Make Heterophily Graphs Better Fit GNN: A Graph Rewiring Approach

Wendong Bi†
bwendong20@mails.ucas.ac.cn
Institute of Computing Technology,
Chinese Academy of Sciences
Beijing, China

Lun Du‡
lun.du@microsoft.com
Microsoft Research Asia
Beijing, China

Qiang Fu
qifu@microsoft.com
Microsoft Research Asia
Beijing, China

Yanlin Wang
yanlwang@microsoft.com
Microsoft Research Asia
Beijing, China

Shi Han
shihan@microsoft.com
Microsoft Research Asia
Beijing, China

Dongmei Zhang
dongmeiz@microsoft.com
Microsoft Research Asia
Beijing, China

ABSTRACT

Graph Neural Networks (GNNs) are popular machine learning methods for modeling graph data. A lot of GNNs perform well on homophily graphs while having unsatisfied performance on heterophily graphs. Recently, some researchers turn their attentions to designing GNNs for heterophily graphs by adjusting message passing mechanism or enlarging the receptive field of the message passing. Different from existing works that mitigate the issues of heterophily from model design perspective, we propose to study heterophily graphs from an orthogonal perspective by rewiring the graph structure to reduce heterophily and making the traditional GNNs perform better. Through comprehensive empirical studies and analysis, we verify the potential of the rewiring methods. To fully exploit its potential, we propose a method named Deep Heterophily Graph Rewiring (DHGR) to rewire graphs by adding homophilic edges and pruning heterophilic edges. The detailed way of rewiring is determined by comparing the similarity of label/feature-distribution of node neighbors. Besides, we design a scalable implementation for DHGR to guarantee a high efficiency. DHGR can be easily used as a plug-in module, i.e., a graph pre-processing step, for any GNNs, including both GNN for homophily and heterophily, to boost their performance on the node classification task. To the best of our knowledge, it is the first work studying graph rewiring for heterophily graphs. Extensive experiments on 11 public graph datasets demonstrate the superiority of our proposed methods.

KEYWORDS

GNN, heterophily, graph rewiring, neighbor distribution

1 INTRODUCTION

Graph-structure data is ubiquitous in representing complex interactions between objects [6, 12, 28]. Graph Neural Network (GNN), as a powerful tool for graph data modeling, has been widely developed for various real-world applications [10, 34, 39]. Based on the message passing mechanism, GNNs update node representations by aggregating messages from neighbors, thereby concurrently exploiting the rich information inherent in the graph structure and node attributes.

Traditional GNNs [16, 19, 31] mainly focus on homophily graphs that satisfy property of homophily (i.e. most of connected nodes belong to the same class). However, these GNNs usually cannot perform well on graphs with heterophily (i.e. most of connected nodes belong to different classes) for the node classification problem, because message passing between nodes from different classes makes their representations less distinguishable, and thus leading to bad performance on node classification task. The aforementioned issues motivate considerable studies around GNNs for heterophily graph. For example, some studies [11, 33, 37] adjust message passing mechanism for heterophily edges, while others [1, 8, 27, 43] enlarge the receptive field for the message passing. Note that, all these works mitigate the distinguishability issue caused by heterophily from the perspective of the GNN model design. While, there is another orthogonal perspective to mitigate the issue caused by heterophily, i.e., rewiring graph to reduce heterophily or increase homophily, which is still under-explored.

Graph rewiring [2, 7, 14, 29] is a kind of method that decouples the input graph from the graph for message passing and boost the performance of GNN on node classification tasks via changing the message passing structure. Many works have utilized graph rewiring for different tasks. However, most existing graph rewiring techniques have been developed for graphs under homophily assumption (sparsity [24], smoothness [17, 26] and low-rank [45]), and thereby can not directly transfer to heterophily graphs. Different from existing solutions that design specific GNN architectures
adapted to heterophily graphs, in this paper, we conduct comprehensive study on graph rewiring and propose an effective rewiring algorithm to reduce graph heterophily, which make GNNs perform better for both homophily and homophily graphs.

First we demonstrate the effects of increasing homophily-level for heterophily graphs in Sec. 3 with comprehensive controlled experiments. Note that the homophily (and heterophily) level can be measured with Homophily Ratio (HR) [27, 43], which is formally defined as an average of the consistency of labels between each connected node-pair. From the analysis in Sec. 3.1, we find that both the node-level homophily ratio [11, 27] and node degree (reflects the recall of nodes from the same class) can affect the performance of GCN on the node classification task, where increasing either of the two variables can lead to better performance of GCN. This finding, i.e., classification performance of GCN on heterophily graphs can be increased by reducing the heterophily-level of graphs, motivates us to design a graph-rewiring strategy to increase homophily-level for heterophily graphs so that GNNs can perform better on the rewired graphs.

Then, we propose a learning-based graph rewiring approach on heterophily graphs, namely Deep Heterophily Graph Rewiring (DHGR). DHGR re-wires the graph by adding/pruning edges on the input graph to reduce its heterophily-level. It can be viewed as a plug-in module for graph pre-processing that can work together with many kinds of GNN models including both GNNs for homophily and heterophily, to boost their performance on node classification tasks. The key idea of DHGR is to reduce the heterophily while keeping the effectiveness by adding more homophilic edges and removing heterophilic edges. However, simply adding homophilic edges and removing heterophilic edges between nodes in the training set may increase the risk of overfitting and lead to poor performance (we prove this in Sec. 5.4). Another challenge is that unlike homophily graphs that can leverage Laplace Smooth to enhance the correlation between node features and labels, heterophily graphs do not satisfy the property of smoothness [17, 26]. In this paper, we propose to use label/feature-distribution of neighbors on the input graph as guidance signals to identify edge polarity (homophily/heterophily) and prove its effectiveness in 3.2.

Under the guidance of the neighbors’ label-distribution, DHGR learns the similarity between each node-pair, which forms a similarity matrix. Then based on the learned similarity matrix, we can rewire the graph by adding edges between high-similarity node-pairs and pruning edges connecting low-similarity node-pairs. Then the learned graph structure can be further fed into GNNs for node classification tasks. Besides, we also design a scalable implementation of DHGR which avoids the quadratic time and memory complexity with respect to the numbers of nodes, making our method available for large-scale graphs. Finally, extensive experiments on 11 real-world graph datasets, including both homophily and heterophily graphs, demonstrate the superiority of our method.

We summarize the contributions of this paper as follows:

1) We propose the new perspective, i.e., graph rewiring, to deal with heterophily graphs by reducing heterophily and make GNNs perform better.
2) We propose to use neighbor’s label-distribution as guidance signals to identify homophily and heterophily edges with comprehensive experiments.
3) We design a learnable plug-in module for graph rewiring on heterophily graphs, namely DHGR. And we design a high-efficient scalable training algorithm for DHGR.
4) We conduct extensive experiments on 11 real-world graphs, including both heterophily and homophily graphs. The results show that GNNs with DHGR consistently outperform their vanilla versions. In addition, DHGR has additional gain even when combined with GNNs specifically designed for heterophily graphs.

2 PRELIMINARY

In this section, we give the definitions of some important terminologies and concepts appearing in this paper.

2.1 Graph Neural Networks

Let \( G = (V, E) \) denotes a graph, where \( V \) is the node set, \( N = |V| \) is the number of nodes in \( G \). Let \( X \in \mathbb{R}^{N \times D} \) denote the feature matrix and the \( l \)-th row of \( X \) denoted as \( x_i \) is the \( D \)-dimensional feature vector of node \( v_i \). \( E = \{(v_i, v_j) | v_i, v_j \in V \text{ and } v_i, v_j \text{ is connected}\} \). GNNs aim to learn representation for nodes in the graph. Typically, GNN models follow a neighborhood aggregation framework, where node representations are updated by aggregating information of its neighboring nodes. Let \( h_i^{(l)} \) denotes the output vector of node \( v_i \) at the \( l \)-th hidden layer and let \( h_i^{(0)} = x_i \). The \( l \)-th iteration of aggregation step can be written as:

\[
    h_i^{(l)} = \text{COMBINE} \left( h_i^{(l-1)}, \text{AGG} \left( \{h_j^{(l-1)} | v_j \in N(v_i)\} \right) \right)
\]

where \( N(v_i) \) is the set of neighbors of \( v_i \). The AGG function indicates the aggregation function aimed to gather information from neighbors and the goal of the COMBINE function is to fuse the information from neighbors and the central node. For graph-level tasks, an additional READOUT function is required to get the global representation of the graph.

2.2 Graph Rewiring

Given a graph \( G = (V, E) \) with node features \( X \in \mathbb{R}^{N \times D} \) as the input, Graph Rewiring (GR) aims at learning an optimal \( G^* = (V, E^*) \) under a given criterion, where the edge set is updated and the node set is constant. Let \( A, A^* \in \mathbb{R}^{N \times N} \) denote the adjacent matrix of \( G \) and \( G^* \), respectively. The rewired graph \( G^* \) is used as input of GNNs, which is expected to be more effective than directly inputting the original graph \( G \). As shown in Fig. 1, the pipeline of
Graph Rewiring models usually involves two stages, the similarity learning and the graph rewiring based on the learned similarity between pairs of nodes. It is obvious that the criterion (i.e., objective function) design plays a critical role for the similarity learning stage. Thus, we first mine knowledge from data in the next section to abstract an effective criterion of graph rewiring.

3 OBSERVATIONS FROM DATA

We observed from data that there exist two important properties of graph (i.e., node-level homophily ratio and degree) that are strongly correlated with the performance of GNNs. The two properties provide vital guidance so that we can optimize the graph structure by graph rewiring. However, we cannot directly calculate node-level homophily ratio because of the partially observable labels during training. Therefore, we introduce two other effective signals, i.e., neighbor’s observable label/feature-distribution, which have strong correlations with the node-level homophily ratio. In this section, we first verify the relations between the two properties and the performance of GNNs. Then we verify the correlations between neighbor distribution and node-level homophily ratio.

3.1 Effects of Node-level Homophily Ratio and Degree

First, we conduct validation experiments to verify the effects of node-level homophily ratio $p$ and degree $k$, on the performance of GCN, as guidance for graph rewiring. Specifically, we first construct graphs by quantitatively controlling the node-level homophily ratio and node degree, and then verify the performance of GCN on the constructed graphs as a basis for measuring the quality of structured graph structure. Note that considering the direction of message passing is from source nodes to target nodes, the node degree mentioned in this paper refers to the in-degree.

For example, given node degree $k$ and node-level homophily ratio $p$, we can construct a directional Graph $G_{k,p}$ where each node on the $G_{k,p}$ has $k$ different neighboring nodes pointing to it and there are $\lfloor p \cdot k \rfloor$ same-class nodes among the $k$ neighbors, with other $\lceil k \cdot (1-p) \rceil$ neighbors randomly selected from remaining different-class nodes on the graph.

As shown in the Fig. 2, we conduct validation experiments on three different graph datasets, including one homophily graph (Cora) and two heterophily graphs (Chameleon, Actor). In this experiments, we construct graphs $G_{k,p}$ with node degree $k$ ranging from 5 to 25 and node-level homophily ratio $p$ ranging from 0.0 to 1.0, totally 35 constructed graphs for each dataset. And then for each constructed graph, we train vanilla GCN [19] on it three times and calculate the average test accuracy on node classification task. From the Fig. 2, we find that both the homophily graph and the heterophily graph follow the same rule: when the degree is fixed, the accuracy of GCN increases with the increase of the node-level homophily ratio; when the homophily ratio is fixed, the accuracy of GCN increases with the increase of the degree. It should be noted that when the homophily ratio $p$ equals 0 (i.e., all neighboring nodes are from different classes), it may have a higher GCN accuracy than that when the homophily ratio is very small (around $p = 0.2$). Besides, when the homophily ratio $p$ is larger than a threshold, the GCN accuracy converges to 100%. In general, the GCN accuracy almost varies monotonically with the node-level homophily ratio and node degree. And this motivates us to use graph rewiring as a way of increasing both node-level homophily ratio and degree.

Figure 3: Mutual Information (MI) between different signals and edge polarity (i.e. homophily or heterophily).
3.2 Effects of Neighbor’s Label/Feature Distribution

From the Sec. 3.1, we conclude that graph rewiring can be used as a way of reducing heterophily to make GNNs perform well on both homophily and heterophily graphs. However, it is not easy to accurately identify the edge polarity (homophily or heterophily) on a heterophily graph so that we can estimate the node-level homophily ratio. For a homophily graph, we can leverage its homophily property and use Laplacian Smoothing [17, 26] to make its node representation more distinguishable. However, heterophily graphs do not satisfy property of smoothness thus the information available is limited. A straightforward idea is to use node features to identify edge polarity, however, the information of this single signal is limited. In this paper, we propose to use similarity between the neighbor’s label-distribution for node-pairs as a measure of edge polarity. Besides, considering that not all node labels are observable, we also introduce neighbor’s feature-distribution (mean of neighbor features), which is completely observable, as signals in addition to neighbor’s label-distribution.

Up to now, we have three signals (i.e. raw node features, label-distribution and feature-distribution of neighbors) that can be used as measures for edge polarity. We quantitatively evaluate the effectiveness of the three signals and find that the distribution signals are more informative than the raw node feature through the following empirical experiments and analysis. To be specific, we consider the label/feature-distribution of the 1st-order and 2nd-order neighbors. Then we calculate the similarity between each node-pair with one of these signals and compute the mutual information between the node-pair similarity and edge polarity on the graph. The formula of Mutual information is written as follows:

\[
I(X; Y) = \int_y \int_x P_{X,Y}(x, y) \cdot \log \frac{P_{X,Y}(x, y)}{P_X(x)P_Y(y)} \, dx \, dy \quad (1)
\]

In the case of discrete random variables, the integral operation is replaced by the sum operation.

As shown in the Fig. 3, we conduct statistical analysis on three datasets (i.e. Cora, Chameleon, Actor). From the Fig. 3, we find that both the similarity of neighbor’s label-distribution and neighbor’s feature-distribution have a strong correlation with edge polarity than that of the raw node features similarity, and neighbor’s label-distribution has a stronger correlation than neighbor’s feature-distribution in most cases. And this rule applies to both homophily graphs and heterophily graphs.

4. METHOD

Based on the observations mentioned above, we design the Deep Heterophily Graph Rewiring method (DHGR) for heterophily graphs, which can be easily plugged into various existing GNN models. Following the pipeline in Fig. 1, DHGR first learns a similarity matrix representing the similarity between each node-pair based on the neighbor distribution (i.e. label-distribution and feature-distribution of neighbors). Then we can rewire the graph structure by adding edges between high-similarity node-pair and pruning low-similarity edges on the original graph. Finally, the rewired graph is further fed into other GNN models for node classification tasks.

4.1 Similarity Learner Based on Neighbor Distribution

Before rewiring the graph, we first learn the similarity between each pair of nodes. According to the analysis in Sec. 3.2, we design a graph learner that learns the node-pair similarity based on the neighbor distribution. Considering that in the training process, only the labels of nodes in the training set are available, we cannot observe the full label-distribution of neighbors. Therefore, we also leverage the feature-distribution of neighbors which can
be fully observed to enhance this similarity learning process with the intuition that node features have correlations to labels for an attributed-graph. Besides, the results shown in Sec. 3.2 also validate the effectiveness of neighborhood’s feature-distribution.

The overview of similarity learner used in DHGR is shown in Fig. 4. Specifically, for an attributed graph, we can first calculate its observable label-distribution \(D_Y^{(k)}\) and feature-distribution \(D_X^{(k)}\) for the \(k\)-hop neighbors of each node using node-labels in the training set and all node-features:

\[
D_Y^{(k)} = (D^{-1}A)^k Y_{Train}, \quad D_X^{(k)} = (D^{-1}A)^k X
\]

\(D_Y^{(k)}\) and \(D_X^{(k)}\) is respectively the label-distribution and feature-distribution of \(k\)-order neighbors in the graph, \(M\) is the maximum neighbor-order and we use \(M \in [1, 2]\) in this paper. \(Y_{Train}\) is the one-hot label matrix, the \(i\)-th row of \(Y_{Train}\) is the one-hot label vector of node \(v_i\) if \(v_i\) belongs to the training set, else use a zero-vector instead. \(A\) is the adjacent matrix and \(D\) is the corresponding degree diagonal matrix. Then for each node, we can get the observed label-distribution vector and feature-distribution vector of its neighbors. Next we calculate the cosine similarity between each node-pair with respect to both label-distribution and feature-distribution, and we can get the similarity matrix of label-distribution \(S_Y^{train}\) and similarity matrix of feature-distribution \(S_X\):}

\[
\begin{align*}
S_Y^{train}[i, j] &= \prod_{k=1}^{M} \cos \left( D_Y^{(k)}[i, :], D_Y^{(k)}[j, :] \right) \\
S_X[i, j] &= \prod_{k=1}^{M} \cos \left( D_X^{(k)}[i, :], D_X^{(k)}[j, :] \right)
\end{align*}
\]

where

\[
\cos(z_i, z_j) = \frac{\bar{z}_i \cdot \bar{z}_j}{|\bar{z}_i| \cdot |\bar{z}_j|}, \quad \bar{z}_i = z_i - \frac{1}{|V|} \sum_{j \in V} z_j
\]

Note that before calculating cosine similarity, we first decentralize the input variable by subtracting the mean of this variable for all nodes. Considering that not all nodes have an observed label-distribution, e.g., if all neighbors of node \(v_i\) do not belong to the training set, then the observed label-distribution of \(v_i\) is a zero vector. Obviously, this is not ideal, so we compensate for this with the feature-distribution of neighbors. In addition, we restrict the utilization condition of neighbor-label-distribution by using a mask. Specifically, for node \(v_i \in V\), we leverage its neighbor label-distribution only when the percentage of its neighbors in the training set is larger than a threshold \(\alpha\):

\[
Masky(v_i) = \begin{cases} 
1, & r_i > \alpha \\
0, & r_i \leq \alpha
\end{cases}, \quad where \ r_i = \frac{|N(v_i) \cap V_{Train}|}{|N(v_i)|}
\]

Masky \(\in \mathbb{R}^{N \times 1}\) is the mask vector, \(N(v_i)\) is the neighbor set of \(v_i\), \(V_{Train}\) is the set of nodes in the training set. Then our similarity learner targets at learning the similarity of node-pairs based on the neighbor distribution. Specifically, the similarity learner first aggregates and transforms the feature of neighboring nodes and then uses the aggregated node representation to calculate cosine similarity for each node-pair:

\[
S_{i,j} = \prod_{k=1}^{M} \cos \left( b_i^{(k)}, b_j^{(k)} \right), \quad b_i^{(k)} = (D^{-1}A)^k \cdot X \cdot W
\]

\(S_{i,j}\) denotes the similarity between \(v_i\) and \(v_j\), and similarity of all node-pairs form a similarity matrix \(S\). In practice, we also optionally use the concatenation of distribution feature \(b_i^{(k)}\) and \(x_{i,1} \cdot W\) (transformed feature of node itself) for similarity calculation in Eq. 6. Finally, we use the \(S_X\) and \(S_Y^{train}\) calculated in advance to guide the training of \(S\). We have the following two objective functions with respect \(S_X\) and \(S_Y^{train}\):

\[
\begin{align*}
L_1(S, S_X) &= ||S - S_X||_F^2 \\
L_2(S, S_Y^{train}) &= ||(S - S_Y^{train}) \odot (Masky \times Mask_T)||_F^2
\end{align*}
\]

In practice, we first use \(S\) to reconstruct \(S_X\) as the pretraining process and then further use \(S\) to reconstruct \(S_Y^{train}\) under Masky as the finetuning process.

### 4.2 A Scalable Implementation of DHGR

However, directly optimizing the objective function mentioned above has quadratic computational complexity. For node attributes \(X \in \mathbb{R}^{N \times D}\), the \(O(N^2)\) complexity is unacceptable for large graphs when \(N >> D\). So we design a scalable training strategy with stochastic mini-batch. Specifically, we randomly select \(k_1 \cdot k_2\) node-pairs as a batch and optimize the similarity matrix \(S\) by a \((k_1 \times k_2)\)-sized sliding window in each iteration. We can assign small numbers to \(k_1, k_2 \in [1, N]\). We give the pseudocode in Algorithm 1.

**Algorithm 1: Training DHGR with stochastic mini-batch**

**Input:** graph \(G(X, A)\), Node set \(V\), label \(Y\), batch-size \([k_1, k_2]\), min-neighbor-ordinal \(m\), MaxIteration, MaskY Epoch1, Epoch2.

**Output:** Similarity matrix \(S\)

```plaintext
for epoch from 1 to Epoch1 do
    for i from 1 to MaxIteration do
        Sample \(k_1\) nodes \(V^1_i \in V\), \(|V^1_i| = k_1\);
        Sample \(k_2\) nodes \(V^2_i \in V\), \(|V^2_i| = k_2\);
        Calculate the similarity matrix \(S, S_X \in \mathbb{R}^{k_1 \times k_2}\)
        between \(V_i^1\) and \(V_i^2\), (see Eq. 6 and Eq. 3);
        Update \(W\) with \(WL_1(S, S_X)\) (see Eq. 7);
    end
end
Node set \(V_Y \leftarrow \{ v \in V \mid MaskY[v] = 1 \}\).
for epoch from 1 to Epoch2 do
    Sample \(k_1\) nodes \(V^1_Y \in V\), \(|V^1_Y| = k_1\);
    Sample \(k_2\) nodes \(V^2_Y \in V\), \(|V^2_Y| = k_2\);
    Calculate the similarity matrix \(S, S_Y^{train} \in \mathbb{R}^{k_1 \times k_2}\)
    between \(V_Y^1\) and \(V_Y^2\), (see Eq. 6 and Eq. 3);
    Update \(W\) with the gradient of \(||(S - S_Y^{train})||_F^2\);
end
Obtain the entry \(S_{i,j}\) with Eq. 6. » Final similarity
```


4.3 Graph Rewiring with Learned Similarity

After we obtain the similarity of each node-pair, we can use the learned similarity $S$ to rewire the graph. Specifically, we add edges between node-pairs with high-similarity and remove edges with low-similarity on the original graph. Three parameters are set to control this process: $K$ indicates the maximum number of edges that can be added for each node; $\epsilon$ constrains that the similarity of node-pairs to add edges mush larger than a threshold $\epsilon$. Finally another parameter $\gamma$ is set for pruning edges with similarity smaller than $\gamma$. The details of the Graph Rewiring process are given in Algorithm 2. Finally, we can feed the rewired graph $\hat{G}(X, \hat{A})$ into any GNN-based models for node classification tasks.

Algorithm 2: Graph Rewiring with DHGR

| Input: | original graph $G(V, E)$, learned similarity matrix $S$, max number of added edges $K$, growing threshold $\epsilon$, pruning threshold $\gamma$ |
|---|---|
| Output: | Rewired Graph $\hat{G}(X, \hat{A})$ |
| 1 | foreach node $v_i \in V$ do |
| 2 | Select $K$ nodes from $V$ which have top-$K$ largest similarity with $v_i$ to form a node set $C_i$; |
| 3 | Calculate candidate node set $C'_i \leftarrow \{v_j \in C_i \mid S_{j,i} \geq \epsilon\}$; |
| 4 | Adding edges $\{(v_j, v_i) \mid v_j \in C'_i\}$ to $G$; |
| 5 | foreach $(v_j, v_i) \in E$ do |
| 6 | if $S_{j,i} < \gamma$ then |
| 7 | Remove edges $(v_j, v_i)$ from $G$; |

4.4 Complexity Analysis

We analyze the computational complexity of Algorithm 1 and Algorithm 2 with respect to the number of nodes $|V|$. For Algorithm 1, the complexity of random sampling $k_1 + k_2$ nodes is $O(k_1 + k_2)$. Let's denote the feature dimension as $D$ and denote the one-hot label dimension as $|C| < D$. Considering that the complexity of calculating cosine similarity between two $D$-dimension vectors is $O(D)$, the complexity of calculating the similarity matrix $\hat{S}$, $\hat{S}_X$, $\hat{S}_Y$ is $O(Dk_1k_2)$. The complexity of calculating $L_1$ and $L_2$ equals to $O(k_1k_2)$. Therefore, the final computational complexity of one epoch of Algorithm 1 is $O(Dk_1k_2)$ where $k_1$, $k_2$ are two constants. For Algorithm 2, we use Ball-Tree to compute the top-K nearest neighbors, the complexity of one top-K query is $O(D \cdot |V| \log(|V|))$. Therefore, the time complexity of the first FOR-loop which performs the topk algorithm is approximately $O(D \cdot |V| \log(|V|)+K \cdot |V|)$. The second FOR-loop filters each edge in the original Graph and thus its complexity is $O(|E|)$. Therefore the final complexity of Algorithm 2 is $O(D \cdot |V| \log(|V|)+K \cdot |V|+|E|)$.

5 EXPERIMENTS

In this section, we first give the experimental configurations, including the introduction of datasets, baselines and setups used in this paper. Then we give the results of experiments comparing DHGR with other graph rewiring methods on the node classification task under transductive learning scenarios. Besides, we also conduct extensive hyper-parameter studies and ablation studies to validate the effectiveness of DHGR.

5.1 Datasets

We evaluate the performances of DHGR and the existing methods on eleven real-world graphs. To demonstrate the effectiveness of DHGR, we select eight heterophily graph datasets (i.e. Chameleon, Squirrel, Actor, Cornell, Texas, Wisconsin, FB100, Flickr) and three homophily graph datasets (i.e. Cora, CiteSeer, PubMed). The detailed information of these datasets are presented in the Table 1. For graph rewiring methods, we use both the original graphs and the rewired graphs as the input of GNN models to validate their performance on the node classification task.

5.2 Baselines

DHGR can be viewed as a plug-in module for other state-of-the-art GNN models. And we select five GNN models tackling homophily, including GCN [19], GAT [31], GraphSAGE [16], APPNP [29] and GCNII [4]. To demonstrate the significant improvement on heterophily graphs caused by DHGR, we also choose two GNNs tackling heterophily (i.e. GPRGNN [8], H2GCN [43]). Besides, to validate the effectiveness of DHGR as a graph rewiring method, we also compare DHGR with two Graph Structure Learning (GSL) methods (i.e. LDS [14] and IDGL [7]) and one Graph Rewiring methods (i.e. SDRF [29]), which are all aimed at optimizing the graph structure. For GPRGNN and H2GCN, we use the implementation from the benchmark [23], and we use the official implementation of other GNNS provided by Torch Geometric. For all Graph Rewiring methods except SDRF whose code is not available, we all use their official implementations proposed in the original papers.

5.3 Experimental Setup

For datasets in this paper, we all use their public released data splits. For Chameleon, Squirrel, Actor, Cornell, Texas, and Wisconsin, ten random generated splits of data are provided by [27]. And we therefore train models on each data split with 3 random seeds for model initialization (totally 30 trails for each dataset) and finally we calculate the average and standard deviation of all 30 results. And we use the official splits of other datasets (i.e. Cora, CiteSeer, PubMed, Flickr, FB100) from the corresponding papers. We train our DHGR models with 200 epochs for pretraining and 30 epochs for finetuning in all datasets. And we search the hyper-parameters of DHGR in the same space for all datasets. $M$ (the max order of neighbors) is searched in $[1, 2, 3]$, $K$ (the growing threshold) is searched in $[3, 6, 8, 16]$ and $\gamma$ (the pruning threshold) is searched in $[0, 0.3, 0.6]$, where we do not prune edges for homophily datasets which equals to set $\gamma$ to -1.0. The batch size for training DHGR is searched in $[5000, 10000]$. For other GSL methods (i.e. LDS [14], IDGL [7]), we adjust their hyper-parameters according to the configurations used in their papers. For GNNs used in this paper, we adjust the hyper-parameters in the same searching space for fairness. We search the hidden dimensions in $[32, 64]$ for all GNNs and set the number of model layers to 2 for GNNs except for GCNII which is designed with deeper depth and we search the number of layers for GCN2 in $[2, 64]$ according to its official implementation. We train 200/300/400 epoch for all models and
select the best parameters via the validation set. The learning rate is searched in [1e-2, 1e-3, 1e-4], the weight decay is searched in [1e-2, 1e-3, 1e-4], and we use Adam optimizer to optimize all the models on Nvidia Tesla V100 GPU.

5.4 Main Results

We conduct experiments of node classification task on both heterophily and homophily graph datasets, and the results are presented in Table 2 and Table 3 respectively. We evaluate the performance of DHGR by comparing the classification accuracy of GNN with original graphs and graphs rewired by DHGR respectively. We also calculate the average gain (AG) of DHGR for all models on each dataset. The formula of average gain is given as follows:

\[
AG = \frac{1}{|M|} \sum_{m_i \in M} \left( ACC(m_i(\mathcal{G})) - ACC(m_i(\mathcal{G})) \right)
\]

where \(M\) is the set of GNN models, \(ACC\) is the short form of accuracy, \(\mathcal{G}\) is the original graph and \(\hat{\mathcal{G}}\) is the graph rewired by DHGR. We also compare the proposed DHGR with other Graph Rewiring methods on their performance and running time, and the results of different graph rewiring methods are reported in Table 4 and Fig. 5. By analyzing these results, we have the following observations:

(1) All GNNs enhanced by DHGR, including GNNs for homophily and GNNs for heterophily, outperform their vanilla versions on the eight heterophily graph datasets. The average gain of DHGR on heterophily graph can be up to 32.44% on Squirrel. However, vanilla GNN on Squirrel only has 26.39% classification accuracy on the test set. Even with the state-of-the-art GNNs for heterophily (i.e. GPRGNN, H2GCN), an test accuracy of no more than 40% can be achieved. The H2GCN enhanced by DHGR can achieve an astonishing 72.24% test accuracy on Squirrel, almost doubling. For most other heterophily datasets, GNN with DHGR can provide significant accuracy improvements. It demonstrates the importance of graph rewiring strategy for improving GNN’s performance on heterophily graphs. Besides, the significant average gain by DHGR also demonstrates the effectiveness of DHGR. For large-scale and edge-dense datasets such as Flickr and FB100 (\(N >> D\)), graph rewiring with DHGR can still provide a competitive boost for GNNs,
Table 3: Node classification accuracy (%) on the test set of homophily graphs. The bold numbers indicate that our method improves the base model.

| GNN Model | Cora         | CiteSeer     | PubMed       |
|-----------|--------------|--------------|--------------|
| GCN       | vanilla 81.09±0.39 | 70.13±0.45   | 78.38±0.39   |
|           | DHGR 82.70±0.41  | 70.79±0.12   | 79.10±0.33   |
| GAT       | vanilla 81.90±0.73 | 69.60±0.63   | 78.1±0.63    |
|           | DHGR 82.93±0.51  | 70.43±0.65   | 78.81±0.93   |
| GraphSAGE | vanilla 80.62±0.47 | 70.30±0.57   | 77.1±0.23    |
|           | DHGR 81.30±0.26  | 71.11±0.65   | 77.63±0.16   |
| APPNP     | vanilla 83.25±0.42 | 70.46±0.31   | 78.9±0.45    |
|           | DHGR 83.86±0.40  | 71.60±0.35   | 79.61±0.53   |
| GCNII     | vanilla 83.11±0.37 | 70.90±0.73   | 79.46±0.33   |
|           | DHGR 83.93±0.28  | 71.96±0.67   | 79.49±0.39   |
| Avg Gain  | 0.95 ↑         | 0.90 ↑       | 0.54 ↑       |

which verifies the effectiveness and scalability of DHGR on large-scale graphs.

(2) For homophily graphs (i.e., Cora, CiteSeer, Pubmed), the proposed DHGR can still provide competitive gain of node classification performance for the GNNs. Note that homophily graphs usually have a higher homophily ratio (i.e., 81%, 74%, 80% for Cora, CiteSeer, and Pubmed), so even vanilla GCNs can achieve great results and thus the benefit of adjusting the graph structure to achieve a higher homophily ratio is less than that for heterophily graphs. To be specific, DHGR gains best average gain on Cora, e.g., the classification accuracy of vanilla GCN on Cora is improved from 81.1% to 82.6%. For another two datasets, DHGR also provide average gain no less than 0.5% accuracy for all GNN models. These results demonstrate that our method can provide significant improvements for heterophily graphs while maintaining competitive improvements for homophily graphs.

(3) To demonstrate the effectiveness of DHGR as a method of graph rewiring, we also compare the proposed approach with other graph rewiring methods (i.e., LDS, IDGL, SDRF). Besides, we also use two random graph structure transformation by adding or removing edges on the original graph with a probability of 0.5, namely RandAddEdge and RandDropEdge. To validate the effect of adding edges between same-class nodes with training label, we also design a method named RandAddEdge_Y^train, which only use training label to add edges, though increases the homophily ratio, it cannot add edges beyond nodes in the training set. Only adding homophilic edges within the training set cannot guarantee an improvement of GCN’s performance and make the nodes in the training set easier to distinguish, increasing the risk of overfitting. The significant improvements made by DHGR demonstrates the effectiveness of DHGR as a graph rewiring method.

(4) Note that the traditional paradigm of GSL methods (e.g., LDS, IDGL) is training a graph learner and a GNN through an end2end manner and based on the dense matrix optimization, which have larger complexity. The running time of DHGR and two other GSL methods is presented in Fig. 5, we find that the running time of DHGR is significantly smaller than that of GSL methods under the same device environment. We did not present the running time of SDRF because its code has not been released publicly yet.

5.5 Hyper-Parameter Study

To demonstrate the robustness of the proposed approach, we study the effect of the four main hyper-parameter of DHGR, i.e. Batchsize, K (maximum number of added edges for each node), e (the threshold of lowest-similarity when adding edges) and training ratio of datasets in this section.

5.5.1 The effect of batchsize and training set ratio. Table 5 shows the results of GCN with DHGR on two heterophily datasets varying with different batchsize for DHGR and training ratio (percentage of nodes in the training set). The batchsize is ranging from [100×100] to [N×N], where N is the number of nodes and [N×N] indicates using full-batch for training. Note that for the Squirrel dataset
which has only 5201 nodes, the batchsize of 10000 × 10000 equals full-batch. The results in Table 5 show that the proposed approach has stable improvements with different batchsize and training ratio. To be specific, GCN with DHGR only has a 3% decrease in accuracy when decreasing the batchsize to 100, which is extremely small and with no more than 2% decrease in accuracy with training ratio ranging from 40% to 10%. Besides, we usually set the batchsize of DHGR ranging from 5000 to 10000 in real applications, because the overhead of 10000×10000 matrix storage and operation is completely acceptable. These results demonstrate the robustness of DHGR when adjusting the batchsize and training ratio.

![Homophily Ratio of rewired graphs (a) and GCN Accuracy on rewired graphs (b)](image)

Figure 6: Results of experiments with different K and ε. K is the maximum number of edges that can be added for each node. ε is the minimum similarity threshold of node-pairs between which edges can be added. Note that we remove all edges on the original graph for this experiment and only to verify the effects of edges added by DHGR.

5.5.2 The effect of K and ε. We have two important hyperparameters when rewiring graphs with DHGR, the maximum number of edges added for each node (denoted as K) and the threshold of lowest-similarity when adding edges (denoted as ε). Given the learned similarity by DHGR, the two hyper-parameters almost determine the degree and homophily ratio of the rewired graph. Motivated by the observations presented in Sec. 3, we verify the effectiveness of DHGR for graph rewiring by using different K and ε. Fig. 6 (a) shows the homophily ratio of rewired graphs using different K and ε and Fig. 6 (b) shows the node classification accuracy of GCN on the rewired graphs using different K and ε. We observe that the homophily ratio usually increases when increasing K with fixed ε, while decreases when increasing K with fixed K. Besides, the change of GCN node classification accuracy basically matches the change of homophily ratio with different K and ε. This demonstrates the effectiveness and robustness of the rewired graphs learned by DHGR.

| Methods                | Cora     | Cornell | Texas    | FB100    |
|------------------------|----------|---------|----------|----------|
| DHGR \_label \_dist    | 80.97±0.05 | 65.38±5.53 | 79.67±1.79 | 75.95±0.16 |
| DHGR \_feat \_dist     | 81.3±0.13  | 67.08±6.08  | 82.02±1.06  | 76.68±0.56  |
| DHGR \_feat \_self     | 81.7±0.11  | 62.21±4.49  | 78.58±1.02  | 75.65±0.26  |
| DHGR                   | 82.63±0.41 | 67.38±3.33  | 81.78±0.82  | 77.01±0.14  |

Table 6: Node classification accuracy (%) of the ablation studies to compare GCN with DHGR and its variants which remove certain component from the original DHGR architecture.

6 RELATED WORK

6.1 Graph Representation Learning

Graph Neural Networks (GNNs) have been popular for modeling graph data [3, 5, 9, 35, 38]. GCN [19] proposed to use graph convolution based on neighborhood aggregation. GAT [31] proposed to use attention mechanism to learn weights for neighbors. GraphSAGE [16] was proposed with graph sampling for inductive learning on graphs. These early methods are designed for homophily graphs, and they perform poorly on heterophily graphs. Recently,
some studies [1, 8, 11, 27, 43] propose to design GNNs for modeling heterophily graphs. MixHop [1] was proposed to aggregate representations from multi-hop neighbors to alleviate heterophily. Geom-GCN [27] proposed a bi-level aggregation scheme considering both node embedding and structural neighborhood. GPR-GNN [8] proposed to adaptively learn the Generalized PageRank (GPR) weights to jointly optimize node feature and structural information extraction. More recently, GBK-GNN [11] was designed with bi-kernels for homophilic and heterophilic neighbors respectively.

6.2 Graph Rewiring

The traditional message passing GNNs usually assumes that messages are propagated on the original graph [4, 16, 19, 31]. Recently, there is a trend to decouple the input graph from the graph used for message passing. For example, graph sampling methods for inductive learning [16, 42], motif-based methods [25] or graph filter leveraging multi-hop neighbors [1], or changing the graph either as a preprocessing step [2, 21] or adaptively for the downstream task [18, 36]. Besides, Graph Structure Learning (GSL) methods [7, 14, 15, 22, 32, 44] aim at learning an optimized graph structure and its corresponding node representations jointly. Such methods of changing graphs for better performance of downstream tasks are often generically named as graph rewiring [29]. The works of [2, 29] proposed rewiring the graph as a way of reducing the bottleneck, which is a structural property in the graph leading to over-squashing. Some GSL methods [15, 32] directly make adjacent matrix a learnable parameter and optimize it with GNN. Other GSL methods [7, 14] use a bilevel optimization pipeline, in which the inner loop denotes the downstream tasks and the outer loop learns the optimal graph structure with a structure learner. Some studies [13, 40] also use transformer-like GNNs to construct global connections between all nodes. However, both GSL methods and graph transformer-based methods usually have a higher time and space complexity than other graph rewiring methods. Most of existing Graph Rewiring methods are under the similar assumption (e.g., sparsity [24], low-rank [45], smoothness [17, 26]) on graphs. However, the property of low-rank and smoothness are not satisfied by heterophily graphs. Thus, graph rewiring methods for modeling heterophily graphs still need to be explored.

7 CONCLUSION

In this paper, we propose a new perspective of modeling heterophily graphs by graph rewiring, which targets at improving the homophily ratio and degree of the original graphs and making GNNs gain better performance on the node classification task. Besides, we design a learnable plug-in module of graph rewiring for heterophily graphs namely DHGR which can be easily plugged into any GNN models to improve their performance on heterophily graphs. DHGR improves homophily of graph by adjusting structure of the original graph based on neighbor’s label-distribution. And we design a scalable optimization strategy for training DHGR to guarantee a linear computational complexity. Experiments on eleven real-world datasets demonstrate that DHGR can provide significant performance gain for GNNs under heterophily, while gain competitive performance under homophily. The extensive ablation studies further demonstrate the effectiveness of the proposed approach.

REFERENCES

[1] Sami Abu-El-Haija, Bryan Perozzi, Amol Kapoor, Nazanin Alipourfard, Kristina Lerman, Hrany Harutyunyan, Greg Ver Steeg, and Aram Galstyan. 2019. Mixhop: Higher-order graph convolutional architectures via sparsified neighborhood mixing. In Proceedings of International Conference on Machine Learning. 21–29.

[2] Uri Alon and Eran Yahav. 2020. On the bottleneck of graph neural networks and its practical implications. arXiv preprint arXiv:2006.05205 (2020).

[3] Wendong Bi, Lun Du, Qiang Fu, Yanlin Wang, Shi Han, and Dongmei Zhang. 2022. M3-GNN: Mix-Moment Graph Neural Network towards Modeling Neighborhood Feature Distribution. arXiv preprint arXiv:2208.07012 (2022).

[4] Ming Chen, Zhewei Wei, Zengfeng Huang, Bolin Ding, and Taliang Li. 2020. Simple and deep graph convolutional networks. In Proceedings of International Conference on Machine Learning. 1725–1735.

[5] Xu Chen, Lun Du, Mengyu Chen, Yun Wang, Qingqing Long, and Kunqing Xie. 2021. Fast Hierarchy Preserving Graph Embedding via Subspace Constraints. In ICASSP 2021-2021 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP). IEEE. 3580–3584.

[6] Xu Chen, Yuanxing Zhang, Lun Du, Zheng Fang, Yi Ren, Kaiyu Bian, and Kunqing Xie. 2020. TSNRGCN: Temporal Spectral Spatial Retrival Graph Convolutional Network for Traffic Flow Forecasting. In 2020 IEEE International Conference on Data Mining (ICDM). 954–959 https://doi.org/10.1109/ICDM50108.2020.00108.

[7] Yu Chen, Lingfei Wu, and Mohammed Zakii. 2020. Iterative deep graph learning for graph neural networks: Better and robust node embeddings. Advances in Neural Information Processing Systems 33 (2020), 19314–19326.

[8] Eli Chien, Jianhao Peng, Fan Li, and Olgica Milenkovic. 2020. Adaptive Universal Generalized PageRank Graph Neural Network. In Proceedings of International Conference on Learning Representations.

[9] Lun Du, Xu Chen, Fei Gao, Quan Pu, Kunqing Xie, Shi Han, and Dongmei Zhang. 2022. Understanding and Improvement of Adversarial Training for Network Embedding from an Optimization Perspective. In Proceedings of the Fifteenth ACM International Conference on Web Search and Data Mining. 230–240.

[10] Lun Du, Fei Gao, Xu Chen, Ran Jia, Junshan Wang, Jiang Zhang, Shi Han, and Dongmei Zhang. 2021. TabularNet: A neural network architecture for understanding semantic structures of tabular data. In Proceedings of the 27th ACM SIGKDD Conference on Knowledge Discovery & Data Mining. 322–331.

[11] Lun Du, Xiaohou Shi, Quan Pu, Xiaojun Ma, Hengyu Liu, Shi Han, and Dongmei Zhang. 2022. GBK-GNN: Gated Bi-Kernel Graph Neural Networks for Modeling Both Homophily and Heterophily. In Proceedings of the ACM Web Conference 2022. 1550–1558.

[12] Lun Du, Guojie Song, Yiming Wang, Jipeng Huang, Mengfei Ruan, and Zhanyuan Yu. 2018. Traffic events oriented dynamic traffic assignment model for expressway network: a network flow approach. IEEE Intelligent Transportation Systems Magazine 10, 1 (2018), 107–120.

[13] Vijay Prakash Dwivedi, Ank Tuan Luu, Thomas Laurent, Yoshua Bengio, and Xavier Bresson. 2021. Graph neural networks with learnable structural and positional representations. arXiv preprint arXiv:2110.07875 (2021).

[14] Luca Franceschi, Mathias Niepert, Massimiliano Fancelli, and Xiao He. 2019. Learning discrete structures for graph neural networks. In Proceedings of International conference on machine learning. 1972–1982.

[15] Xiang Gao, Wei Hu, and Zongming Guo. 2020. Exploring structure-adaptive graph learning for robust semi-supervised classification. In Proceedings of 2020 IEEE International Conference on Multimedia and Expo (ICME). 1–6.

[16] William L Hamilton, Rex Ying, and Jure Leskovec. 2017. Inductive representation learning on large graphs. In Proceedings of the 31st International Conference on Neural Information Processing Systems. 1025–1035.

[17] Vasileia Kalofolias. 2016. How to learn a graph from smooth signals. In Proceedings of International Conference on Machine Learning. 1972–1982.

[18] Anees Kazi, Luca Cosmo, Seyed-Ahmad Ahmadi, Nassir Navab, and Michael Bronstein. 2022. Differentiable graph module (dgm) for graph convolutional networks. IEEE Transactions on Pattern Analysis and Machine Intelligence (2022), 1–1.

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

[20] Johannes Klünera, Aleksandar Bojchevski, and Stephan Günnemann. 2018. Predict then propagate: Graph neural networks meet personalized pagerank. arXiv preprint arXiv:1810.05997 (2018).

[21] Johannes Klüner, Stefan Welling, and Stephan Günnemann. 2019. Diffusion improves graph learning. arXiv preprint arXiv:1911.05485 (2019).

[22] Ruoyu Li, Sheng Wang, Feiyun Zhu, and Junzhou Huang. 2018. Adaptive graph convolutional networks. In Proceedings of the AAAI Conference on Artificial Intelligence. 3546–3553.

[23] Derek Lim, Xiuyu Li, Felix Hohne, and Ser-Nam Lim. 2021. New benchmarks for learning on non-homophilous graphs. arXiv preprint arXiv:2104.01404 (2021).
[24] Christos Louizos, Max Welling, and Diederik P Kingma. 2017. Learning sparse neural networks through $L_0$ regularization. *arXiv preprint arXiv:1712.01312* (2017).

[25] Federico Monti, Karl Otter, and Michael M Bronstein. 2018. Motifnet: a motif-based graph convolutional network for directed graphs. In *Proceedings of 2018 IEEE Data Science Workshop (DSW)*. 225–228.

[26] Antonio Ortega, Pascal Frossard, Jelena Kovačević, José MF Moura, and Pierre Vandergheynst. 2018. Graph signal processing: Overview, challenges, and applications. *Proc. IEEE* 106, 5 (2018), 808–828.

[27] Hongbin Pei, Bingzhe Wei, Kevin Chen-Chuan Chang, Yu Lei, and Bo Yang. 2020. Geom-gcn: Geometric graph convolutional networks. *arXiv preprint arXiv:2002.05287* (2020).

[28] Guojie Song, Yuanhao Li, Junshan Wang, and Lun Du. 2020. Inferring explicit and implicit social ties simultaneously in mobile social networks. *Science China Information Sciences* 63, 4 (2020), 1–3.

[29] Jake Topping, Francesco Di Giovanni, Benjamin Paul Chamberlain, Xiaowen Dong, and Michael M Bronstein. 2021. Understanding over-squashing and bottlenecks on graphs via curvature. *arXiv preprint arXiv:2111.14522* (2021).

[30] Amanda L Traud, Peter J Mucha, and Mason A Porter. 2012. Social structure of Facebook networks. *Physica A: Statistical Mechanics and its Applications* 391, 16 (2012), 4165–4180.

[31] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. 2017. Graph attention networks. *arXiv preprint arXiv:1710.10903* (2017).

[32] Guohong Wan and Harsha Kokel. 2021. Graph Sparsification via Meta-Learning. *DLG@ AAAI* (2021).

[33] Tao Wang, Rui Wang, Di Jin, Dongxiao He, and Yuxiao Huang. 2021. Powerful Graph Convolutional Networks with Adaptive Propagation Mechanism for Homophily and Heterophily. *arXiv preprint arXiv:2112.13562* (2021).

[34] Yanlin Wang, Lun Du, Ensheng Shi, Yuxuan Hu, Shi Han, and Dongmei Zhang. 2020. Cocogum: Contextual code summarization with multi-relational gnn on umls. *Microsoft, Tech. Rep. MSR-TR-2020-16* (2020).

[35] Yun Wang, Lun Du, Guojie Song, Xiaojuo Ma, Lichen Jin, Wei Lin, and Fei Sun. 2019. Tag2Gauss: Learning Tag Representations via Gaussian Distribution in Tagged Networks. In *ICML* 3799–3805.

[36] Yue Wang, Yongbin Sun, Ziwei Liu, Sanjay E Sarma, Michael M Bronstein, and Justin M Solomon. 2019. Dynamic graph cnn for learning on point clouds. *ACM Transactions On Graphics (tog)* 38, 5 (2019), 1–12.

[37] Yujun Yan, Milad Hashemi, Kevin Swersky, Yaoqing Yang, and Danai Koutra. 2021. Two sides of the same coin: Heterophily and oversmoothing in graph convolutional neural networks. *arXiv preprint arXiv:2102.06662* (2021).

[38] Shuwen Yang, Guojie Song, Yilun Jin, and Lun Du. 2021. Domain adaptive classification on heterogeneous information networks. In *Proceedings of the Twenty-Ninth International Conference on International Joint Conferences on Artificial Intelligence*. 1410–1416.

[39] Di Yao, Haonan Hu, Lun Du, Gao Cong, Shi Han, and Jingping Bi. 2022. Traj-GAT: A Graph-based Long-term Dependency Modeling Approach for Trajectory Similarity Computation. In *Proceedings of the 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*. 2275–2285.

[40] Chengxuan Yin, Tianle Cai, Shengjie Luo, Shuzin Zheng, Guolin Ke, Di He, Yanming Shen, and Tie-Yan Liu. 2021. Do Transformers Really Perform Badly for Graph Representation? *Advances in Neural Information Processing Systems* 34 (2021).

[41] Haqing Zeng, Hongkuan Zhou, Ajitesh Srivastava, Rajgopal Kannan, and Viktor Prasanna. 2019. Graphsaint: Graph sampling based inductive learning method. *arXiv preprint arXiv:1907.04931* (2019).

[42] Yingxue Zhang, Soumyasundar Pal, Mark Coates, and Deniz Ustebay. 2019. Bayesian graph convolutional neural networks for semi-supervised classification. In *Proceedings of the AAAI conference on artificial intelligence*, Vol. 33. 5829–5836.

[43] Jiong Zhu, Yujun Yan, Lingxiao Zhao, Mark Heimann, Leman Akoglu, and Danai Koutra. 2020. Beyond homophily in graph neural networks: Current limitations and effective designs. *Advances in Neural Information Processing Systems* 33 (2020), 7793–7804.

[44] Yanqiao Zhu, Weizhi Xu, Jinghao Zhang, Yuqing Liu, Cagnn: Cluster-aware graph neural networks for unsupervised graph representation learning. *arXiv preprint arXiv:2009.01674* (2020).