Learning heterophilious edge to drop: A general framework for boosting graph neural networks

Jincheng Huang
Southwest Petroleum University
Chengdu, China
huangjc0429@gmail.com

Ping Li
Southwest Petroleum University
Chengdu, China
dping.li@gmail.com

Rui Huang
Southwest Petroleum University
Chengdu, China
huangrui1104@foxmail.com

Na Chen
Southwest Petroleum University
Chengdu, China
dpnanachen@gmail.com

ABSTRACT
Graph Neural Networks (GNNs) aim at integrating node contents with graph structure to learn nodes/graph representations. Nevertheless, it is found that most of existing GNNs do not work well on data with high heterophily level that accounts for a large proportion of edges between different class labels. Recently, many efforts to tackle this problem focus on optimizing the way of feature learning. From another angle, this work aims at mitigating the negative impacts of heterophily by optimizing graph structure for the first time. Specifically, on assumption that graph smoothing along heterophilious edges can hurt prediction performance, we propose a structure learning method called LHE to identify heterophilious edges to drop. A big advantage of this solution is that it can boost GNNs without careful modification of feature learning strategy. Extensive experiments demonstrate the remarkable performance improvement of GNNs with LHE on multiple datasets across full spectrum of homophily level.

CCS CONCEPTS
• Computer systems organization → Embedded systems; Redundancy; Robotics; • Networks → Network reliability.

KEYWORDS
graph neural networks, heterophily, learning to drop, node classification

1 INTRODUCTION
The surprising expressiveness of graph neural networks (GNNs) has aroused an explosion of interests in graph representation learning [6], resulting in extensive applications ranging from social network analysis [17] to molecular biology [4, 10], even to regular data processing like text mining [16] and image processing [24]. Despite their practical success, it is not yet guaranteed that GNNs can be effective for arbitrary graph data.

One notable feature in graphs is heterophily [29]: connected nodes may have different class labels or properties. In real-world systems, many graphs exhibit strong heterophily. For instance, matchmaking website tends to connect people to those with the opposite gender, the hierarchical organization structure of many natural and man-made systems shows the leader-member relations. When applying GNNs on such graph data, the implicit assumption underlying GNNs that node features should be similar (smooth) among neighboring nodes is violated, which makes it very possible to learn undiscriminating features for different classes.

To tackle this issue, a few recent work has made efforts to capture node feature encoded in the topology from different respects. For example, by looking into the distribution of class labels in a graph, Zhu et al. [29] find that the 2-hop neighborhood is less heterophilious than the nearest neighborhood, thus it is expected to
improve the power of graph learning by leveraging the second-order neighbors. Geom-GCN [15] maps a graph to a continuous space to capture long-range dependencies between nodes such that the information on distant nodes with the same label is able to be exploited in node representation learning. Though the prior work has carefully redesigned the way of information integration, to optimize representation learning strategy needs to exhaustively examine the characteristics of class label distribution in a graph, which remains a great challenge.

Clearly the block is the presence of heterophilious edges. As shown in Figure 1, if we remove all heterophilious edges in graph data, the performance of a state-of-the-art model SGC [23] can be improved by about 30 percentage points, compared to the original data. This inspires us to propose a solution by optimizing not representation learning but the structure, on top of which existing GNN models can be boosted. This solution, termed LHE, is able to improve GNNs by a large margin and achieve near optimal results that are quite close to the performance bound on the homophily graph, as shown with the orange bar in Figure 1.

Our idea is simple: we divide the edges into two categories, namely, homophilous edge and heterophilous edge, where homophilous edges refer to the edges connecting nodes in the same class, and heterophilous edges represent the edges connecting nodes between different classes. Based on the edge labeling on the training set, a binary classification model is learned to discriminate between heterophilous and homophilous edges, with which the heterophilous edges are identified from the unlabeled set and removed from the graph. As a result, the changed graph will lessen the misleading effect on message passing caused by heterophily. Further more, in order to search for the optimal deletion, we propose two joint learning methods. Since the changed graph structure is to be fed to GNN module, a task-oriented edge classifier can be learned by passing GNN loss to edge classification model. Alternatively, edge classifier and GNN module can be updated independently.

The contribution of this paper is summarized as follows:

• We propose a new solution to the problem of heterophily, by optimizing the graph structure instead of careful design of feature learning strategy.
• We prove the rationality of our assumption through pilot study. Based on that, we devise a simple yet effective method to learn the heterophily of the connectivity and devise two training approaches for joint learning.
• Extensive experiments on the benchmark graph data with low homophily validate the superiority of the proposed method over the state-of-the-art models.

2 PRELIMINARIES

Let $G = (V, E)$ be an undirected and unweighted graph with node set $V$ and edge set $E$. The nodes are described by the feature matrix $X \in \mathbb{R}^{n \times f}$, where $f$ denotes the number of features per node and $n$ is the number of nodes. Each node is associated with a class label, which is depicted in the label matrix $Y \in \mathbb{R}^{n \times c}$ with a total of $c$ classes. We represent the graph by its adjacency matrix $A \in \mathbb{R}^{n \times n}$ and the graph with self-loops by $A = A + I_n$.

Graph Convolutional Network and Its Simplification Message passing graph convolutional networks have been proved to be powerful on a number of graph data, among which graph convolutional network(GCN) proposed by Kipf et al. [12] is a widely used one. A typical GCN makes prediction according to a series of operations on node features:

$$\hat{Y} = \text{softmax}(S_{sym} \text{ReLU}(S_{sym}XW_0)W_1),$$

where $\hat{Y} \in \mathbb{R}^{n \times c}$ are the predicted node labels, $W_0$ and $W_1$ are for feature mapping at the first and second layer respectively. Besides, $S_{sym} = D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ denotes the symmetrically normalized adjacency matrix with self-loops, where $D$ refers to the diagonal degree matrix of $A$.

The above Equation 1 reveals three core components in GCN, namely, feature propagation, linear transformation, non-linear activation. However, Wu et al. [23] have shown that the latter two components are redundant and detrimental to performance, so they simplify the vanilla GCN as

$$\hat{Y} = \text{softmax}(S^K_{sym}XW),$$

where $K$ is the number of graph convolutions, and $W \in \mathbb{R}^{d \times c}$ denotes the learnable parameters of a logistic regression classifier. The simplified GCN is referred to as SGC.

Homophily and heterophily In this work, we use the homophily measure given in [29] to quantify the homophily level of a graph data, as described in DEFINITION 2. Moreover, we define homophilous and heterophilous edge as:

DEFINITION 1. Homophilous edge: Edge which connects nodes that have the same label. On the contrary, heterophilous edges are the edges which connect nodes with different labels. We say a graph is homophily if there is no heterophilous edges in the graph.

DEFINITION 2. [29] The edge homophily ratio is defined as $h = \frac{\|\{(u,v) \in E \mid y_u = y_v\}\|}{\|E\|}$, where $\|E\|$ denotes the total number of edges in the graph.

3 PILOT STUDY

To encode topological interaction between nodes into feature representations, GNNs generally integrate information from various neighborhoods via message passing. The consequence is that nodes in close proximity are more likely to be similar in feature representation. In other words, GNNs attempt to smooth out the difference in close proximity are more likely to be similar in feature representation. However, in some settings where graphs have low edge homophily ratios, the vanilla GNNs have been found to underperform MLPs [29]. We conjecture that a large number of heterophilous edges in graphs with weak homophily (i.e., strong heterophily) may be noisy and interfere in feature representation learning, since they allow the “messages” to pass between classes.

Assumption 3.1. The fewer heterophilous edges, the more effective GNNs can be. Messaging within the same class is the ideal messaging mode for GNNs.

To investigate whether the intra-class messaging is ideal, we conduct a pilot study to test the node classification performance of vanilla GNNs in the ideal situation where the homophilous edges
Table 1: Summary of node classification results (in percent). The suffix bound represents the ideal situation, and \( l \) represents the number of convolution layer. SGC\(_2\) uses a two-layer MLPs with linear map as the predictor, which is detailed in Section 4.3

| Dataset | Homo.ratio | Cora | Cite. | Film. | Texas | Wisc. | Corn. | Cham. | Squi. |
|---------|------------|------|-------|-------|-------|-------|-------|-------|-------|
|         |            |      |       |       |       |       |       |       |       |
| GCN     | 0.81       | 87.2 | 76.4  | 30.1  | 59.5  | 59.8  | 57.3  | 60.3  | 36.7  |
| GCN\(_l\) bound | 0.74       | 95.1 | 84.1  | 51.4  | 82.7  | 87.5  | 84.1  | 86.6  | 81.9  |
| GAT     | 0.86       | 87.6 | 76.3  | 29.0  | 59.1  | 53.1  | 58.4  | 45.1  | 28.3  |
| GAT\(_l\) bound | 0.79       | 95.4 | 84.0  | 53.6  | 84.9  | 88.4  | 83.8  | 87.0  | 82.5  |
| SGC\(_l\) bound(l=2) |          | 95.6 | 84.2  | 59.4  | 83.5  | 87.7  | 83.0  | 87.2  | 81.9  |
| SGC\(_l\) bound(l=50) |          | 96.2 | 84.9  | 61.9  | 82.5  | 87.5  | 84.1  | 87.9  | 81.5  |

in the graph are retained, while all heterophilous edges are deleted. From the table 1 (see Section 5 for the details of datasets and data split), we have the following observations:

- On the ideal graph structure, the performance of the GNNs is greatly improved.
- Deeply stacking convolution layers (e.g. SGC with 50 convolution layers) does not result in drops in GNNs’ performance. It is manifested that the over-smoothing effect is only negative for inter-class messaging, but helpful for intra-class messaging.

We further study the impact of heterophilous edges in the training phase. Figure 3 shows the variations of training losses of SGC under the configurations where heterophilous edges are randomly removed with deletion rate of 0%, 50%, and 100%, respectively. Note that 100% deletion corresponds to the ideal situation. It is shown from the figure that the lowest loss of the model is achieved when there are no heterophilous edges, while the highest loss corresponds to the original graph structure, and deleting even a portion of heterophilous edges can help to better fit the training samples. The experimental results verify our assumption on the influence of heterophilous edges on GNNs’ performance and inspire us to design a strategy that is able to spot those edges to drop.

4 METHODOLOGY

We propose Learning Heterophilous Edge to drop (LHE), a novel method that aims to resolve the major limitation of message passing based GNNs when confronted with graph data that has strong heterophily. Instead of devising better feature aggregation strategy, LHE learns potential heterophilous edges and remove them from the graph such that message passing along those edges is not allowed. To achieve this, we introduce an edge classifier that is pre-trained on training set at the first place, and then join it with a GNN model for further end-to-end training. The overall framework is diagrammatically illustrated in Figure 2.
4.1 Model Pretraining

To optimize graph structure towards the ideal configuration (i.e., homophilous graph), we first pre-train a binary classifier to initialize the graph update procedure.

Pretraining task We introduce a supervised edge classification task that predicts which type a given edge belongs to, where edges are divided into two categories, namely, homophilous and heterophilious edges. The edges among labeled nodes (i.e., the training set) are used for edge classifier pre-training, whose labels are obtained according to DEFINITION 1. In a similar way, the validation edge set and test edge set can also be obtained.

Pre-training model The representation of the edge between node $i$ and node $j$ is determined by the representations of the two endpoints:

$$e_{ij} = R(Wx_i, Wx_j, \gamma)$$

where $x_i$ denotes the feature representation of node $i$, $W \in \mathbb{R}^{f \times f}$ is a shared parameter matrix that maps node representations into a lower dimensional subspace, and $R(\cdot)$ can be any permutation invariance function. Here we consider two operations, namely, element-wise summation or squared difference,

$$R(Wx_i, Wx_j, \gamma) = \begin{cases} Wx_i + Wx_j & \text{if } \gamma = 0 \\ (Wx_i - Wx_j)^2 & \text{if } \gamma = 1 \end{cases}$$

The differences between these two operations are demonstrated using a toy example, as shown in Figure 4. We empirically find that element-wise squared difference is more suitable for capturing distinct information among different types of edges (i.e., homophilous and heterophilous edges), when in-class nodes have similar feature representations and between-class nodes are dissimilar in feature representations, while summation is a better choice when in-class nodes are less similar. In practical application, node attributes can be used to estimate which measure will be appropriate, which will be further discussed in the experiments.

End-To-End training. In this scheme, GNNs’ downstream task is used to supervise the feature learning and structure update.
Specifically, task-relevant training loss will be back propagated to the edge classifier and GNN at the same time. However, to propagate the loss to the edge classifier is challenging. The reason is that as the output of edge classifier, the discrete graph structure is not differentiable. We tackle this problem by proposing a BackMax method inspired by Gumbel-Softmax [9].

Our BackMax is detailed as follows.
1. For any arbitrary edge with endpoints \( u, v \), the probability that the edge belongs to one of two classes is given by Equation 5, i.e.,

\[
    z_{u,v} = \text{edge\_classifier}(x_u, x_v)
\]

where \( z_{u,v} \in \mathbb{R}^2 \).

2. The softmax function is employed to amplify the probability distribution,

\[
    \pi_{u,v} = \frac{\exp(z_{u,v})}{\sum \exp(z_{u,v})}
\]

3. Then in the forward propagation phase,

\[
    y_{\text{hard}} = \text{one\_hot}(\text{argmax}(\pi_{u,v}))
\]

which is adopted to update the graph structure, while in the backward propagation phase, the error will be fed back to the continuous counterpart of \( y_{\text{hard}} \): \( y = \pi_{u,v} \) for updating the parameters of the edge classifier. The following expression combines two variables together:

\[
    \hat{y} = \text{detach}(y_{\text{hard}} - \pi_{u,v}) + \pi_{u,v}
\]

where the function \( \text{detach()} \) is to disconnect the backpropagation. In comparison to Gumbel-softmax estimator [9], BackMax does not involve any sampling for reparameterization and hyper-parameter for annealing, which can reduce the computational complexity.

**Separate Training.** The difference between separate training and end-to-end training lies in the way of training edge classifier. In separate training, downstream task loss will not be propagated back to the edge classifier(structure learning). To update the edge classifier, we leverage the characteristics of the Adam optimizer, which allows a model to be updated slowly along the momentum direction of the gradient. This way, the structure is able to be updated.

As for GNN, it is updated independently based on downstream task loss and then takes graph structure renewed at this epoch as input to obtain new node representations.

Note that it is also possible to train GNN on top of the one-off optimized structure, that is, the structure is first optimized by the edge classifier that is trained on the whole training set, and then GNN learning is performed on this structure. This manner, however, is found to be slightly inferior to the joint learning scheme. We conjecture that the joint learning results in sub-optimal structure that corresponds to optimal GNN.

4.3 **Base Model**

We consider two powerful GNNs, namely, GCN and its simplification variant SGC. Though vanilla SGC employs one-layer perceptron for prediction, we empirically find it is insufficient to give appropriate prediction, especially when the dimension of node features is relatively high\(^1\). In our model, we use two-layer MLPs for SGC and denote it as SGC\(_2\) which can be formulated as,

\[
    \hat{Y} = \text{softmax}(\sum_{i=0}^{2} x_i w_i)
\]

In the following section, we will show that SGC\(_2\) with 2-layer MLPs, when applied to node classification, is much superior in terms of test accuracy.

**Proposition 4.1.** LHE(\(\cdot\)) unifies MLP(\(\cdot\)) and GNN(\(\cdot\)) in supervised graph learning.

Given a GNN \( Y = f(A, X, W) \), in one extreme case where the edges among training nodes are all heterophilous, LHE will learn to delete all connections in the graph, i.e., the adjacency matrix \( A = I \) at the convergence. Then LHE-GNN and MLP are equivalent (i.e., \( Y = f(A, X, W) = f(X, W) \)). On the other end of the spectrum, there are only homophilous edges in the training set, which makes the edge classifier bias to homophilous edges, so LHE will not remove any links in the graph. In this case, LHE-GNN equals GNN. When the training set is in between, LHE will adaptively drop heterophilous edges that are assumed to be adverse to GNN’s message passing. After structure optimization, for the nodes that are disconnected from the graph, LHE behaves like MLP, while for the connected components, GNN will be performed.

**Complexity.** The time complexity of SGC\(_2\) is \( O(|E|) + O(n f_0 (f+c)) \), where \( f_0 \) denotes the hidden size of two-layer MLP, \( c \) is the number of classes and \( |E| \) denotes edge count. The complexity of edge classifier module is \( O(f_0 (2nf+nc+|E|)) \). So the total computational complexity of LHE(\(\cdot\)) is \( O(|E|) + f_0 (2nf+nc+|E|) \), which is linear with the sum of node and edge counts and introduces additional computation of an edge classifier, compared to the vanilla SGC\(_2\).

5 **EXPERIMENTS**

In this section, we evaluate the performance of LHE on transductive node classification task on a wide variety of benchmark graph datasets.

**Datasets.** We conduct experiments on nine open graph datasets [15, 20, 21, 25] across the full spectrum of homophily ratio \( h \). The statistics of the datasets is listed in Table 2. For fair comparison, we follow the data partition in [15] (i.e., 48%/32%/20% of nodes per class for train/validation/test) and adopt the shared 10 random splits for each dataset.

| Datasets   | Nodes | Edges | Features | Classes |
|------------|-------|-------|----------|---------|
| Cora       | 2708  | 5429  | 1433     | 7       |
| Citeseer   | 3327  | 4732  | 3703     | 6       |
| Pubmed     | 1271  | 44338 | 500      | 3       |
| Chameleon  | 2277  | 36101 | 2325     | 5       |
| Squirrel   | 5201  | 217073| 2089     | 5       |
| Film       | 7600  | 33544 | 931      | 5       |
| Cornell    | 183   | 295   | 1703     | 5       |
| Texas      | 183   | 309   | 1703     | 5       |
| Wisconsin  | 251   | 499   | 1703     | 5       |

**Baseline Models.** We compare our method to strong baselines and state-of-the-art approaches, including GCN [12], SGC [23],
Table 3: Test node classification accuracies (in percent) on graph datasets. Average accuracy and standard deviation over different spirts is reported from [29]. Prefix (e2e) denotes results with end-to-end training, (st) indicates that separate training is adopted in LHE. The best results are in bold and the second best results are underlined.

| Datasets | Homo.ratio h | Cora | Cite. | Pubm. | Cham. | Squi. | Film | Corn. | Texa. | Wisc. | Avg. Rank |
|----------|--------------|------|-------|-------|-------|-------|------|-------|-------|-------|-----------|
| SGC      | 0.81         | 83.72±1.4 | 74.01±1.7 | 83.62±0.5 | 47.41±2.5 | 36.68±1.4 | 25.49±1.5 | 59.45±5.2 | 58.37±4.2 | 51.50±8.8 | 14        |
| SGC2     | 0.90±1.6     | 76.31±1.4 | 76.31±1.4 | 87.03±0.7 | 61.70±2.0 | 42.43±1.8 | 26.30±1.0 | 63.70±4.0 | 59.18±4.4 | 54.20±3.6 | 10.6      |
| GCN      | 0.84±1.7     | 76.41±1.6 | 76.41±1.6 | 87.30±0.7 | 60.26±2.4 | 36.68±1.7 | 30.09±1.0 | 57.03±4.7 | 59.46±5.3 | 59.80±7.0 | 10.3      |
| GAT      | 0.85±1.7     | 76.33±2.2 | 76.62±0.5 | 45.13±1.9 | 28.39±1.4 | 29.03±0.9 | 58.38±3.7 | 59.10±4.3 | 53.14±4.5 | 13        |
| MixHop†  | 83.10±2.0    | 70.75±3.0 | 80.75±2.3 | 46.10±4.7 | 29.08±3.8 | 25.43±1.9 | 67.84±9.4 | 74.59±8.9 | 71.96±3.7 | 14.7      |
| GraphSAGE† | 86.60±1.8 | 75.61±1.6 | 88.01±0.8 | 58.71±2.3 | 41.05±1.1 | 34.37±1.3 | 75.59±5.2 | 82.70±5.9 | 81.76±5.6 | 8.4       |
| GCN-Cheby† | 86.68±1.0 | 76.25±1.8 | 88.08±0.5 | 63.38±1.4 | 40.86±1.5 | 33.80±0.9 | 71.35±5.9 | 78.65±5.8 | 77.45±4.8 | 8.2       |
| GEOM-GCN† | 85.27        | 77.99    | 90.05   | 60.90   | 38.14   | 31.63   | 60.18   | 67.57   | 64.12   | 8.4       |
| H2GCN-1  | 86.35±1.6    | 76.85±1.5 | 88.50±0.6 | 58.84±2.1 | 34.82±2.0 | 35.94±1.3 | 79.45±5.7 | 84.56±1.1 | 82.55±3.7 | 5.7       |
| H2GCN-2  | 88.13±1.4    | 76.73±1.4 | 88.46±0.7 | 59.56±1.8 | 35.65±1.9 | 35.55±1.6 | 78.38±4.8 | 84.59±6.8 | 82.35±4.3 | 5.2       |
| FAGCN    | 87.88±0.8    | 76.76±1.6 | 88.80±0.6 | 45.13±2.2 | 31.77±2.1 | 34.51±0.7 | 72.43±6.6 | 67.84±4.8 | 77.06±6.5 | 9.0       |
| CFGNN-MLP| 86.84±0.7    | 76.61±1.7 | 88.02±0.4 | 46.56±2.0 | 32.41±1.3 | 35.69±1.0 | 81.09±4.0 | 80.42±5.3 | 83.16±7.6 | 6.7       |
| CFGNN-Cheby | 85.27±0.7 | 75.56±2.3 | 87.14±0.2 | 46.34±3.1 | 29.58±2.3 | 35.10±1.2 | 80.54±6.0 | 80.27±4.3 | 83.14±3.3 | 9.6       |
| RPGNN    | 87.98±1.2    | 77.08±1.7 | 87.53±0.4 | 46.64±1.7 | 31.58±1.2 | 34.61±1.2 | 80.25±5.1 | 78.44±4.4 | 83.02±4.2 | 7.4       |
| MLP      | 75.13±2.7    | 73.26±1.7 | 85.69±0.3 | 46.93±1.7 | 29.95±1.6 | 34.78±1.2 | 79.79±4.2 | 79.19±4.3 | 83.15±5.7 | 10.8      |
| LHE-SGC(e2e) | 87.21±1.6 | 76.83±1.8 | 87.15±0.8 | 53.20±2.1 | 33.31±2.2 | 34.96±1.0 | 81.12±6.1 | 81.42±4.8 | 84.52±4.0 | 5.9       |
| LHE-SGC(st) | 87.16±1.2 | 76.85±1.8 | 86.64±0.5 | 63.54±2.2 | 44.15±1.6 | 35.20±1.0 | 80.30±5.9 | 80.90±4.0 | 84.90±3.3 | 4.4       |

GAT [22], GCN-Cheby [5], graphSAGE [7], and Mixhop [1]. We also compare our model with heterophily-oriented methods, namely, two variants of H2GCN (i.e., H2GCN-1 and H2GCN-2) [29], GEOM-GCN [15] which quantitatively analyzes the homogeneity of a graph for the first time and the every recent work GPRGNN, CFGNN [3, 27]. In particular, we choose the best two among the four variants of CPFGNN for comparison. Moreover, we compare our model with recently proposed FAGCN [2] that leverages high-frequency signals to relieve the over-smoothing effect on disassortative networks, because similar to heterophily, dissatisfactoriness accounts for the feature that nodes from different classes tend to connect with each other.

**Setup.** We implement models in Pytorch and use Adam optimizer for parameter updates. We set learning rate to 0.005 for the pre-training module, dimension to 64 for linear transformation and use L2 regularizer with regularization factor of 0.0005 on the weights of the linear layer. For SGC, SGC2 and GCN, we use two-layer MLPs as the classification model on all datasets, whose hidden units are 64, learning rate is 0.01, and weight decay is 0.0005. Furthermore, dropout ratio of 0.6 is applied to both layers. For edge representation in LHE model, we use element-wise squared difference on Cora, Citeseer, Pubmed, Cornell, Texas, Wisconsin datasets, while on the remaining datasets, namely, Chameleon, Squirrel and Film, we use summation method. In the later section, we justify the choice of summation and element-wise squared difference for different data.

5.1 Results

The experimental results on real data are reported in Table 3. We observe that LHE using SGC as base model shows consistently strong performance across the full spectrum of homophily. Specifically, LHE-SGC(st) achieves state-of-the-art performance on average, and LHE-SGC(e2e) is comparative to the strong state-of-the-art method H2GCN. Note that graphSAGE and GCN-Cheby perform well on the datasets with high heterophily, demonstrating the benefits of separate embedding of ego and its neighbors and learning higher order neighbors, which consists of design factors of H2GCN [28]. Compared to vanilla SGC, it is shown that our design for structure optimization is able to significantly improve the expressiveness of GNNs and thus boost the base model. Another observation on graph data with low homophily levels is that among several heterophily-oriented methods, namely, GEOM-GCN, two best H2GCN models, FAGCN, CPFGNN, GPRGNN and ours, optimizing structure (ours) is more effective than optimizing feature extraction (prior work). We also note that SGC2 with 2-layer MLPs remarkably outperforms the original SGC which uses one-layer linear discriminator. It should also be noted that if a graph has strong heterophily (e.g., Texas and Wisconsin), our model will delete a large proportion of the edges in the graph. In this case, the learned SGC model is close but still better than MLP.

Besides, it is observed that the performance of separate training is better than end-to-end training sometimes. We explain it based on the feedback loop. Specifically, in end-to-end mode, graph structure is finetuned according to updated feature representations, which will be affected by heterophily, while separating training searches structures independently, so it is less susceptible to heterophily.

5.2 Structure Change after Learning

To investigate how much the original graph structure changes due to deletion after the model converges, we calculate the ratio of deleted edges to the total number of edges in original graph, which
is termed total deletion ratio. Moreover, to validate whether LHE
can effectively delete heterophilous edges, we consider the ratio of
deleted heterophilous edge to the total of deleted edges, termed
heterophilous edge deletion ratio.

![Figure 5: Average edge deletion rate after LHE-SGC convergence.](image)

As is shown in Figure 5, the heterophilous edge deletion ratio is
always much higher than the total edge deletion ratio on eight real
datasets. This is because our model will delete some homophilous
dges in three graph datasets with strong heterophily.

The reason that LHE performs better on some graph data than
others is that the homophily level affects edge classification bias.
More precisely, in graphs that have strong homophily/heterophily,
homophilous/heterophilous edges are far more than heterophil-
strong homophily/heterophily. On the other hand, it will be
undesirable for structure optimization when homophilous edges
dominate, as in this setting the classifier has a higher chance to
mistakenly infer an edge to be homophilous, whose ground-truth
actually is heterophilous.

We also note that LHE-SGC successfully deletes all heter-
ophilous edges in three graph datasets with strong heterophily
(i.e., Cornell, Texas, and Wisconsin), there is still a little gap between
the heterophilous/homophilous edges. This imbalance is favorable when it is
biased towards heterophilous edges. On the other hand, it will be
undesirable for structure optimization when homophilous edges
dominate, as in this setting the classifier has a higher chance to
mistakenly infer an edge to be homophilous, whose ground-truth
actually is heterophilous.

5.3 Comparison to DropEdge

We compare our goal-directed edge deletion with DropEdge [19],
the random deletion approach to verify the effectiveness of our
method. Note that DropEdge randomly removes a portion of edges
in the graph during training, so for fair comparison, we set the
drop ratio in DropEdge to be equal to the total edge deletion ratio
obtained by our method on each dataset.

Table 4 shows the change of accuracy when we apply two meth-
ods of dropping edge on two base models (SGC2, GCN and GAT).
We can see that our goal-directed method is evidently superior to
random deletion, while random deletion (i.e., DropEdge) may even
degrade the performance of base models, especially GAT. Another
advantage of our method compared to DropEdge is that LHE-GNNs
does not introduce any additional hyperparameters, e.g., edge dele-
tion ratio, the model learns target edges to drop adaptively.

5.4 Analysis of Edge Representation

![Figure 6: Between-class distance and in-class distance distri-
bution.](image)

as is shown in Figure 6, the between-class distance and in-class distance
distribution ratio, the model learns target edges to drop adaptively.
distance between nodes is given by

\[ d_{i,j} = \| e_{i,j} \|_2 \quad \text{s.t.} \quad e_{i,j} = x_i - x_j \] (11)

Then the mean and variance of in-class/between-class node distance distribution are as follows,

\[ \mu = \frac{1}{c} \sum_{l \in L} \sum_{i \in V_l} \mathbb{1}(E_{i,l}) \sum_{j \in V_{l'}} A_{i,j} d_{i,j} \]

\[ \sigma^2 = \frac{1}{c} \sum_{l \in L} \sum_{i \in V_l} \mathbb{1}(E_{i,l}) \sum_{i \in V_l,j \in V_{l'}} A_{i,j} (\mu(l,l') - d_{i,j})^2 \] (12)

where \( \mathbb{1}(\cdot) \) is the indicator function that is 1 when there is an edge between two classes, otherwise 0. \( V_l \) indicates the set of nodes in class \( l \) and \( N \) denotes the neighborhood of node \( i \). Particularly, \( l' = l \), \( \mu \) and \( \sigma^2 \) are the statistics of the in-class distance distribution, otherwise they are for between-class distribution.

Figure 6 shows the between-class distance distributions in graphs with different homophily levels. It can be found that there is no significant association between distribution pattern and homophily ratio. However, we observe that for some graphs (i.e., Citeseer in Figure 6(a) and Texas in Figure 6(b)), the distributions of between-class distances and in-class distances are distinguishing, while in other graphs the distributions of between-class distances and in-class distances are close to each other, as shown in Figure 6(c) and (d). This implies that element-wise difference cannot always be helpful for discriminating homophilous edges (in-class connections) and heterophilous edges (between-class connections). From a practical viewpoint, we can adopt different edge representation methods for different data. Specifically, for the graphs whose between-class distance distribution is different from in-class distance distribution, it will be effective to choose element-wise squared difference. Otherwise, summation may be more appropriate.

5.5 Analysis of Graph Spectrum

To look into the underlying change of graph resulted from structure optimization, we compare the spectrums of a graph before and after performing LHE. It is observed in Figure 7 that the graph spectrum has been expanded towards the extremum. In particular, the smallest eigenvalue that is known to correspond to the ability of feature smoothing [14] becomes smaller when the graph exhibits strong homophily, as shown in Figure 7(a)(b), indicating that LHE facilitates the feature smoothing for homophilous graphs. In contrast, in graphs with low homophily level (as shown in Figure 7(c)(d)), there is an increasing number of maximum eigenvalues (i.e., eigenvalues equal to 1), demonstrating that edge deletion in LHE leads to some isolated nodes or connected components. This makes a local feature smoothing.

6 RELATED WORK

Homophily and Heterophily. Homophily describes the consistency between node class labels and the graph structure. Prior work has shown the homophily plays a crucial role in graph learning. GeomGNNs [15] first pays attention to this property and provides a metric to measure the homophoby level of a graph. In particular,

Geom-GCN leverages non-Euclidean embedding technique to better capture structural information and long-distance dependence. In recent work, Kim et al. [11] find that homophily can affect the power of attention mechanism. Recent work by Hou et al. [8] synthetically study the ability of GNN to capture graph information, and also propose metrics to measure feature smoothing and label smoothing quantitatively. To allow the model to be aware of the information not only about node features but about class labels, graph markov neural networks [18] models the joint label distribution with conditional random field, which can be effectively trained with the variational EM algorithm. On the other hand, to mitigate the negative effect of heterophily on performance, H2GCN [29] studies the distribution of heterophilous edges in graph and finds that on a graph with a high level of heterophily, the 2-hop neighborhood is always dominated by homophily nodes, so it can be used for feature representation learning. GPRGNN [3] adaptively learns generalized pagerank weights so as to jointly optimize node feature and topological information extraction. In addition, CPGNN [27] shares similar motivations to ours, i.e., both works attempt to identify connected label pairs that are incompatible/compatible. But unlike CPGNN that learns compatibility for all label pairs via belief diffusion, our method directly learns an incompatible/compatible classifier connections. A recent work FAGCN [2] can be regarded as another prevalent work. FAGCN aims at disassortative data, in which nodes belonging to different communities (or classes) are connect to each other. To enrich the feature representation, FAGCN utilizes the differences between nodes (the so-called high frequency part of signal). HOG-GCN measures the homophily between node pairs through topology and feature information, and designs GNN that can automatically change the promotion and aggregation process. LINKX [13] is the first method proposed in large-scale heterophilous graph datasets. It can achieve better results on large-scale heterophilous datasets simply by sending the feature matrix and adjacency matrix into MLP for learning and fusion. Generally, previous work mainly focuses on enhancing the expressivity of feature representations. To the best of our knowledge, this work is the first attempt to resolve the heterophily challenge from the angle of structure optimization.

Graph Sparsification. The operation of discarding heterophilous edges in our work can be viewed as a way of graph sparsification. A popular graph sparsification model is graphSAGE [7], whose goal is to allow graph convolution to be available in large-scale graphs. Likewise, Dropedge [19] randomly drops edges to overcome the oversmoothness of graph networks. However, most of the existing work on graph sparsification ignores the relatedness between edges and tasks, except for NeuralSparce [26] that learns k-neighbor subgraphs for deleting task-irrelevant edges. In contrast, our model performs task-oriented sparsification.

7 CONCLUSION AND DISCUSSION

We propose a framework to boost GNNs on graph data with low homophily levels by optimizing the graph structure. On the conjecture that heterophilous edges mislead GNNs to aggregate information from different classes, we focus on learn an optimal structure that has as less heterophilous edges as possible, instead of careful design of feature learning strategy. Our experimental investigation
Figure 7: Statistics of eigenvalue distribution of Laplacian matrix of a graph data before and after LHE’s edge deletion. The red histogram represents the spectrum of the original graph, while the blue one is for the updated graph of LHE.

Broader Impact. Over the past years, the representation ability of GNNs on heterophily data has received great attention, with the majority of efforts devoted to designing advanced and complex GNN architectures for heterophily problem. Instead of heading towards that direction, this work is dedicated to looking at heterophily from the perspective of structural optimization. We hope that this work could provide insights on the homophily limitations of existing graph learning models and help researchers design more general models that work well in the full homophily regime.

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 international conference on machine learning. PMLR, 21–29.

[2] Deyu Bo, Xiao Wang, Chuan Shi, and Huawei Shen. [n. d.]. Beyond Low-frequency Information in Graph Convolutional Networks. In Thirty-Fifth AAAI Conference on Artificial Intelligence, AAAI 2021, Thirty-Third Conference on Innovative Applications of Artificial Intelligence, IAAI 2021, The Eleventh Symposium on Educational Advances in Artificial Intelligence, EAAI 2021, Virtual Event, February 2-9, 2021. AAAI Press, 3950–3957.

[3] Eli Chien, Jianhao Peng, Pan Li, and Olga Milenkovic. [n. d.]. Adaptive Universal Generalized PageRank Graph Neural Network. In 9th International Conference on Learning Representations, ICLR 2021, Virtual Event, Austria, May 3-7, 2021.

[4] Connor W. Coley, Wengong Jin, Luke Rogers, Timothy F. Jamison, Tommi S. Jaakkola, William H. Green, Regina Barzilay, and Klavs F. Jensen. 2019. A graph-convolutional neural network model for the prediction of chemical reactivity. Chemical science 10, 2 (2019), 370–377.

[5] Michael Defferrard, Xavier Bresson, and Pierre Vandergheynst. 2016. Convolutional neural networks on graphs with fast localized spectral filtering. Advances in neural information processing systems 29 (2016), 3844–3852.

[6] William L Hamilton. 2020. Graph representation learning. Synthesis Lectures on Artificial Intelligence and Machine Learning 14, 3 (2020), 1–159.

[7] 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.

[8] Yifan Hou, Jian Zhang, James Cheng, Kaili Ma, Richard T. B. Ma, Hongshi Chen, and Ming-Chang Yang. [n. d.]. Measuring and Improving the Use of Graph Information in Graph Neural Networks. In 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020.

[9] Eric Jang, Shixiang Gu, and Ben Poole. [n. d.]. Categorical Reparameterization with Gumbel-Softmax. In 5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings. OpenReview.net.

[10] Meng Qu, Yoshua Bengio, and Jian Tang. 2019. Gmnn: Graph markov neural network. In Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 1073–1082.

[11] Dongkwan Kim and Alice Oh. 2020. How to find your friendly neighborhood: Graph attention design with self-supervision. In International Conference on Learning Representations.

[12] Thomas N. Kipf and Max Welling. 2017. Semi-Supervised Classification with Graph Convolutional Networks. In 5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings.

[13] Derek Lim, Felix Hohne, Xiuyu Li, Siuja Linda Huang, Vaishnavi Gupta, Omkar Bhalekar, and Ser-Nam Lim. [n. d.]. Large Scale Learning on Non-Homophilous Graphs: New Benchmarks and Strong Simple Methods. CoRR abs/2110.14446 (n.d.).

[14] Hongbin Pei, Bingzhe Wei, Kevin Chen-Chuan Chang, Yu Lei, and Bo Yang. [n. d.]. Geom-GCN: Geometric Graph Convolutional Networks. In 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020.

[15] Mao Peng, Jianxin Li, Yu He, Yaqiong Liu, Mengjiao Bao, Lihong Wang, Yangqiu Song, and Qiang Yang. 2018. Large-scale hierarchical text classification with recursively regularized deep graph-cnn. In Proceedings of the 2018 world wide web conference. 1063–1072.

[16] Jiezhong Qiu, Jian Tang, Hao Ma, Yuxiao Dong, Kuansan Wang, and Jie Tang. 2018. DeepInf: Social influence prediction with deep learning. In Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 2110–2119.

[17] Meng Qi, Yoshua Bengio, and Jian Tang. 2019. Gmnn: Graph markov neural networks. In International conference on machine learning. PMLR, 5241–5250.

[18] Yu Rong, Wenbing Huang, Tingyang Xu, and Junzhou Huang. [n. d.]. DropEdge: Towards Deep Graph Convolutional Networks on Node Classification. In 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020.

[19] Benedek Rozemberczki, Carl Allen, and Rik Sarkar. 2021. Multi-scale attributed node embedding. Journal of Complex Networks, 9, 2 (2021), cnab014.

...
[21] Jie Tang, Jimeng Sun, Chi Wang, and Zi Yang. 2009. Social influence analysis in large-scale networks. In Proceedings of the 15th ACM SIGKDD international conference on Knowledge discovery and data mining. 807–816.

[22] Petar Veličkovic, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. 2018. Graph Attention Networks. In 6th International Conference on Learning Representations, ICLR 2018, Vancouver, BC, Canada, April 30 – May 3, 2018, Conference Track Proceedings. OpenReview.net.

[23] Felix Wu, Amauri Souza, Tianyi Zhang, Christopher Fifty, Tao Yu, and Kilian Weinberger. 2019. Simplifying graph convolutional networks. In International conference on machine learning. PMLR, 6861–6871.

[24] Jianwei Yang, Jiasen Lu, Stefan Lee, Dhruv Batra, and Devi Parikh. 2019. Graph r-cnn for scene graph generation. In Proceedings of the European conference on computer vision (ECCV). 670–685.

[25] Zhilin Yang, William Cohen, and Ruslan Salakhutdinov. 2016. Revisiting semi-supervised learning with graph embeddings. In International conference on machine learning. PMLR, 40–48.

[26] Cheng Zheng, Bo Zong, Wei Cheng, Dongjin Song, Jingchao Ni, Wenchao Yu, Haifeng Chen, and Wei Wang. 2020. Robust graph representation learning via neural sparsification. In International Conference on Machine Learning. PMLR, 11458–11468.

[27] Jiong Zhu, Ryan A. Rossi, Anup Rao, Tung Mai, Nedim Lipka, Nesreen K. Ahmed, and Danai Koutra. [n. d.]. Graph Neural Networks with Heterophily. In Thirty-Fifth AAAI Conference on Artificial Intelligence, AAAI 2021, Thirty-Third Conference on Innovative Applications of Artificial Intelligence, IAAI 2021, The Eleventh Symposium on Educational Advances in Artificial Intelligence, EAAI 2021, Virtual Event, February 2-9, 2021, AAAI Press, 11168–11176.

[28] Jiong Zhu, Yujun Yan, Lingxiao Zhao, Mark Heimann, Leman Akoglu, and Danai Koutra. [n. d.]. Beyond Homophily in Graph Neural Networks: Current Limitations and Effective Designs. In Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual.

[29] Jiong Zhu, Yujun Yan, Lingxiao Zhao, Mark Heimann, Leman Akoglu, and Danai Koutra. 2020. Generalizing graph neural networks beyond homophily. arXiv preprint arXiv:2006.11468 (2020).