We conduct extensive experiments on nine well-known benchmark datasets to verify the effectiveness, interpretability, and robustness of CAGNNs.* Our framework can be easily applied to enhance the performance of most GNNs on heterophilic graphs with an additional mixer module.

To present our contributions, we organised this paper into seven sections. In Section II, we survey related work. Section III introduces the notations and background. In Section IV, we present the proposed novel metric for measuring class-level and graph-level neighbor effect in detail. In Section V, we describe the proposed CAGNN framework and implementation in detail. Evaluation results on nine benchmark datasets and ablation studies are presented in Section VI to verify the effectiveness, interpretability and robustness of the proposed framework. The final section concludes this paper.

## II. RELATED WORKS

### A. Graph Neural Networks

GNNs models can be roughly categorized into spectral and spatial methods. Early on, Bruna et al. [16] first proposed a spectral graph-based extension of convolutional networks to graphs. In a follow-up work, ChebyNets [17] define graph convolutions using Chebyshev polynomials to remove the computationally expensive Laplacian eigendecomposition. GCNs [18] further simplify graph convolutions by stacking layers of first-order Chebyshev polynomial filters with a redefined propagation matrix. Also, the GCN bridges the spectral and spatial domain gap since it can also be regarded as a mean

aggregator to aggregate neighbor information to each node. Further, in the spatial domain, Graph Attention Network (GAT) introduces the attention mechanism to learning edge weights to improve the aggregation step. Xu et al. [19] studied the expressiveness of graph neural networks and introduce Graph Isomorphism Network (GIN), which is proved to be as powerful as the Weisfeiler-Lehman test. There are many other graph neural models [2], [20], [21]; we refer to [1], [22] for a more comprehensive review.

To investigate why and when graph neural networks work well for node classification, there are some works aiming at understanding the behavior of GNNs. Ni and Machara [23] indicated that graph neural networks only perform low-pass filtering on feature vectors and do not have the non-linear manifold learning property from signal processing perspective. Li et al. [3] pointed out that the GCN model's graph convolution is actually a special form of Laplacian smoothing, which is consistent with the homophily assumption. However, it also brings potential concerns of making the features of connected nodes from different labels indistinguishable. On the other hand, Ma et al. [14] theoretically reveal that homophily is not a necessary assumption for the GCN model. Moreover, for the attention-based GNNs, Wang et al. [24] found that stacking multiple attention layers causes excessive smoothing of node features due to information exchanging over inter-class edges. [10], [11] summarized the current popular message-passing scheme in GNNs and argued that the message between intra-class edges would help nodes receive information gain. In contrast, the inter-class edges may introduce negative disturbance.

### B. GNNs for Heterophily

Recently, heterophilic graph learning is becoming an upward trending research topic and various specific structured GNNs have been proposed to tackle heterophily. Most argue that message passing during inter-class edges is harmful to the downstream node classification task and try to avoid the harmfulness. Current kinds of literature can be divided into three lines:

(1) Some works aim to deal with heterophily from spectral domain: The FAGCN [5] divides the message from each edge into low-frequency and high-frequency signals and shows that both the low and high-frequency are necessary for heterophilic graph learning. In addition, some works aim at extracting high-order approximation with graph spectral filters. GPRGNN [13] modifies the convolution to the generalized page rank and learns an arbitrary K-order polynomial graph filter. GCNII [21] proposes the initial residual and identity mapping for vanilla GCN and theoretically proves that it can express a K-order polynomial filter with arbitrary coefficients. BernNet [25] learns arbitrary graph spectral filters via Bernstein approximation to oversimplified or ill-posed filters.

(2) Some works aim to discover the neighbor from latent space to reorganize the graph structure with a homophilic signal. Geom-GCN [9] utilizes geometric aggregation to capture structural similarity in the latent space and long-range dependencies. NLGNN [26] leverages the attention-guide sort-

ing to generate a re-connected graph and conducts non-local aggregation. SLAPS [27] combines the self-supervised technique to infer a homophily latent structure. GDAMN [10] proposes the decoupling attention mechanism on both features and labels to increase the intra-class and reduce inter-class edges weights.

(3) Some work aims to capture high-order neighbor information, which was proved to be homophily-dominant [5]. MixHop [28] repeatedly mixes feature representations of neighbors at various distances to achieve higher-order message passing. JK-Nets [29] jumps the intermediate representations to the last layer to enable better structure-aware representation. H2GCN [5] proposes three designs with separate ego and neighbors, higher-order neighbors and a combination of intermediate representations to combine the message from neighbors.

Unlike these specific GNN architectures to avoid the harmfulness from inter-class edges. Instead, we consider the inter-class edges from an identifiable neighbor distribution perspective. Further, we propose a simple and general Conv-Agnostic framework. This framework can be regarded as a plug-in component and compatible with traditional GNNs to improve their performance on heterophilic graphs.

### III. PRELIMINARY

#### A. Problem Setup

Consider an undirected graph  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  with adjacency matrix  $\mathbf{A} \in \mathbb{R}^{N \times N}$ , where  $\mathcal{V}$  and  $\mathcal{E}$  are the sets of nodes and edges, respectively. For each node  $v_i \in \mathcal{V}$ , we denote  $\mathcal{N}(v_i) = \{j : (i, j) \in \mathcal{E}\}$  as its neighbor set. Each node is given a  $d$ -dimensional feature representation  $\mathbf{x}_i$  and a  $c$ -dimensional one-hot class label  $\mathbf{y}_i$ . The feature inputs are then formed by  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N]$ , and the labels are  $\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_N]$ . Given the labels  $\mathbf{Y}_{\mathcal{L}}$  of a subset of nodes  $\mathcal{L} \subset \mathcal{V}$ , the task of semi-supervised node classification is to predict the labels  $\mathbf{Y}_{\mathcal{U}}$  of the unlabeled nodes  $\mathcal{U} = \mathcal{V} \setminus \mathcal{L}$  by exploiting the graph structure  $\mathcal{E}$  and the features of all the nodes  $\mathbf{X}$ .

#### B. Graph Neural Networks

From a probabilistic view, most GNNs assume the local Markov property on node features, i.e., for each node  $v_i$ , the label  $\mathbf{y}_i$  only depends on the node self-feature  $x_i$  and its neighbor-features  $\mathbf{x}_j : j \in \mathcal{N}(v_i)$ . For the  $l$ -th layer of a GNN, we use  $\mathbf{h}_i^l$  to represent the embedding of node  $v_i$  and  $\mathbf{h}_i^0$  to represent  $\mathbf{x}_i$  or a projection of  $\mathbf{x}_i$  for dimension reduction. Then, the general  $l$ -th layer Graph Convolution for node  $i$  can be formulated as

$$\mathbf{h}_i^{(l)} = f \left( \mathbf{h}_i^{(l-1)}, \left\{ \mathbf{h}_j^{(l-1)} : j \in \mathcal{N}(v_i) \right\} \right), \quad (1)$$

where the graph convolution operator  $f$  can be implemented by a weighted sum of each node based on the adjacent matrix  $\mathbf{A}$  as in GCN [18] and GIN [19] or the attention mechanism in GAT [30]. The formulations of three well-known graph convolution layers are summarized in Table I.

The final output  $\mathbf{Z} \in \mathbb{R}^{N \times c}$  of the label prediction is evaluated using a *softmax* function to embed the last layer

Models	Aggregation for each layer $l(1 \leq l \leq L)$
GCN	$h_v^{(l)} = \sigma \left( \sum_{v' \in \mathcal{N}_v \cup \{v\}} \frac{1}{\sqrt{( \mathcal{N}_v +1) \cdot ( \mathcal{N}_{v'} +1)}} \cdot W^{(l-1)} \cdot h_{v'}^{(l-1)} \right)$
GIN	$h_v^{(l)} = \text{MLP}^{(l)} \left( (1 + \epsilon^{(l)}) \cdot h_v^{(l-1)} + \sum_{v' \in \mathcal{N}(v)} h_{v'}^{(l-1)} \right)$
GAT	$h_{v_i}^{(l)} = \sigma \left( \sum_{v_j \in \mathcal{N}_{v_i} \cup \{v_i\}} a_{i,j}^{(l-1)} \cdot W^{(l-1)} \cdot h_{v_j}^{(l-1)} \right)$

TABLE I: The different neighborhood aggregation schemes. Here  $\sigma$  means the ReLu activation,  $a$  means attention weights,  $W$  means the weight matrix and MLP means multiple layer perceptron.

$\mathbf{H}^L$ . The objective function is the cross-entropy of the ground truth labels  $\mathbf{Y}$  and the output of the network  $\mathbf{Z}$ :

$$\mathcal{O} = - \sum_{i \in \mathcal{L}} \sum_{j=1}^c \mathbf{Y}_{ij} \ln \mathbf{Z}_{ij}. \quad (2)$$

It is worth noting that these GNNs straightforwardly feed the current aggregation features to the following graph convolution layer and merely use the last layer aggregation feature  $\mathbf{H}^L$  for the downstream node classification task. Consequently, the entangling of aggregation and classification may cause the node classification boundary to be over-smoothed by the corresponding inter-class neighbors. Moreover, they ignore that each node's entire neighbors' effect may be different.

#### C. Homophily/Heterophily Metrics on Graphs

The homophily ratio  $h$  aims to measure the overall homophily level in a graph. By definition, the ratio  $h \in [0, 1]$ . Graphs with  $h$  closer to 1 tend to have more intra-class edges indicating stronger homophily; on the other hand, graphs with  $h$  closer to 0 have more edges connecting different classes and it indicates stronger heterophily. The node-level [9] and edge-level [8] homophily metrics are usually defined by

$$\mathcal{H}_{\text{edge}}(\mathcal{G}) = \frac{|\{e_{uv} \mid e_{uv} \in \mathcal{E}, Y_u = Y_v\}|}{|\mathcal{E}|}, \quad (3)$$

$$\mathcal{H}_{\text{node}}(\mathcal{G}) = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \frac{|\{u \mid u \in \mathcal{N}_v, Y_u = Y_v\}|}{d_v}. \quad (4)$$

However, as reported in previous literature [8], these metrics are not significantly relevant to the prediction performance of GCNs. For example, for three well-known heterophily datasets (Chameleon, Squirrel, and Actor), although their homo-ratios are all 0.22, the reported accuracy of node classification for GCN varies, i.e., 60%, 37% and 30%, respectively [8]. The traditional node/edge-level homo-ratio indicators evaluating the proportion of inter-class edges may ignore the entire local neighbor effect. On the contrary, we find that these datasets have different neighbors identifiability, and each node's local neighbor distribution may contain discrimination information for classification.

### IV. A NOVEL METRIC: VON NEUMANN ENTROPY TO MEASURE THE NEIGHBOR EFFECT

As noted in Fig. 1, when the label distribution of neighbors is random, i.e., every node is connected to other neighbors with random labels, there is no helpful information we can

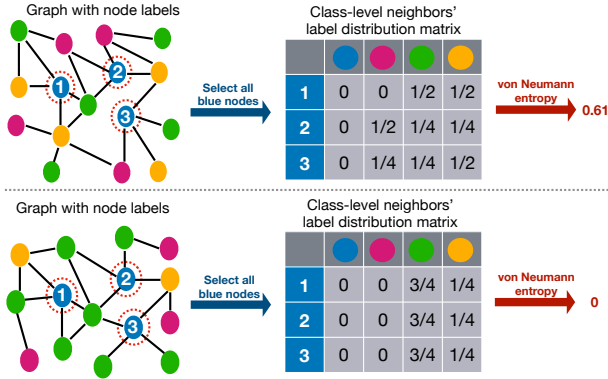


Fig. 2: Class-level Von Neumann entropy, which measures the information of neighbors’ label distribution matrix. This metric ranges from  $[0, 1]$  and can quantify the identifiability of neighbors for a specific class (the lower means the more identifiable).

learn from the aggregation step. However, when the neighbor distribution of each class’s nodes forms a certain identifiable distribution, regardless of whether the connected edges are intra-class or inter-class, graph convolution can extract useful information from this non-random neighbor distribution for the downstream tasks. Therefore, we need a new metric to measure the randomness/identifiability of the neighbor distribution as the neighbor effect for the node classification task.

We define the identifiability of neighbors as the information of the nodes’ neighbor distribution. As Fig. 2 shows, to measure the identifiability of neighbors, we group the nodes by class and form a class-level neighbor’s label distribution matrix  $A_N^k \in \mathbb{R}^{n_k \times C}$  for each class  $k$ , where  $k = 1, \dots, C$  for different class and  $n_k$  indicates the number of nodes with label  $k$ . Then, our task is to evaluate the information of the matrix to quantify the identifiability of neighbors. Inspired by the Von Neumann entropy in quantum statistical mechanics [15], which extends the idea of entropy for positive definite symmetric matrices, we generalize this idea to our task of evaluating neighbors’ identifiability.

Specifically, suppose  $\sigma_1^k, \sigma_2^k, \dots, \sigma_C^k$  denote singular values of  $A_N^k$ , we then normalize them so that  $\sum_{i=1}^C \sigma_i^k = 1$ , where  $i = 1, \dots, C$  for index of singular values. Then the Von Neumann entropy of class  $k$  is computed by

$$\mathcal{H}_{neighbor}^k = \frac{-\sum_{i=1}^C \sigma_i^k \log(\sigma_i^k)}{\log(C)}. \quad (5)$$

The above metric ranges from  $[0, 1]$  and can be used to quantify the identifiability of neighbors for a specific class (the lower, the more identifiable). Considering the problem of class imbalance, we compute the weighted sum of class-level Von Neumann entropy to evaluate the neighbors’ identifiability of a graph

$$\mathcal{H}_{neighbor}(\mathcal{G}) = \sum_{k=1}^C \frac{n_k}{N} \mathcal{H}_{neighbor}^k. \quad (6)$$

Compared with the node/edge-level homophily metrics, our measurement and the GCNs’ performance for different

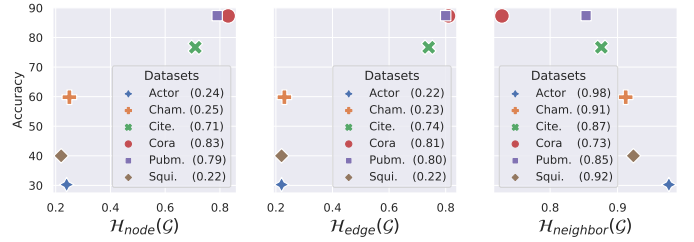


Fig. 3: The relation between hom-metric and GCN’s performance from [8] on different graph node classification datasets<sup>1</sup>. Our metric  $\mathcal{H}_{neighbor}$  is more monotonous with the models’ performance. Moreover, compared with other metrics, it can distinguish the Actor dataset, which has a random neighbor distribution and the lowest accuracy from the Squirrel and Chameleon. More details can be found in Section VI-C.

datasets are more monotonous as shown in Fig. 3. In addition, we can observe that the Actor, Chameleon, and Squirrel datasets have a similar node/edge-level homophily metrics (proportion of inter-class edges) in the left and middle part of Fig. 3. However, the performance of these datasets is inconsistent, especially for the Actor dataset, which has the poorest performance (accuracy=30%) and is totally different from the others. On the contrary, as shown in Fig. 3 (right), our metric can distinguish the Actor dataset from others since it has a nearly random neighbor distribution ( $\mathcal{H}_{neighbor}=0.98$ ). This indicates that the proposed metric can be used to guide the application of GCNs on different datasets. Furthermore, our metric reveals that the inter-class edges are not always harmful for the node classification during aggregation, and the entire local neighbor perspective can provide more information. It motivates us to learn the effectiveness of each node’s local neighbors during aggregation to help traditional GNNs deal with heterophily.

However, to guide the aggregation during the training process, we cannot directly utilize the entropy measurement and need to evaluate the node-level neighbor effect in another way. The reasons are two-fold: 1) Similar to  $\mathcal{H}_{edge}$  and  $\mathcal{H}_{node}$ , the computation of the entropy  $\mathcal{H}_{neighbor}$  also requires the labels of all the nodes, which are unavailable in the training process. 2) The class-level neighbor distribution identifiability  $\mathcal{H}_{neighbor}^c$  is not consistent with the entropy of the node-level label distribution. Namely, the entropy of a node does not represent the identifiability of the neighbor distribution of this class. In the next section, we will elaborate how to adaptively learn the node-level neighbor effect from the downstream supervision signal and the features of a node with its neighbor.

## V. PROPOSED METHOD AND SPECTRAL ANALYSIS

In this section, we first propose the Conv-Agnostic GNNs framework (CAGNNs) to adaptively learn the neighbor effect of each node, followed by a spectral analysis to show the expressive power of the node classification task of the proposed framework. Lastly, we describe the difference between

<sup>1</sup>We ignore the datasets that have fewer than 500 nodes. Their performances are highly sensitive to the data splits.

our framework and the GNNs with decoupling design and skip connection.

### A. Conv-Agnostic GNNs Framework

The proposed CAGNNs aim to empower traditional GNNs to generate suitable representations for each node for both homophilic and heterophilic graphs. The core idea is to decouple the representation for discrimination and aggregation and learn a mixer module. The mixer module can adaptively evaluate each node’s neighbor effect and determine whether to incorporate the information from neighbors. As shown in Fig. 4, our framework is composed of four major components: Encoder, Graph Convolution (GC), Mixer, and Decoder. Below, we elaborate each component in order. Moreover, we append the normalization operation after the Encoder, GC, and Mixer to maintain the numerical stability, which will be discussed later.

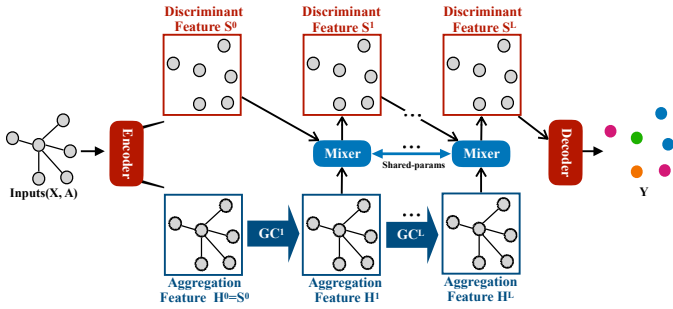


Fig. 4: The GC operator indicates any Graph Convolutions. The shared-parameter Mixer function can help each node to determine whether to absorb neighbors’ information by considering the neighbor effect based on the node’s feature.

**Encoder:** We use linear layers as the encoder to transform the node features  $\mathbf{X}$ . Then we feed it into two streams. One is the node’s own feature  $\mathbf{S}^0$  for downstream-task discrimination, and the other is the aggregation feature  $\mathbf{H}^0$  for the graph convolution. These two streams decouple the discriminant feature and the information from the neighbor, which may prevent the classification boundary of nodes from blurring by their neighbors during aggregation. Moreover, this decoupling operation gives each node the freedom to evaluate the neighbor effect for downstream discrimination tasks in the following aggregation step.

$$\mathbf{H}^0 = \mathbf{S}^0 = \text{Norm}(f_{\text{encoder}}(\mathbf{X})). \quad (7)$$

**Graph Convolution (GC):** Since our framework is Conv-Agnostic, in this part, any standard graph convolution layers (e.g., GCN, GAT, and GIN) can be applied to aggregate each node’s neighborhood information to update the aggregation representation  $\mathbf{H}$ . Moreover, this graph convolution layer can be stacked multiple times to enhance the receptive field of each node by considering the information of more neighbors. The embedding  $\mathbf{H}^l$  can also be regarded as the  $l$ -hop neighbors’ information. However, the information from neighbors is not always beneficial for the classification task of each node.

Hence, we propose the following mixer operator to determine the neighbor effect of each hop.

$$\mathbf{H}^{l+1} = \text{Norm}(\text{GraphConvolution}(\mathbf{A}, \mathbf{H}^l)). \quad (8)$$

**Mixer:** From the view of node  $v_i$  at layer  $l$ , it needs to combine the discrimination feature  $\mathbf{S}_i^l$  and  $l$ -hop neighbors feature  $\mathbf{H}_i^l$  according to the neighbor effect to update the representative embedding for the downstream task. Therefore, the goal of the mixer function is to evaluate the neighbor effect of each node and then to selectively incorporate the neighbors’ information. As discussed in Section IV, we do not need to inject the entropy function to evaluate the node-level neighbor effect. We have already encoded the neighbor information of each node into  $\mathbf{H}^l$  by the graph convolution. According to the universal approximation theorem [31], [32], we hypothesize that the MLP can adaptively learn the node-level neighbor effect based on  $\mathbf{S}^l$  and  $\mathbf{H}^l$  and the downstream objective  $\mathcal{O}$ . For simplicity and better generalization power, we implement the mixer by

$$\alpha^l = \sigma(f_{\text{mix}}(\mathbf{S}^{l-1}, \mathbf{H}^l)), \quad (9)$$

$$\mathbf{S}^l = \text{Norm}((\mathbf{1} - \alpha^l) * \mathbf{S}^{l-1} + \alpha^l * \mathbf{H}^l). \quad (10)$$

The  $f_{\text{mix}}$  is a linear layer function  $\mathbb{R}^{2d \times 1} \rightarrow \mathbb{R}^{N \times 1}$ . It maps the discrimination feature  $\mathbf{S}^{l-1}$  and neighbor feature  $\mathbf{H}^{l-1}$  at layer  $l$  to a vector  $\alpha^l \in \mathbb{R}^{N \times 1}$ . With the Sigmoid function  $\sigma$ , each alpha element is normalized to an importance score ranging from 0 to 1 and can be regarded as the neighbor effect of the node.

Based on the importance score  $\alpha^l$ , we use the convex combination of discriminant feature  $\mathbf{S}^{l-1}$  and neighbor information  $\mathbf{H}^{l-1}$  at each layer to adaptively update the discriminant feature  $\mathbf{S}^l$ . This convex combination strategy has the advantages of numerical stability and interpretability, which was widely used in modern deep learning, such as the Highway network [33] and Attention mechanism [34].

Note that the parameters of all the  $f_{\text{mixer}}$  functions are shared across layers to learn the neighbor effect of each node. Moreover, the mixer function maintains the expressive power of the chosen graph convolution, since it can easily degenerate to the normal graph convolution when  $\alpha^l = 1$ . As shown in the ablation study, our implementation of this mixer function is very effective with minimal parameter cost.

**Decoder:** With the last layer discriminant  $\mathbf{S}^L$  at hand, the task of decoder is to produce the final prediction  $\mathbf{Z}$  for classification. For simplicity, we use the linear layer with *softmax* operator as our decoder  $f_{\text{decoder}}$ .

$$\mathbf{Z} = \text{softmax}(f_{\text{decoder}}(\mathbf{S}^L)). \quad (11)$$

Note that we also apply the Norm layer to maintain numerical stability at the end of the Encoder, GC and Mixer module. Specifically, we use the L2 normalization for each node. Compared with the widely used BatchNorm and LayerNorm, we experimentally show that the L2 normalization of each node is parameter-free and can achieve better performance for our task.

In summary, our CAGNNs contribute three prominent advantages. First, it decouples the discrimination features from the aggregation features in the embedding space for the downstream task so that the graph convolution operator may not directly interact with the node’s discrimination feature and blur the classification boundary. Second, it leverages a learnable mixer function to determine the neighbor’s effect for each node based on these features. It can help each node choose to absorb or discard the neighbors’ information adaptively, thus leading to more discriminative node representations. Third, our framework can easily enhance the performance of most traditional graph convolution with only one additional layer.

### B. Spectral Analysis

We now study CAGNNs from a spectral perspective. We demonstrate that CAGNNs correspond to a polynomial graph filter with arbitrary coefficients on the graph spectral domain. Since using a polynomial graph filter can approximate any graph filter [35], the ability to express a polynomial graph filter with arbitrary coefficients is essential to prevent over-smoothing [21] and to learn from heterophilic graphs [13].

*Theorem 1: Considering the propagation matrix  $\mathbf{P}$  used for the basic graph convolution layer and a graph signal  $\mathbf{X}$ , a  $K$ -layer CAGNNs has the ability to express a  $K$ -order polynomial filter  $(\sum_l^K \theta^l \mathbf{P}^l) \mathbf{X}$  with different arbitrary coefficients  $\theta$  for each node.*

The above theorem indicates the expressive power on node classification of our framework. Intuitively, the important score  $\alpha$  allows CAGNNs to simulate the coefficient  $\theta$  of the polynomial graph filter for each node. Note that with a proper choice of  $\theta$ , the discriminant feature  $\mathbf{S}^K$  of each node can carry information from both the input feature and the high-order neighbor’s information adaptively with the increment of the order  $K$ . The detailed proof is presented below.

For simplicity, we neglect the L2 normalization at each layer because the simplified version also produces comparable performance. Moreover, we assume the input feature  $\mathbf{X}$  to be non-negative and remove the nonlinear Relu activation in the graph convolution layer [21], [36]. Then, for the simplified graph convolution layer, we have

$$\mathbf{H}^l = \mathbf{P}\mathbf{H}^{l-1}\mathbf{W}^l \quad (12)$$

$$= \mathbf{P}^l \mathbf{H}^0 \prod_{j=0}^{l-1} \mathbf{W}^j \quad (13)$$

$$= \mathbf{P}^l \mathbf{X} \tilde{\mathbf{W}}^l, \quad \text{where } \tilde{\mathbf{W}}^l = \prod_{j=0}^{l-1} \mathbf{W}^j. \quad (14)$$

Further, we can express the final representation as

$$\mathbf{S}^L = (\mathbf{1} - \alpha^L) * \mathbf{S}^{L-1} + \alpha^L * \mathbf{H}^L \quad (15)$$

$$= \sum_{l=0}^L \alpha^l \prod_{k=l+1}^L (1 - \alpha^k) * \mathbf{H}^l \quad (16)$$

$$= \sum_{l=0}^L \vartheta^l * \mathbf{H}^l, \quad \text{where } \vartheta^l = \alpha^l \prod_{k=l+1}^L (1 - \alpha^k) \quad (17)$$

$$= \sum_{l=0}^L \vartheta^l * \mathbf{P}^l \mathbf{X} \tilde{\mathbf{W}}^l \quad (18)$$

However,  $\vartheta^l \in [0, 1]$  which limits the expressive power of the polynomial filter. Thanks to the weight matrix  $\tilde{\mathbf{W}}^l$ , the coefficients of the polynomial can be extended to arbitrary values. Inspired by [21], we consider a weaker version of CAGNNs by fixing the weight matrix  $\tilde{\mathbf{W}}^l$  to be  $\gamma^l$ , where  $\gamma^l$  is a learnable parameter. We have

$$\mathbf{S}^L = \sum_{l=0}^L \vartheta^l * \mathbf{P}^l \mathbf{X} \gamma^l \quad (19)$$

$$= \sum_{l=0}^L \theta^l * \mathbf{P}^l \mathbf{X}, \quad \text{where } \theta^l = \vartheta^l \gamma^l \quad (20)$$

The polynomial coefficients  $\theta^l$  for each layer  $l$  can be set to arbitrary values with the help of the scalable parameter  $\gamma^l$ , so that our framework can help each node to learn arbitrary polynomial graph filters. Notice that, compared with other spectral GNNs that learn polynomial filters  $(\sum_l^K \theta^l \mathbf{P}^l) \mathbf{X}$  [13], [17], our models can empower each node with distinct polynomial coefficients by vectorized  $\theta$ . As in Section VI-B, our framework achieves higher performance than other spectral GNNs experimentally.

### C. Relation to other Decouple or Skip Connection GNNs

In this section, we discuss the relation of our two techniques (decouple operation and mixer module) in the framework with other models.

**Relation to GNNs with Decouple Design:** We remark that the decouple operation, which we study in this work, is a distinct concept from other decouple GNNs. The well-known decoupled GNNs, like APPNP [20],  $\mathbf{S}^2\text{GC}$  [37], and GPRGNN [13], aim to decouple the propagation and transformation of graph convolution. Without the loss of generalizability, they can be formulated as follows.

$$\mathbf{H}^l = \underbrace{\left( \sum_{i=0}^l \theta_i \mathbf{P}^i \right)}_{\text{propagate}} \overbrace{\mathbf{H}^0 \mathbf{W}}^{\text{transform}}, \quad (21)$$

where  $\theta$  is a scalar and  $\mathbf{P}$  is the propagation matrix. This operation make node have the ability to received high-order neighbor informaiton in one layer. In addition, the learnable parameter  $\theta$  ensures that it can learn the arbitrary coefficient of polynomial graph filters beyond the low-pass filters and perform well in heterophily [13]. However, it needs to decouple the weight matrix  $\mathbf{W}$  to reformulate the graph convolution operator, which restricts the adaption to other graph convolutions.

In contrast, our approach aims to decouple the discriminant feature and the aggregation feature, which can be easily compatible with most standard GNNs. Moreover, we theoretically prove that our framework can learn different arbitrary coefficients of  $K$ -order polynomial graph filters for each node, and achieve higher performance experimentally.

**Relation to GNNs with Skip Connection:** To better understand the mixer module, we compare it with respect to

the DeepGNNs with skip connection. Notice that, we aim at the heterophily problem, and our approach is different from the DeepGNNs designed to reduce the oversmoothing problem [3]. In order to alleviate the oversmoothing problem when the model becomes deeper, most DeepGNNs equip the residual connection or initial connection to combine previous layers’ features to prevent forgetting the original feature when models become deeper [21], [38]. The standard DeepGNN with skip connection can be formulated as follows.

$$\mathbf{H}^l = \sigma(\mathbf{P}\mathbf{H}^l\mathbf{W} + \{\mathbf{H}^{l-1}/\mathbf{H}^0\})(\text{residual/init connection}) \quad (22)$$

However, as in Section VI-B, this type of DeepGNNs also cannot perform well when dealing with heterophilic graphs. Since it just prevents forgetting the initial feature but not adaptively to aggregation of each node. For instance, the recent well-known SOTA of this type model is GCNII, where

$$\mathbf{H}^l = \sigma(((1 - \alpha_l)\mathbf{P}\mathbf{H}^l + \alpha_l\mathbf{H}^0) ((1 - \beta_l)\mathbf{I}_n + \beta_l\mathbf{W}^l)). \quad (23)$$

Since the scalar  $\alpha_l$  in GCNII is a hyper-parameter that must be manually chosen, it is shared for all nodes and is not the best choice to guide how to aggregate neighbors’ information on heterophilic datasets.

On the contrary, as shown in Equations (9), we use the mixer function to explicitly learn the importance score  $\alpha$  to evaluate the node-level neighbor effect for feature fusion explicitly. Moreover, compared with the skip connection, we separate the discriminant features of nodes at each layer and do not feed them into the next layer graph convolution component.

## VI. EXPERIMENTS

In this section, we report and compare the results for node classification on both real-world heterophily and homophily datasets to investigate the effectiveness, robustness and interpretability of the proposed heterophily GNN framework CAGNNs.

### A. Experimental Setup

1) *Datasets*: We evaluate the performance on nine well-known real-world node classification datasets, including three homophily datasets (Citeseer, Pubmed, and Cora) and six heterophily datasets (Texas, Wisconsin, Actor, Squirrel, Chameleon, and Cornell). For all benchmarks, we use the same feature vectors, graph structure, class labels, and 10 fixed random splits (48%/32%/20% of nodes per class for train/validation/test) provided in literature [8], [9].

- Homophily Datasets

- *Citeseer, Pubmed, Cora* [18]: For the basic citation datasets [39], nodes correspond to papers; edges correspond to citation links; the sparse bag-of-words are the feature representation of each node. Finally, the label of each node represents the topic of the paper.

- Heterophily Datasets

- *Texas, Wisconsin, Cornell* [9]: Cornell, Texas, and Wisconsin are the web page networks captured from the computer science departments of these universities in the WebKB<sup>2</sup> dataset. In these networks, nodes and edges represent the web pages and hyperlinks. Similar to the Citations networks, words in the web page represent the node features in the bag-of-word form. The web pages are labeled into five categories: student, project, course, staff, and faculty.
- *Squirrel, Chameleon* [9]: Chameleon and Squirrel are web pages extracted from different topics in Wikipedia [40]. Similar to WebKB, nodes and edges respectively denote the web pages and hyperlinks among them, and informative nouns in the web pages are employed to construct the node features in the bag-of-word form. Webpages are labeled in terms of the average monthly traffic level.
- *Actor* [9]: Actor network contains the co-occurrences of actors in films, which are extracted from the heterogeneous information networks. It describes the complex relationships among films, directors, actors and writers [41]. In this network, nodes and edges stand for actors and their co-occurrences in films, respectively. The actor’s Wikipedia page is exploited to extract features and node labels.

2) *Baselines*: We compare our method with the following baselines: (1) classical standard GNNs: GCN [18], GAT [30] and GIN [19]; (2) recent state-of-the-art GNNs of specific structure tackling heterophily: Geom-GCN [9], MixHop [28], H2GCN [8], GPRGNN [13], FAGCN [5], GCN-Cheby [17], JK-Net [29], GCNII [21]; and (3) standard 2-layer MLP. To show the effectiveness and generalizability of our framework, we choose three simple GCN, GAT, and GIN as the graph convolution component in CAGNNs. For ease of comparison, we use the reported results of baselines in literature [8], [9]. Moreover, for the missing results under these splits, we rerun the released code for 10 times and reported the mean and standard deviation.

- Classical GNNs

- *GCN* [18]: GCN can be seen as a laplacian smoother since it uses the mean aggregator to smooth each node and its neighbor’s features.
- *GIN* [19]: GIN utilized the MLP to model the injective function when aggregation and generalizes the WL test.
- *GAT* [30]: GAT is a graph neural network that applies the attention mechanism on node features to learn edge weights for aggregation.

- Heterophily GNNs

- *H2GCN* [5]: H2GCN proposed three designs with separate ego and neighbors, higher-order neighbors and a combination of intermediate representations to combine the message from neighbors.

<sup>2</sup><https://www.cs.cmu.edu/afs/cs.cmu.edu/project/theo-11/www/wwkb>

TABLE II: Performance comparison on various real-world heterophily and homophily datasets. Mean test accuracy and standard deviation are reported over 10 random data splits. The best performance is highlighted. “\*\*” denotes the results obtained from [8].

	Texas	Wisconsin	Actor	Squirrel	Chameleon	Cornell	Citeseer	Pubmed	Cora	Average
<b>Nodes</b>	183	251	7,600	5,201	2,277	183	3,327	19,717	2,708	-
<b>Edges</b>	295	466	26,752	198,493	31,421	280	4,676	44,327	5,278	-
<b>Features</b>	1,703	1,703	931	2,089	2,325	1,703	3,703	500	1,433	-
<b>Classes</b>	5	5	5	5	5	5	7	3	6	-
$\mathcal{H}_{node}$	0.06	0.16	0.24	0.22	0.25	0.11	0.71	0.79	0.83	-
$\mathcal{H}_{edge}$	0.11	0.21	0.22	0.22	0.23	0.30	0.74	0.80	0.81	-
$\mathcal{H}_{neighbor}$	0.45	0.72	<b>0.98</b>	0.92	0.91	0.55	0.87	0.85	0.72	-
GEOM-GCN [9]*	67.57	64.12	31.63	38.14	60.90	60.81	<b>77.99</b>	<b>90.05</b>	85.27	64.05
MixHop [28]*	77.84±7.73	75.88±4.90	32.22±2.34	43.80±1.48	60.50±2.53	73.51±6.34	76.26±1.33	85.31±0.61	87.61±0.85	68.21
H2GCN-1 [8]*	84.86±6.77	86.67±4.69	<b>35.86±1.03</b>	36.42±1.89	57.11±1.58	82.16±4.80	77.07±1.64	89.40±0.34	86.92±1.37	70.72
H2GCN-2 [8]*	82.16±5.28	85.88±4.22	35.62±1.30	37.90±2.02	59.39±1.98	82.16±6.00	76.88±1.77	89.59±0.33	87.81±1.35	70.87
GPRGNN [13]	82.12±7.72	81.16±3.17	33.29±1.39	43.29±1.66	61.82±2.39	81.08±6.59	75.56±1.62	86.85±0.46	86.98±1.33	70.15
JK-Net [29]*	66.49±6.64	74.31±6.43	34.18±0.85	40.45±1.61	63.42±2.00	64.59±8.68	74.51±1.75	88.41±0.45	86.79±0.92	65.79
GCN-Cheby [17]*	77.30±4.07	79.41±4.46	34.11±1.09	43.86±1.64	60.50±2.53	73.51±6.34	76.26±1.33	85.31±0.61	87.61±0.85	68.65
FAGCN [5]	78.11±5.01	81.56±4.64	35.41±1.18	42.43±2.11	56.31±3.22	76.12±7.65	74.86±2.42	85.74±0.36	83.21±2.04	68.18
GCNII [21]	69.72 ±8.90	75.29±4.64	35.58±1.25	47.21±1.73	60.79±2.35	79.19±6.12	76.82±1.67	89.26±0.48	<b>87.89±1.88</b>	69.07
MLP*	81.89±4.78	85.29±3.61	35.76±0.98	29.68±1.81	46.36±2.52	81.08±6.37	72.41±2.18	86.65±0.35	74.75±2.22	65.99
GIN [19]	71.89±6.64	77.84±4.53	32.15±1.56	35.78±1.34	56.18±1.94	75.94±7.47	75.68±1.89	88.64±0.54	86.49±1.91	66.73
CAGNN <sub>GIN</sub>	82.51±4.49	84.41±2.98	35.09±1.07	54.07±1.39	67.32±1.95	<b>82.97±5.56</b>	76.64±1.27	89.46±0.48	87.06±1.02	73.28
Gain	↑ 14.77%	↑ 8.44%	↑ 9.14%	↑ 51.12%	↑ 19.83%	↑ 9.26%	↑ 1.21%	↑ 0.93%	↑ 0.66%	↑ 9.81%
GAT [30]*	58.38±4.45	55.29±8.71	26.28±1.73	30.62±2.11	54.69±1.95	58.92±3.32	75.46±1.72	84.68±0.44	82.68±1.80	58.56
CAGNN <sub>GAT</sub>	83.52±6.17	<b>86.68±3.74</b>	34.95±1.36	55.52±1.45	68.50±1.32	81.35±5.28	75.51±1.54	89.51±0.54	87.48±1.10	73.67
Gain	↑ 43.06%	↑ 56.77%	↑ 32.99%	↑ 81.32%	↑ 25.27%	↑ 38.07%	↑ 0.07%	↑ 5.70%	↑ 5.81%	↑ 25.81%
GCN [18]*	59.46±5.25	59.80±6.99	30.26±0.79	36.89±1.34	59.82±2.58	57.03±4.67	76.68±1.64	87.38±0.66	87.28±1.26	61.62
CAGNN <sub>GCN</sub>	<b>85.13±5.73</b>	82.55±4.17	35.83±0.73	<b>61.82±1.45</b>	<b>69.16±1.90</b>	81.35±5.47	76.03±1.16	89.74±0.55	87.28±1.01	<b>74.32</b>
Gain	↑ 43.17%	↑ 38.04%	↑ 18.41%	↑ 67.58%	↑ 15.61%	↑ 42.64%	↓ 0.85%	↑ 2.70%	→ 0.00%	↑ 20.61%

- *FAGCN* [5]: FAGCN divided the message from each edge into low-frequency and high-frequency signals during aggregation.
- *GCN-Cheby* [17]: GCN-Cheby combines higher-order neighbor information with Chebyshev polynomials from the spectral domain.
- *GEOM-GCN* [9]: GEOM-GCN utilized structural similarity to capture the smooth structure in the latent space and long-range dependencies.
- *MixHop* [28]: MixHop repeatedly mixed feature representations of neighbors at various distances to achieve higher-order message passing.
- *GPRGNN* [13]: GPRGNN modified the convolution to the generalized page rank and learned an arbitrary polynomial graph filter to incorporate multi-scale information.
- *JK-Net* [29]: It combine intermediate node representations from each layer by concatenating them in the final layer.
- *GCNII* [21]: The state-of-the-art deep model combines initial connections and identity mapping to train a very deep GCN.

3) *Hyper-parameters.*: We adopt the same set of default hyper-parameters (2 layers and 64 hidden dimensions) for GCN, GAT, and GIN and corresponding CAGNNs. And for the CAGNNs, we only add one linear layer with 128 hidden units. We employ the Adam [42] optimizer and select the learning rate  $\in \{0.001, 0.01, 0.05\}$ , weight decay  $\in \{0.00005, 0.0005\}$  and dropout rate  $\in \{0, 0.5\}$  based on the validation sets. For other models, we utilize their best default

parameters in the original papers.

### B. Performance Comparison with SOTA

We report and compare the performance for the standard node classification task in Table II. For the classic GNNs (GCN, GAT and GIN), we first note that they outperform the MLP in the homophily datasets. It indicates that the homophily assumption and connected same-class neighbors provide helpful node classification information. However, we also notice that they sometimes also perform better than the MLP under heterophily datasets. For instance, in the Actor dataset, the performance of MLP is about 36%, but the traditional GCN only gets 26%. But in the Chameleon dataset, the performance comparison between GCN and MLP is (60% vs. 46%). Hence, it implies that not all the inter-class edges in the heterophily datasets are harmful to the node classification.

In addition, we note that the GNNs with specific designs for the heterophily datasets outperform the traditional GNNs with a large margin for six heterophily datasets. Most of them (e.g., MixHop, JK-Net, and H2GCN) explicitly aggregates high-order neighbors’ information to avoid the harmfulness of inter-class edges. For instance, the strong baseline H2GCN proves that the neighbor’s high-order information is expectedly homophily-dominant and achieves 70.87% average performance. In comparison, the average performance of two-layer GCN is only 61.62%.

In contrast, instead of considering the inter-class edges are all harmful, we take each node’s entire neighbor effect into account. As a result, compared with recently state-of-the-art heterophily GNNs, our CAGNNs framework helps tradi-



tional standard GNNs achieve competitive performance while maintaining the performance on three homophily datasets. Moreover, in the perspective of the spectral domain, our framework performs better than the spectral GNNs sharing the same polynomial filters coefficients for all nodes (e.g., GPRGNN and GCNII). Since CAGNN can help traditional GNNs adaptively learn different coefficients of K-order polynomial graph filters for each node. Under our framework, the average performance on nine datasets of GIN, GAT, and GCN outperforms all the baselines, and the average performance gains are 9.81%, 25.81%, and 20.61%, respectively. Among them, the proposed CAGNNs with 2-layers GCN achieves the best average performance (74.32) over all datasets. It verifies the effectiveness of decoupling design and consideration of the neighbor effect when performing graph convolution.

### C. Relation between the Metrics and Performance

Table II also shows the different metrics for all datasets. All the metrics range from  $[0, 1]$  and a higher score of  $\mathcal{H}_{\text{node}}$  and  $\mathcal{H}_{\text{edge}}$  denotes higher homophily. However, a higher  $\mathcal{H}_{\text{neighbor}}$  means lower identifiability of neighbors' distribution and a more challenging dataset, i.e., the neighbor distribution provides less useful information for classification. Note that our  $\mathcal{H}_{\text{neighbor}}$  can distinguish the dataset Actor (0.98) from others, in which the neighbors' distribution is nearly random and the best test classification accuracy is very low, i.e., 35.86. Therefore, neighbor distribution identifiability might provide a new way to understand the heterophily problem in GNNs.

Moreover, we also report the Kendall rank correlation coefficient between the metrics and the performance of CAGNN in Table III. The  $\mathcal{H}_{\text{neighbor}}$  is more correlated with the performance over different datasets. Therefore, the proposed metric can be considered a rough evaluator to measure the difficulty of graphs for the node classification task using GNNs, especially for medium-scale graphs with more than 500 nodes. Since we must have a sufficient number of nodes to have meaningful stats information.

For the class-level  $\mathcal{H}_{\text{neighbor}}^c$ , we show the relation with our CAGNN's performance under different datasets in Fig. 5. For clarity, we apply the negative  $\mathcal{H}_{\text{neighbor}}^c$  for each class to show a positive correlation between the model's class-wise performance and the class-wise neighbor distribution identifiability. At the class level, we can see that the performance of CAGNN<sub>GCN</sub> is highly consistent with the neighbor distribution identifiability for most datasets, which indicates that the neighbor perspective can help explain the model performance on various datasets. It also verifies that our framework can adaptively evaluate the neighbor effect and guide each node to absorb helpful information for the downstream node classification task.

### D. Ablation Study

In this section, we compare CAGNN with its variants for Mixer and Normalization to validate the effectiveness of each component. When testing different Mixer variants, we fix the Normalization to L2. Also, we set the Mixer to linear

TABLE III: Kendall correlation between different metrics and the performance of CAGNN<sub>GCN</sub>. The higher coefficient and the lower p-value are better and more significant.

Datasets	Kendall	$\mathcal{H}_{\text{node}}$	$\mathcal{H}_{\text{edge}}$	$\mathcal{H}_{\text{neighbor}}$
>500 nodes	coefficient	0.733	0.828	<b>0.867</b>
	p-value	0.056	0.022	<b>0.017</b>
All datasets	coefficient	0.11	0.25	<b>0.59</b>
	p-value	0.7	0.34	<b>0.02</b>

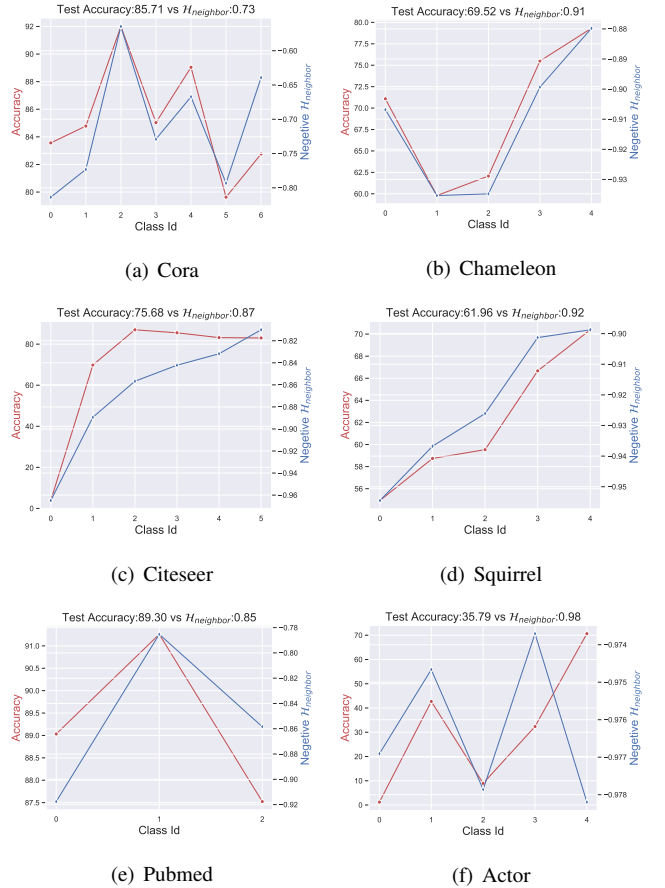


Fig. 5: Class-level comparison between our CAGNN<sub>GCN</sub> performance (red) and the negative class-level  $\mathcal{H}_{\text{neighbor}}^c$  (blue) for Homophily (Cora, Citeseer, and Pubmed) and Heterophily (Chameleon, Squirrel, and Actor). The class-level performance of CAGNN<sub>GCN</sub> is highly consistent with the neighbor distribution identifiability for most datasets.

to test different Normalization variants. We select the best hyper-parameters of each variant and run experiments for each dataset under 10 random splits to report the average performance on all datasets.

**Variants of Mixer.** The mixer module is a critical part of our framework to evaluate the neighbor effect and feature fusion. We compared our results with five variants.

- *Add*: The Add mixer is implemented by  $\mathbf{S}^l = \text{Norm}(\mathbf{S}^{l-1} + \mathbf{H}^l)$ .
- *Concat*: The Concat mixer is implemented by  $\mathbf{S}^l =$

TABLE IV: The average performance on all datasets for the ablation study of different types of Mixers and Normalization.

	Variants	CAGNN <sub>GIN</sub>	CAGNN <sub>GAT</sub>	CAGNN <sub>GCN</sub>
Mixer	Add	71.91	70.63	71.41
	Concat	69.50	71.27	72.23
	Global	72.17	72.52	73.43
	MLP-2	72.84	73.15	<b>74.38</b>
	MLP-3	72.57	73.47	74.20
Norm	None	72.29	73.03	73.01
	BatchNorm	65.11	61.61	64.92
	LayerNorm	72.41	72.19	72.45
	Ours	<b>73.28</b>	<b>73.67</b>	74.32

Norm( $[\mathbf{S}^{l-1}||\mathbf{H}^l]$ ). Notice that, we only apply the Norm at the first and last layer for the Concat variant to maintain stability.

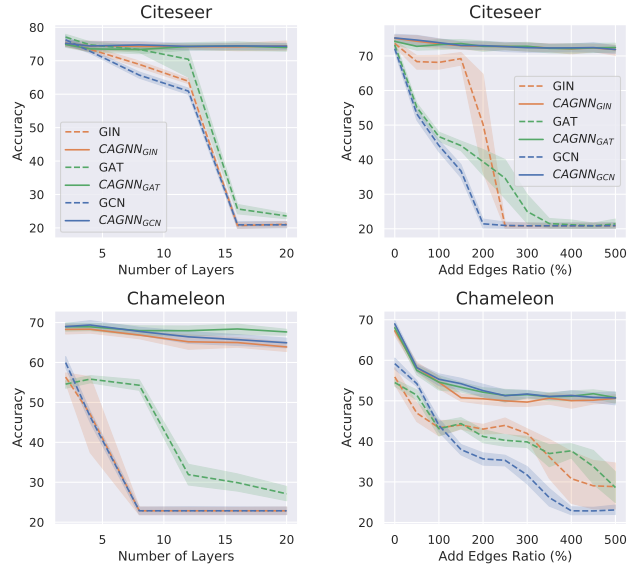
- *Global*: The Global mixer is  $\mathbf{S}^l = \text{Norm}((1 - \alpha_l)\mathbf{S}^{l-1} + \alpha_l\mathbf{H}^l)$ , where the learnable scalar  $\alpha_l$  is shared for all nodes.
- *MLP-2/3*: It replace the linear layer in  $f_{mixer}$  with 2 or 3 layers MLP.

From the results of these mixer variants in Table IV, we can draw the following conclusions: (1) The results of the Global mixer are better than the Add and Concat mixer, indicating neighbor effect is diverse under different datasets. (2) Our 1-layer mixer and multiple layer MLPs variants achieve consistently better performance than the Global. These mixers can adaptively learn each node’s neighbor effect, which verifies that the learnable node-level neighbor effect plays a more vital role than global. (3) Compared with different layers in the current  $f_{mixer}$  module, the result shows that the current one-layer is simple yet effective compared with multiple layer MLPs.

**Variants of Normalization.** We also compare the L2 norm for each node with three variants (None, BatchNorm [43] and LayerNorm [44]) to show its effectiveness. We first observe that the None normalization version achieves comparable performance, demonstrating that our framework is stable and competitive. However, the BatchNorm usually assumes the independent and identical distribution of each sample in deep learning, which may not be reasonable for the heterophilic graph and results in worse performance. Moreover, LayerNorm is also not beneficial, since the layer norm introduces learning parameters that may be redundant for GNNs. Compared with these variants, our simple yet effective L2 Norm achieves the best average performance.

### E. Robustness Analysis

In order to investigate whether the proposed CAGNN framework can help basic GNNs become more robust, we report the performance comparison between the basic GNNs and corresponding CAGNN in the oversmoothing and noisy edges scenario, respectively.



(a) Robustness of oversmooth (b) Robustness of noisy edges

Fig. 6: Performance comparison with traditional GNNs and the variants under the proposed CAGNNs framework in terms of (a) *number of layers*, and (b) *ratio of adding noisy edges* on Homophily (Citeseer) and Heterophily (Chameleon) datasets.

**Alleviating oversmooth.** It is well known that the traditional graph convolution is sensitive to the number of convolution layers due to the oversmoothing problem [3]. Our CAGNNs is able to increase the robustness of traditional graph convolution to avoid oversmoothing. As shown in Fig. 6(a), when the number of layers increases, the performance of traditional GNNs drops rapidly due to oversmoothing. Moreover, due to the massive inter-class edges, the oversmoothing phenomenon occurs earlier in the heterophily datasets. In contrast, the methods under the proposed framework are more stable and more consistent on both the Homophily (Citeseer) and Heterophily (Chameleon) datasets. The reason is that our framework has the ability to avoid incorporating the over-smoothing features to maintain the discrimination power for each node.

**Alleviating noisy edges.** Most GNNs are also sensitive to the noisy edges in graphs [45], [46]. To evaluate the robustness of the proposed framework on noisy graphs, we construct graphs with random edge addition according to the literature [47]. Specifically, we randomly add 25%~500% edges in the original graphs. As shown in Fig. 6(b), our CAGNNs achieves significantly better prediction for those noisy graphs compared with the basic GNNs. It also demonstrates that our decouple design and the mixer module are able to learn to discard the noisy features from neighbors.

### F. Visualization and Interpretability

To verify whether CAGNNs can adaptively learn the different neighbor effect of each node, we visualize the neighbor importance score  $\alpha$  distribution on both homophily and

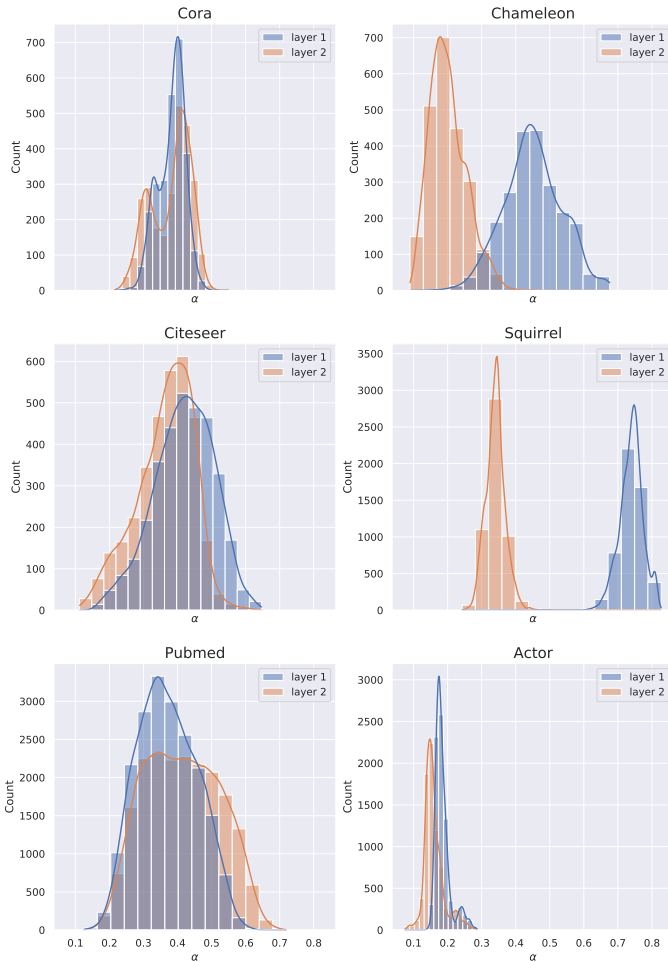


Fig. 7: Visualization of nodes’ neighbor importance score of the first and second layer on different datasets.

heterophilic datasets, where the results are shown in Fig. 7. We have the following observation: (1) As we can see, for homophilic datasets (Cora, Citeseer, and Pubmed), the coefficients are near 0.4 for most nodes. This indicates that the information from neighbors is helpful for the downstream classification, which is consistent with the homophilic assumption. (2) However, we observe similar trends in heterophilic datasets (Chameleon and Squirrel) that most nodes still absorb the neighbors’ information. Moreover, the distribution of the second layer score shows that 1-hop neighbors are more important than the 2-hop neighbors. This phenomenon is contrary to the previous study that the inter-class edges are all harmful, which implies that graph convolution can still extract classification information from an inter-class neighbor with non-random distribution. (3) As for the Actor dataset, that has a similar proportion of inter-class edges with Chameleon and Squirrel, but the neighbor distribution is nearly random (the  $\mathcal{H}_{neighbor}$  is 0.98). The neighbor importance score  $\alpha$  of nodes tends to be 0, which verifies that the inter-class edges with random distribution are harmful and guides the model to discard neighbors’ information when aggregation.

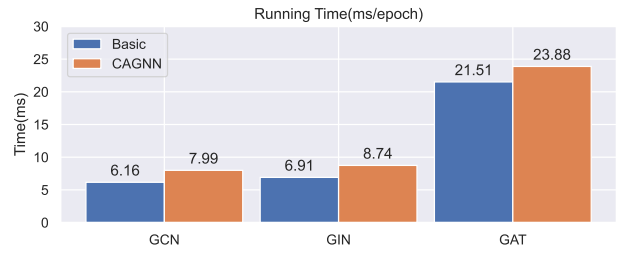


Fig. 8: Average running time per epoch (ms)

### G. Complexity

Finally, we investigate the complexity of the proposed framework. The complexity of computing the neighbor importance score and mixing for all nodes is  $O(Nd)$  where  $N$  is the total number of nodes and  $d$  is the dimension of hidden nodes. The computational complexity is on par with the neighborhood aggregation operation in GNNs, which is also  $O(Nd)$ . Hence, the complexity of ours and classic GNNs are on the same level. We also report the average training time of each epoch over all datasets of the standard graph convolution and our method in Fig. 8. It indicates that our model scales similarly to the basic GNNs with a small computation cost for the mixer module.

## VII. CONCLUSION

In this paper, we have investigated the neighbor effect on heterophilic datasets. Unlike the previous works that argue that the inter-class edges are harmful for the node classification, we find that the inter-class edges may be helpful when the neighbor distribution is identifiable and quantify the neighborhood identifiability with Von Neumann entropy. This new metric sheds new light on the heterophily problem of GNNs. It enables us to explain the performance variation of GNNs for different datasets and can be used to guide the application of GNNs.

We also proposed a general heterophily GNN framework to improve the performance of traditional GNNs by adding only one mixer layer. Specifically, we first decouple the features of nodes into the discrimination and aggregation parts. Then, we use a mixer module to adaptively fuse these features by evaluating the neighbor effect of each node. Our experiments on nine well-known benchmark datasets demonstrate the effectiveness of our framework to improve existing GNNs on heterophilic graphs consistently.

## REFERENCES

- [1] Z. Wu, S. Pan, F. Chen, G. Long, C. Zhang, and P. S. Yu, “A comprehensive survey on graph neural networks,” *IEEE Transactions on Neural Networks and Learning Systems*, vol. 32, no. 1, pp. 4–24, 2021.
- [2] W. L. Hamilton, R. Ying, and J. Leskovec, “Inductive representation learning on large graphs,” in *Advances in Neural Information Processing Systems*, 2017, pp. 1025–1035.
- [3] Q. Li, Z. Han, and X.-M. Wu, “Deeper insights into graph convolutional networks for semi-supervised learning,” in *Proceedings of the AAAI Conference on Artificial Intelligence*, vol. 33, no. 1, 2018, pp. 3538–3545.

- [4] Y. Yan, M. Hashemi, K. Swersky, Y. Yang, and D. Koutra, "Two sides of the same coin: Heterophily and oversmoothing in graph convolutional neural networks," *preprint arXiv:2102.06462*, 2021.
- [5] D. Bo, X. Wang, C. Shi, and H. Shen, "Beyond low-frequency information in graph convolutional networks," in *Proceedings of the AAAI Conference on Artificial Intelligence*, vol. 35, no. 5, 2021, pp. 3950–3957.
- [6] J. Zhu, R. A. Rossi, A. Rao, T. Mai, N. Lipka, N. K. Ahmed, and D. Koutra, "Graph neural networks with heterophily," in *Proceedings of the AAAI Conference on Artificial Intelligence*, vol. 35, no. 12, 2021, pp. 11 168–11 176.
- [7] X. Zheng, Y. Liu, S. Pan, M. Zhang, D. Jin, and P. S. Yu, "Graph neural networks for graphs with heterophily: A survey," *preprint arXiv:2202.07082*, 2022.
- [8] J. Zhu, Y. Yan, L. Zhao, M. Heimann, L. Akoglu, and D. Koutra, "Beyond homophily in graph neural networks: Current limitations and effective designs," in *Advances in Neural Information Processing Systems*, vol. 33, 2020.
- [9] H. Pei, B. Wei, K. C.-C. Chang, Y. Lei, and B. Yang, "Geom-gcn: Geometric graph convolutional networks," in *International Conference on Learning Representations*, 2020.
- [10] J. Chen, S. Chen, M. Bai, J. Pu, J. Zhang, and J. Gao, "Graph decoupling attention markov networks for semisupervised graph node classification," *IEEE Transactions on Neural Networks and Learning Systems*, pp. 1–15, 2022.
- [11] Y. Hou, J. Zhang, J. Cheng, K. Ma, R. T. B. Ma, H. Chen, and M.-C. Yang, "Measuring and improving the use of graph information in graph neural networks," in *International Conference on Learning Representations*, 2020.
- [12] O. Stretcu, K. Viswanathan, D. Movshovitz-Attias, E. A. Platanios, S. Ravi, and A. Tomkins, "Graph agreement models for semi-supervised learning," in *Advances in Neural Information Processing Systems*, 2019.
- [13] E. Chien, J. Peng, P. Li, and O. Milenkovic, "Adaptive universal generalized pagerank graph neural network," in *International Conference on Learning Representations*, 2021.
- [14] Y. Ma, X. Liu, N. Shah, and J. Tang, "Is homophily a necessity for graph neural networks?" in *International Conference on Learning Representations*, 2022.
- [15] I. Bengtsson and K. Życzkowski, *Geometry of quantum states: an introduction to quantum entanglement*. Cambridge university press, 2017.
- [16] J. Bruna, W. Zaremba, A. Szlam, and Y. LeCun, "Spectral networks and locally connected networks on graphs," *preprint arXiv:1312.6203*, 2013.
- [17] M. Defferrard, X. Bresson, and P. Vandergheynst, "Convolutional neural networks on graphs with fast localized spectral filtering," *Advances in neural information processing systems*, vol. 29, 2016.
- [18] T. N. Kipf and M. Welling, "Semi-supervised classification with graph convolutional networks," in *International Conference on Learning Representations*, 2017.
- [19] K. Xu, W. Hu, J. Leskovec, and S. Jegelka, "How powerful are graph neural networks?" in *International Conference on Learning Representations*, 2018.
- [20] J. Klicpera, A. Bojchevski, and S. Günnemann, "Predict then propagate: Graph neural networks meet personalized pagerank," in *International Conference on Learning Representations*, 2019.
- [21] M. Chen, Z. Wei, Z. Huang, B. Ding, and Y. Li, "Simple and deep graph convolutional networks," in *International Conference on Machine Learning*. PMLR, 2020, pp. 1725–1735.
- [22] P. W. Battaglia, J. B. Hamrick, V. Bapst, A. Sanchez-Gonzalez, V. Zambaldi, M. Malinowski, A. Tacchetti, D. Raposo, A. Santoro, R. Faulkner *et al.*, "Relational inductive biases, deep learning, and graph networks," *preprint arXiv:1806.01261*, 2018.
- [23] H. Nt and T. Maehara, "Revisiting graph neural networks: All we have is low-pass filters," *preprint arXiv:1905.09550*, 2019.
- [24] G. Wang, R. Ying, J. Huang, and J. Leskovec, "Improving graph attention networks with large margin-based constraints," *preprint arXiv:1910.11945*, 2019.
- [25] M. He, Z. Wei, H. Xu *et al.*, "Bernnet: Learning arbitrary graph spectral filters via bernstein approximation," *Advances in Neural Information Processing Systems*, vol. 34, 2021.
- [26] M. Liu, Z. Wang, and S. Ji, "Non-local graph neural networks," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2021.
- [27] B. Fatemi, L. El Asri, and S. M. Kazemi, "Slaps: Self-supervision improves structure learning for graph neural networks," *Advances in Neural Information Processing Systems*, vol. 34, 2021.
- [28] S. Abu-El-Haija, B. Perozzi, A. Kapoor, N. Alipourfard, K. Lerman, H. Harutyunyan, G. Ver Steeg, and A. Galstyan, "Mixhop: Higher-order graph convolutional architectures via sparsified neighborhood mixing," in *International Conference on Machine Learning*. PMLR, 2019, pp. 21–29.
- [29] K. Xu, C. Li, Y. Tian, T. Sonobe, K.-i. Kawarabayashi, and S. Jegelka, "Representation learning on graphs with jumping knowledge networks," in *International Conference on Machine Learning*. PMLR, 2018, pp. 5453–5462.
- [30] P. Veličković, G. Cucurull, A. Casanova, A. Romero, P. Liò, and Y. Bengio, "Graph attention networks," in *International Conference on Learning Representations*, 2018.
- [31] K. Hornik, M. Stinchcombe, and H. White, "Multilayer feedforward networks are universal approximators," *Neural networks*, vol. 2, no. 5, pp. 359–366, 1989.
- [32] K. Hornik, "Approximation capabilities of multilayer feedforward networks," *Neural networks*, vol. 4, no. 2, pp. 251–257, 1991.
- [33] R. K. Srivastava, K. Greff, and J. Schmidhuber, "Highway networks," *preprint arXiv:1505.00387*, 2015.
- [34] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, and I. Polosukhin, "Attention is all you need," in *Advances in Neural Information Processing Systems*, 2017, pp. 5998–6008.
- [35] D. I. Shuman, S. K. Narang, P. Frossard, A. Ortega, and P. Vandergheynst, "The emerging field of signal processing on graphs: Extending high-dimensional data analysis to networks and other irregular domains," *IEEE Signal Processing Magazine*, vol. 30, no. 3, pp. 83–98, 2013.
- [36] F. Wu, A. Souza, T. Zhang, C. Fifty, T. Yu, and K. Weinberger, "Simplifying graph convolutional networks," in *International Conference on Machine Learning*. PMLR, 2019, pp. 6861–6871.
- [37] H. Zhu and P. Koniusz, "Simple spectral graph convolution," in *International Conference on Learning Representations*, 2021.
- [38] G. Li, M. Muller, A. Thabet, and B. Ghanem, "Deepgcn: Can gcns go as deep as cnns?" in *Proceedings of the IEEE/CVF international conference on computer vision*, 2019, pp. 9267–9276.
- [39] P. Sen, G. Namata, M. Bilgic, L. Getoor, B. Galligher, and T. Eliassi-Rad, "Collective classification in network data," *AI magazine*, vol. 29, no. 3, pp. 93–93, 2008.
- [40] B. Rozemberczki, C. Allen, and R. Sarkar, "Multi-scale attributed node embedding," *Journal of Complex Networks*, vol. 9, no. 2, 2021.
- [41] J. Tang, J. Sun, C. Wang, and Z. Yang, "Social influence analysis in large-scale networks," in *Proceedings of the 15th ACM SIGKDD international conference on Knowledge discovery and data mining*, 2009, pp. 807–816.
- [42] D. P. Kingma and J. Ba, "Adam: A method for stochastic optimization," *preprint arXiv:1412.6980*, 2014.
- [43] S. Ioffe and C. Szegedy, "Batch normalization: Accelerating deep network training by reducing internal covariate shift," *preprint arXiv:1502.03167*, 2015.
- [44] J. Ba, J. R. Kiros, and G. E. Hinton, "Layer normalization," *preprint arXiv:1607.06450*, 2016.
- [45] L. Franceschi, M. Niepert, M. Pontil, and X. He, "Learning discrete structures for graph neural networks," in *International Conference on Machine Learning*. PMLR, 2019, pp. 1972–1982.
- [46] K. Xu, H. Chen, S. Liu, P.-Y. Chen, T.-W. Weng, M. Hong, and X. Lin, "Topology attack and defense for graph neural networks: An optimization perspective," in *International Joint Conference on Artificial Intelligence*, 2019.
- [47] Y. Chen, L. Wu, and M. Zaki, "Iterative deep graph learning for graph neural networks: Better and robust node embeddings," *Advances in Neural Information Processing Systems*, vol. 33, 2020.