Label-Wise Message Passing Graph Neural Network on Heterophilic Graphs

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Abstract

Graph Neural Networks (GNNs) have achieved remarkable performance in modeling graphs for various applications. However, most existing GNNs assume the graphs exhibit strong homophily in node labels, i.e., nodes with similar labels are connected in the graphs. They fail to generalize to heterophilic graphs where linked nodes may have dissimilar labels and attributes. Therefore, in this paper, we investigate a novel framework that performs well on graphs with either homophily or heterophily. More specifically, to address the challenge brought by the heterophily in graphs, we propose a label-wise message passing mechanism. In label-wise message-passing, neighbors with similar pseudo labels will be aggregated together, which will avoid the negative effects caused by aggregating dissimilar node representations. We further propose a bi-level optimization method to automatically select the model for graphs with homophily/heterophily. Extensive experiments demonstrate the effectiveness of our proposed framework for node classification on both homophilic and heterophilic graphs.

1 Introduction

Graph-structured data is very pervasive in the real-world such as knowledge graphs, traffic networks, and social networks. Therefore, it is important to model the graphs for downstream tasks such as traffic prediction (Yu, Yin, and Zhu 2017), recommendation system (Hamilton, Ying, and Leskovec 2017) and drug generation (Bongini, Bianchini, and Scarselli 2021). Inspired by the homophily of graphs, i.e., linked nodes tend to have similar features and belong to the same class (McPherson, Smith-Lovin, and Cook 2001), Graph Neural Networks (GNNs) (Wu et al. 2020) adopt a message-passing mechanism which learns a node’s representation by iteratively aggregating the representations of its neighbors. This can enrich the node features and preserve the node attributes and local topology for downstream tasks, especially the semi-supervised node classification.

Despite the great success of GNNs in modeling graphs, most GNNs design their message-passing mechanisms based on the homophily assumption of graphs; while heterophilic graphs also widely exist in the real world due to “opposite attract”. For instance, in dating websites, people are more likely to connect with people of different genders. In the trading network, fraudsters tend to contact accomplices instead of other fraudsters (Pandit et al. 2007).

The heterophily of graphs challenges many existing GNNs with homophily assumption. For example, GCN (Kipf and Welling 2016) will smooth the representations of central nodes and their neighbors, which can lead to similar embeddings within a cluster (Li, Han, and Wu 2018). This will facilitate the node classification on homophilic graphs. However, in heterophilic graphs, the neighbors of central nodes can have different labels and features with each other. Directly aggregating the information of neighbors and central node in different classes will induce similar representations for nodes in different classes, making the learned representations less discriminative, even resulting in poorer performance than multilayer perceptrons (Zhu et al. 2020). Fig. 1 gives an example, where the node color is the node label and the number on the node denotes the node attribute. For node $v_A$ and $v_B$ with labels, adopting one step aggregation of GCN will result in similar representations of $v_A$ and $v_B$, i.e., 3.5 and 3.0, which could worsen the classification. Attention mechanism such as GAT (Velickovic et al. 2018) also cannot address the issue due to the high heterophily of the graphs. For example, for node $v_A$, all of its neighbors are of different classes with $v_A$. Applying attention won’t be able to assign larger weights to nodes of the same label as $v_A$ to help learn better representation of $v_A$.

Though heterophilic graphs challenge existing GNNs, we observe that the heterophilic neighborhood contexts itself provides useful information. Generally, two nodes of the same class are more likely to have similar heterophilic neighborhood contexts while two nodes of different classes are more likely to have different heterophilic neighborhood contexts. Thus, if we can learn representations that keep such contexts, we can learn more discriminative representations. One promising way is to conduct label-wise aggregation, i.e., separately aggregate neighbors in each class. As shown in Fig. 1 for node $v_A$, with label-wise aggregation, $v_A$ will be represented as $[1.0, 5.0, 3.0, non-existence]$, corresponding to $v_A$’s attribute, blue, green, and orange neighbors, respectively. Compared with $v_B$, $v_A$’s representations of central node and neighborhood context differ significantly with $v_B$. In other words, we obtain more discriminative features. Though promising, there is no existing work...
exploring label-wise message passing to address the challenge of heterophilic graphs (Bo et al. 2021; Jin et al. 2021).

Therefore, in this paper, we investigate a novel label-wise massage passing for node classification on heterophilic graphs. In essence, we are faced with two challenges: (i) the label-wise aggregation needs the label of each node; while for node classification, we are only given a small set of labeled nodes. How to design label-wise message passing to facilitate node classification on sparsely labeled heterophilic graphs? (ii) Generally, we don’t know the homophily level of the given graph. The label-wise message passing might not work well on graphs with high homophily. How to ensure the performance on both heterophilic and homophilic graphs? In an attempt to address these challenges, we propose a novel framework Label-Wise GNN (LW-GNN)\(^1\). LW-GNN adopts a pseudo label predictor to predict pseudo labels and designs a novel label-wise message-passing to preserve the heterophilic contexts with pseudo labels. To handle both heterophilic and homophilic graphs, apart from label-wise message passing GNN, LW-GNN also utilizes a GNN for homophilic graphs, and adopts bi-level optimization on the validation data to automatically select the better model for the given graph. The main contributions are:

- We propose a novel label-wise message passing mechanism to benefit node classification on heterophilic graphs;
- We further add an automatic model selection module to ensure the performance of LW-GNN on both heterophilic and homophilic graphs; and
- We conduct extensive experiments on real-world graphs with heterophily and homophily to demonstrate the effectiveness of LW-GNN.

\(^1\)The code will be released upon acceptance

## 2 Related Work

Graph neural networks (GNNs), which generalize deep learning for graph structured data, have shown great success for various applications such as social networks (Hamilton, Ying, and Leskovec 2017; Dai and Wang 2021), financial transaction networks (Wang et al. 2019; Dou et al. 2020), and traffic networks (Yu, Yin, and Zhu 2017; Zhao et al. 2020). Based on the definition of the graph convolution, GNNs can be categorized into two categories, i.e., spectral-based (Bruna et al. 2014; Defferrard, Bresson, and Vandergheynst 2016; Kipf and Welling 2016) and spatial-based (Veličković et al. 2018; Xu et al. 2018b; Abu-El-Haija et al. 2019). Graph convolution in spectral-based GNN models is defined according to spectral graph theory (Bruna et al. 2014). Firstly, generalize convolution operation to graph-structured data from spectral domain. Graph Convolutional Network (GCN) (Kipf and Welling 2016) simplifies the graph convolution by first-order approximation. For spatial-based graph convolution, it aggregates the information of the neighbors nodes (Niepert, Ahmed, and Kutzkov 2016). Hamilton, Ying, and Leskovec (2017) for instance, spatial graph convolution that incorporates the attention mechanism is applied in GAT (Veličković et al. 2018) to facilitate the information aggregation. Graph Isomorphism Network (GIN) (Xu et al. 2018a) is proposed to learn more powerful representations of the graph structures. Recently, to learn better node representations, deep graph neural networks (Chen et al. 2020; Klügl, Bojchevski, and Günnemann 2018; Li et al. 2019) and self-supervised learning methods (Sun, Zhu, and Lin 2020; Kim and Oh 2021; Zhu, Du, and Yan 2020; Qiu et al. 2020; You et al. 2020) have been investigated.

However, the aforementioned methods are generally designed based on the homophily assumption of the graph. Low homophily level in some real-world graphs can largely degrade their performance (Zhu et al. 2020). Some initial efforts (Pei et al. 2020; Bo et al. 2021; Jin et al. 2021; Zhu et al. 2020) have been taken to address the problem of heterophilic graphs. For example, H2GCN (Zhu et al. 2020) investigated three key designs for GNNs on heterophilic graphs. Jin et al. propose a node similarity preserving mechanism to handle graphs with heterophily. Our proposed LW-GNN is inherently different from these methods: (i) we propose a novel label-wise aggregation to better capture the neighbors’ information in heterophilic graphs; and (ii) Automatic model selection is deployed to achieve state-of-the-art performance on both homophilic and heterophilic graphs.

## 3 Preliminaries

In this section, we first discuss the inner working of GNNs to show the challenge of heterophilic graphs. We then present the formal problem definition of node classification on graphs with homophily/heterophily.

### 3.1 Notations and Definition

Let \(G = (\mathcal{V}, \mathcal{E}, \mathbf{X})\) denote an attributed graph, where \(\mathcal{V} = \{v_1, ..., v_N\}\) is the set of \(N\) nodes, \(\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}\) is the set of edges, and \(\mathbf{X} = \{x_1,...,x_N\}\) is the set of node attributes. Only a part of nodes \(\mathcal{V}_L \subseteq \mathcal{V}\) are provided with labels \(\mathcal{V}_L\). And \(\mathcal{V}_L\) is split into a training set \(\mathcal{V}_{train}\) and a validation set \(\mathcal{V}_{val}\). \(\mathbf{A} \in \mathbb{R}^{N \times N}\) represents the adjacency matrix of the graph \(G\), where \(A_{ij} = 1\) indicates that there is an edge between nodes \(v_i\) and \(v_j\); otherwise, \(A_{ij} = 0\). Based on how likely edges link nodes in the same class, graphs can be...
categorized to homophilic graphs and heterophilic graphs. Specifically, the graph homophily level can be evaluated by the following measure:

**Definition 1 (Homophily Ratio)** It is the fraction of edges in a graph that connect nodes of the same class, i.e., intra-class edges. The homophily ratio \( h \) is calculated as:

\[
    h = \frac{|\{(v_i, v_j) \in E : y_i = y_j\}|}{|E|}.
\]

When the homophily ratio is small, most of the edges will link nodes from different classes, which indicates a heterophilic graph. In homophilic graphs, connected nodes are more likely to belong to the same class, which will lead to a homophily ratio close to 1.

### 3.2 Message Passing in GNNs

Generally, GNNs adopt message passing to incorporate node features and the graph structure in node representations, i.e., each layer of GNNs will update the representations of the nodes by aggregating information of their neighbors. The updating process of the \( k \)-th layer in GNN can be written as:

\[
\begin{align*}
    a_v^{(k)} &= \text{AGGREGATE}^{(k)}(\{h_u^{(k-1)} : u \in \mathcal{N}(v)\}), \\
    h_v^{(k)} &= \text{COMBINE}^{(k)}(h_v^{(k-1)}, a_v^{(k)}),
\end{align*}
\]

where \( h_v^{(k)} \) is the representation vector of the node \( v \in \mathcal{V} \) at \( k \)-th layer and \( \mathcal{N}(v) \) is a set of neighbors of \( v \). Existing GNNs (Kipf and Welling, 2016; Chen et al., 2020) generally follow the process described by Eq. 2. Though they have shown great ability in modeling graph-structured data, most of their aggregate and combine functions are designed for homophilic graphs and cannot handle heterophilic graphs.

For instance, GCN (Kipf and Welling, 2016) and GraphSage (Hamilton, Ying, and Leskovec, 2017) aggregate the information with the implicit assumption that the neighbors have similar features or belong to the same class as the central node. However, in heterophilic graphs, such assumption doesn’t hold, which could mix nodes of different features during message-passing and result in poor representations for node classification on graphs with heterophily.

### 3.3 Intuition and Problem Definition

Though in heterophilic graphs, the neighbors are very likely to belong to diverse classes and simple aggregation could result in noisy representations, we observe that the heterophilic neighbor contexts itself provides useful information. Let \( \mathcal{N}_i(v) \) denote node \( v \)'s neighbors of label class \( i \). Intuitively, for two nodes \( u \) and \( v \) of the same class, i.e., \( y_u = y_v \), the features of nodes in \( \mathcal{N}_i(u) \) are likely to be similar to that of nodes in \( \mathcal{N}_i(v) \); while for nodes \( u \) and \( s \) with \( y_u \neq y_s \), the features of nodes in \( \mathcal{N}_i(u) \) are likely to be different from that in \( \mathcal{N}_i(s) \). This motivate us to develop a novel label-wise message-passing mechanism for heterophilic graphs, which can learn representations that preserve the heterophily of neighbors to avoid mixing neighbors of different classes. In real world, we are usually given a graph with unknown homophily level. Thus, we aim to develop a framework that works for any homophily level. The problem is defined as:

**Problem 1** Given an attributed graph \( G = (\mathcal{V}, \mathcal{E}, \mathcal{X}) \) with a small set of labels \( \mathcal{Y}_U \) for node set \( \mathcal{V}_U \), the homophily ratio \( h \) of \( G \) is unknown, we aim to learn a GNN which accurately predicts the labels of the unlabeled nodes, i.e., \( f(G, \mathcal{Y}_U) \rightarrow \mathcal{Y}_U \), where \( f \) is the function we aim to learn and \( \mathcal{Y}_U \) is the set of predicted labels for unlabeled nodes.

### 4 Methodology

In this section, we give the details of our proposed framework LW-GNN. For heterophilic graphs, the basic idea is to separately aggregate the neighbors in different classes to well preserve the local contextual information. There are two main challenges: (i) how to design and conduct label-wise aggregation on heterophilic graphs with a small number of node labels; and (ii) how to make it work for both heterophilic and homophilic graphs. To address the challenges, LW-GNN estimates the labels of unlabeled nodes and designs a novel label-wise message-passing mechanism with the estimated labels. To ensure the performance on graphs with any homophily level, LW-GNN trains a label-wise aggregation model for heterophily and a GNN model for homophily, and can automatically select which model to apply.

An illustration of the proposed LW-GNN is shown in Fig. 2, which is composed of an MLP-based pseudo label predictor \( f_P \), a GNN \( f_C \) with label-wise message passing, a GNN \( f_G \) for homophilic graph, and an automatic model selection module. The predictor \( f_P \) takes the node attributes as input and predicts the node labels. \( f_C \) utilizes the estimated pseudo labels from \( f_P \) to conduct label-wise aggregation on \( G \) for node classification. \( f_G \) is the GNN for homophilic graphs which also makes predictions from the input graph \( G \). The predictions of \( f_P \) and \( f_G \) are combined with model weights. A bi-level optimization on validation set is applied to learn the model weights for model selection. Next, we give the details of each component.

#### 4.1 Label-Wise Message Passing

Though the message-passing mechanisms in current GNNs have achieved remarkable success in homophilic graphs, they generally fail to deal with heterophilic graphs. This is because nodes and their neighbors have different labels and features in heterophilic graphs, while existing GNNs directly mix the neighbors in various classes together with the central node. Therefore, the aggregated representations...
can poorly preserve the neighbors’ information, resulting in worse performance (Zhu et al. 2020).

Based on the motivation above, we propose to conduct label-wise aggregation, i.e., neighbors in different classes are separately aggregated to help update node representations. However, only a small number of nodes are provided with labels. Thus, a pseudo label predictor is deployed to estimate class labels for label-wise aggregation. Next, we first introduce the pseudo label prediction followed by the design of label-wise message passing for heterophilic graphs.

**Pseudo Label Prediction.** The pseudo label predictor \( f_P \) takes the node attributes as input and estimates the class labels of nodes. Specifically, an MLP is utilized to obtain pseudo label of node \( v \) with \( v \)'s attributes as

\[
\hat{y}_v^P = MLP(x_v),
\]

where \( x_v \) denotes the attributes of node \( v \). Note that, we use MLP as the predictor because message passing of the GNNs can lead to poor representations on heterophilic graphs. The loss function for training the pseudo label predictor \( f_P \) is:

\[
\min_{\theta_P} \mathcal{L}_P = \frac{1}{|\mathcal{V}_{train}|} \sum_{v \in \mathcal{V}_{train}} l(\hat{y}_v^P, y_v),
\]

where \( \mathcal{V}_{train} \) is the set of nodes in the training set, \( y_v \) denote the true label of node \( v \), \( \theta_P \) represents the parameters of the predictor \( f_P \), and \( l(\cdot) \) is the cross entropy loss.(3)

**Design of Label-Wise Message Passing.** With \( f_P \), we can get the pseudo labels \( \hat{Y}_v^P \) for the unlabeled nodes \( \mathcal{V}_U = \mathcal{V} \setminus \mathcal{V}_L \). Combining it with the provided \( \mathcal{Y}_L \), we have labels \( \hat{y}_v^P \in (\hat{Y}_U^P \cup \mathcal{Y}_L) \) necessary for label-wise aggregation. Since in label-wise aggregation, we will separately aggregate the neighbors of each class, which could result in large dimension of node representations. Thus, in each layer of the label-wise message passing, a linear transformation is firstly applied to process the input features to learn a good feature space and reduce the dimension to \( p \) as

\[
z_v^{(k)} = W^{(k)} h_v^{(k)},
\]

where \( h_v^{(k)} \) is the representation vector of node \( v \in \mathcal{V} \) at \( k \)-th layer with \( h_v^{(0)} = x_v \), and \( W^{(k)} \) denotes the parameters. We then aggregate the neighbors of the nodes label-wisely with the estimated labels. Let \( a_{v,i}^{k} \) be the aggregated representation of neighbors whose estimated labels are class \( i \), the label-wise aggregation process can be formally written as:

\[
a_v^{(k),i} = \sum_{u \in \mathcal{N}_i(v)} \frac{1}{n_i(v,u)} z_v^{(k),i},
\]

where \( \mathcal{N}_i(v) = \{ u : (v, u) \in \mathcal{E} \wedge \hat{y}_u^P = i \} \) is node \( v \)'s neighbors with estimated label \( i \), \( n_i(v,u) = \sqrt{d_{v,i} \cdot d_{u,i}} \) is the normalization term with \( d_{v,i} = |\mathcal{N}_i(v)| \). When there is no neighbor belonging to class \( i \), we can assign its value with zero embedding or the average embedding of the class \( i \).

Finally, to preserve the heterophily context, instead of averaging the neighborhood representations, for each node \( v \), we get \( v \)'s representation at layer \( k + 1 \) by concatenating its label-wise neighborhood representations \( a_v^{(k),i} \), \( i = 1, \ldots, c \), together with \( z_v \), followed by the ReLU as the activation function. This can be formally written as

\[
h_v^{(k+1)} = \text{ReLU}(\text{CONCAT}(z_v^{(k)}, a_v^{(k),1}, ..., a_v^{(k),c})),
\]

where \( c \) is the number of classes. \( h_v^{(k+1)} \in \mathbb{R}^{(c+1)p} \) is \( v \)'s representation at layer \( k + 1 \). With Eq. (7) we are able to obtain representations that preserve the target node’s features and capture the information of their neighbors in heterophilic graphs. Thus, for two nodes \( u \) and \( v \) belonging to the same class, their contexts should be similar, which results in similar representations.

Multiple layers of label-wise message passing can be applied to incorporate more hops of neighbors in representation learning. In heterophilic graphs, different hops of neighbors may exhibit different class distributions which can provide useful information for node classification. Therefore, the final node prediction is based on the intermediate representations of all layers. Inspired by (Xu et al. 2018b), max pooling is applied to combine the intermediate representations for a model with \( K \) layers:

\[
\hat{y}_v^{(K)} = \text{softmax}([W_C \cdot \text{MaxPooling}(h_v^{(0)}, ..., h_v^{(K)})]),
\]

where \( W_C \in \mathbb{R}^{c \times (c+1)p} \) is a learnable weight matrix, \( \hat{y}_v^{(K)} \) is predicted label probabilities of node \( v \).

### 4.2 Automatic Model Selection

As it is described in Sec. 4.1, we rely on the pseudo labels to conduct label-wise message passing. In heterophilic graphs, the homophily ratio is very small and even can be around 0.2 (Pei et al. 2020). With a reasonable pseudo label predictor, the label-wise aggregation will mix much less noise than the general GNN aggregation. In contrast, for homophilic graphs such as citation networks, their homophily ratios are close to 1. In this situation, label-wise aggregation may not be effective as (i) the pseudo-labels contain noises, which can bring more negative effects in homophilic graphs; and (ii) most \( \mathcal{N}_i(v), i = 1, \ldots, c \), might be empty. Thus, for homophilic graphs, directly aggregating all the neighbors may introduce less noise in representations than aggregating label-wisely. Therefore, it is necessary to determine whether to apply the label-wise message passing or the state-of-the-art GNN for homophilic graphs. One straightforward way is to select the model based on the homophily ratio. However, the graphs are generally sparsely labeled which makes it difficult to estimate the real homophily ratio. Moreover, an additional hyperparameter i.e., threshold of homophily ratio will be required for model selection. To address this problem, we propose to utilize the validation data to automatically select the model with bi-level optimization.

To achieve good performance on graphs with different homophily ratios, we can combine predictions of the label-wise aggregation model for heterophilic graphs and traditional GNN models for homophilic graphs. Predictions from the GNN \( f_G \) for homophilic graphs are given by:

\[
\hat{y}_v^{(G)} = \text{GNN}(A, X),
\]
where the GNN is flexible to various models for homophilic graphs such as GAT and GIN. Here, we select GCNII (Chen et al. 2020) which achieves state-of-the-art results on homophilic graphs. Here, we select GCNII (Chen et al. 2020) which achieves state-of-the-art results on homophilic graphs. The model selection can be achieved by assigning higher weight to the corresponding model prediction. The combined prediction is given as:

$$\hat{y}_v = \frac{\exp(\phi_1)}{\sum_{i=1}^{2} \exp(\phi_i)} \hat{y}_v^C + \frac{\exp(\phi_2)}{\sum_{i=1}^{2} \exp(\phi_i)} \hat{y}_v^G,$$

where $\hat{y}_v^C \in \hat{y}_v^G$ is the prediction of node $v$ from $f_G, \phi_1$ and $\phi_2$ are the learnable weights to control the contributions of two models in final prediction. $\phi_1$ and $\phi_2$ can be obtained by finding the values that lead to good performance on validation set. More specifically, this goal can be formulated as the following bi-level optimization problem:

$$\min_{\phi_1, \phi_2} L_{val}(\theta_C^*(\phi_1, \phi_2), \theta_G^*(\phi_1, \phi_2), \phi_1, \phi_2)$$

$$s.t. \theta_C^*, \theta_G^* = \arg\min_{\theta_C, \theta_G} L_{train}(\theta_C, \theta_G, \phi_1, \phi_2)$$

where $L_{val}$ and $L_{train}$ are the average cross entropy loss of the combined predictions $\{\hat{y}_v : v \in V_{val}\}$ and $\{\hat{y}_v : v \in V_{train}\}$ on validation set and training set, respectively.

### 4.3 An Optimization Algorithm of LW-GNN

Computing the gradients for $\phi_1$ and $\phi_2$ is expensive in both computational cost and memory. To alleviate this issue, we use an alternating optimization schema to iteratively update the model parameters and the model selection weights.

#### Updating Lower Level $\theta_C$ and $\theta_G$, Instead of calculating $\theta_C^*$ and $\theta_G^*$ per outer iteration, we fix $\phi_1$ and $\phi_2$ and update the model parameters $\theta_G$ and $\theta_C$ for $T$ steps by:

$$\theta_G^{t+1} = \theta_G^t - \alpha_C \nabla_{\theta_C} L_{train}(\theta_C^t, \theta_G^t, \phi_1, \phi_2),$$

$$\theta_C^{t+1} = \theta_C^t - \alpha_G \nabla_{\theta_C} L_{train}(\theta_C^t, \theta_G^t, \phi_1, \phi_2),$$

where $\theta_C^t$ and $\theta_G^t$ are model parameters after updating $t$ steps. $\alpha_C$ and $\alpha_G$ are the learning rates for $\theta_C$ and $\theta_G$.

#### Updating Upper Level $\phi_1$ and $\phi_2$, Here, we use the updated model parameters $\theta_G^t$ and $\theta_C^t$ to approximate $\theta_C^*$ and $\theta_G^*$, Moreover, to further speed up the optimization, we apply first-order approximation (Finn, Abbeel, and Levine 2017) to compute the gradients of $\phi_1$ and $\phi_2$:

$$\phi_1^{k+1} = \phi_1^k - \alpha_{\phi} \nabla_{\phi} L_{val}(\theta_C^t, \theta_G^t, \phi_1^k, \phi_2^k),$$

$$\phi_2^{k+1} = \phi_2^k - \alpha_{\phi} \nabla_{\phi} L_{val}(\theta_C^t, \theta_G^t, \phi_1^k, \phi_2^k),$$

where $\theta_C^t$ and $\theta_G^t$ means stopping the gradient. $\alpha_{\phi}$ is the learning rate for $\phi_1$ and $\phi_2$.

**Training Algorithm.** The training algorithm of LW-GNN is shown in Algorithm 1. In line 1 and 2, we firstly train the $f_P$ to obtain the required pseudo labels for label-wise message passing. From line 4 to 6, we get the combined predictions from $f_C$ and $f_G$ and update the model selection weights with Eq. (13). From line 7 to 10, we update the model parameters $\theta_C$ and $\theta_G$ by minimizing $L_{train}$ with Eq. (12). The updating of model selection weights and model parameters are conducted iteratively until convergence.

### 5 Experiments

In this section, we conduct experiments to demonstrate the effectiveness of LW-GNN. In particular, we aim to answer the following research questions:

- **RQ1** Is our proposed LW-GNN effective in node classification on both homophilic and heterophilic graphs.
- **RQ2** Can our label-wise aggregation learn representations that well capture information for label prediction?
- **RQ3** How do the quality of pseudo labels and the automatic model selection affect LW-GNN?

#### 5.1 Experimental Settings

**Datasets.** To evaluate the performance of our proposed LW-GNN, we conduct experiments on three homophilic graphs and four heterophilic graphs. For homophilic graphs, we choose the widely used benchmark datasets, Cora, Citeseer, and Pubmed (Kipf and Welling 2016). The dataset splits of homophilic graphs are the same as the cited paper. As for heterophilic graphs, we use a webpage dataset Texas (Pei et al. 2020), and three subgraphs of wiki, i.e., Squirrel, Chameleon, and Crocodile (Rozemberczki, Allen, and Sarkar 2021). Following Zhu et al. (2020), 10 splits are used in each heterophilic graph for evaluation. The statistics of the datasets are presented in Table 1.

#### Compared Methods.** We compare LW-GNN with the following representative and state-of-the-art GNNs:
- **MLP:** Multilayer perceptron is applied here to give predictions without using the graph structure information.

| Dataset | Nodes | Edges | Classes | Hom. Ratio |
|---------|-------|-------|---------|------------|
| Texas   | 183   | 309   | 5       | 0.11       |
| Chameleon | 2,277 | 36,101| 5       | 0.24       |
| Squirrel | 5,201 | 217,073| 5       | 0.22       |
| Crocodile | 11,631 | 360,040| 5       | 0.25       |
| Cora    | 2,708 | 5,429 | 6       | 0.74       |
| Citeseer | 3,327 | 4,732 | 7       | 0.80       |
| Pubmed  | 19,717| 44,338| 3       | 0.87       |

Table 1: The statistics of datasets.
Table 2: Node classification performance (Accuracy(%) ± Std.) on heterophilic graphs.

| Method         | Cora   | Citeseer | Pubmed |
|----------------|--------|----------|--------|
| MLP            | 78.4±0.5 | 60.3±0.4 | 72.7±0.4 |
| GCN            | 80.0±0.7 | 71.3±0.3 | 78.4±1.1 |
| MixHop         | 78.4±0.5 | 72.2±0.8 | 78.4±0.5 |
| SuperGAT       | 78.4±0.5 | 72.2±0.8 | 80.2±0.2 |
| GCNII          | 80.0±0.7 | 71.3±0.3 | 78.4±1.1 |
| FAGCN          | 80.0±0.7 | 71.3±0.3 | 78.4±1.1 |
| SimP-GCN       | 80.0±0.7 | 71.3±0.3 | 78.4±1.1 |
| H2GCN          | 80.0±0.7 | 71.3±0.3 | 78.4±1.1 |
| LW-GNN         | 80.0±0.7 | 71.3±0.3 | 78.4±1.1 |
| Weight for f_C | 0.900   | 0.986    | 0.987  |

Table 3: Node classification performance (Accuracy(%) ± Std.) on homophilic graphs.

| Method         | Texas | Chameleon | Squirrel | Crocodile |
|----------------|-------|-----------|----------|-----------|
| MLP            | 78.1±0.6 | 48.0±1.5 | 32.3±1.8 | 65.8±0.7 |
| GCN            | 57.6±5.9 | 63.5±2.2 | 46.7±1.5 | 66.7±1.0 |
| MixHop         | 60.6±7.7 | 61.2±2.2 | 44.1±1.1 | 67.6±1.3 |
| SuperGAT       | 58.6±7.7 | 59.4±2.5 | 38.9±1.5 | 62.6±0.9 |
| GCNII          | 68.6±9.8 | 63.5±2.5 | 49.4±1.7 | 69.0±0.7 |
| FAGCN          | 79.5±4.8 | 63.9±2.2 | 43.3±2.5 | 67.1±0.9 |
| SimP-GCN       | 80.5±5.9 | 63.7±2.3 | 42.8±1.4 | 63.7±2.3 |
| H2GCN          | 83.7±6.0 | 54.2±2.3 | 36.0±1.1 | 66.7±0.5 |
| LW-GNN         | 84.4±5.1 | 69.4±1.4 | 55.8±1.1 | 77.4±0.6 |
| Weight for f_C | 0.960   | 0.986    | 0.987   | 0.999    |

• GCN (Kipf and Welling 2016): This is a popular spectral-based Graph Convolutional Network.
• MixHop (Abu-El-Haija et al. 2019): It adopts a graph convolutional layer mixing powers of the adjacency matrix.
• SuperGAT (Kim and Oh 2020): This is a self-supervised learning method based on GAT (Veličković et al. 2018). Edge prediction is deployed to guide the learning of attention for better information propagation.
• GCNII (Chen et al. 2020): Based on GCN, residual connection and identity mapping are applied in GCNII to have a deep GNN for better performance.

We also compare LW-GNN with the following state-of-the-art GNN models for heterophilic graphs:
• FAGCN (Bo et al. 2021): FAGCN adaptively aggregates low-frequency and high-frequency signals from neighbors to improve the performance on heterophilic graphs.
• SimP-GCN (Jin et al. 2021): A feature similarity preserving aggregation is applied to facilitate the representation learning on graphs with homophily and heterophily.
• H2GCN (Zhu et al. 2020): H2GCN adopts three key designs for node classification on heterophilic graphs.

Implementation Details. For experiments on each heterophilic graph, we run the 10 public dataset splits and report the average results and standard deviations. For homophily graphs, we run each experiment 5 times on the provided public dataset split. A one-hidden layer MLP with 64 filters is applied as the pseudo label predictor f_P. We adopt two layers of label-wise message passing on all the datasets. More discussion about the impacts of the depth on LW-GNN is given in Sec. 5.2. The hidden dimension of f_C is fix as 64 for all graphs. As for the f_C which deploys GCNII (Chen et al. 2020) as the backbone, the hyperparameter settings are the same as the cited paper. During the training phase, the learning rate is set as 0.01 for all the parameters and model selection weights. The inner iteration step T is set as 2. All the hyperparameters of the baselines are tuned on the validation set for fair comparisons.

5.2 Node Classification Performance

To answer RQ1, we conduct experiments on both heterophilic and homophilic graphs with comparison to the state-of-the-art GNN models.

Performance on Heterophilic Graphs. We conduct experiments on 10 dataset splits on each heterophilic graphs. The average accuracy and standard deviations on heterophilic graphs are reported in Table 2. The model selection weight for label-wise aggregation GNN f_C is shown along with the results of LW-GNN. Note that this model selection weight ranges from 0 to 1. When the weight is close to 1, the label-wise aggregation model is selected. When the weight for f_C is close to 0, the GNN f_C for homophilic graph is selected. From this table, we can observe that:
• GNN models designed for homophilic graphs such as GCN and SuperGAT perform poorly on heterophilic graphs. For example, MLP outperforms GCN and other GNNs for homophilic graphs by a large margin on Texas. This indicates the necessity of investigating messaging-passing mechanisms for graphs with heterophily.
• The model selection weight for f_C is close to 1 for heterophilic graphs, which verifies that the proposed LW-GNN can correctly select the label-wise aggregation GNN f_C for heterophilic graphs.
• Compared with SimP-GCN which also aims to preserve node features, our LW-GNN performs significantly better on heterophilic graphs. This is because SimP-GCN only focuses on the similarity of central node attributes. In contrast, our label-wise aggregation can preserve both the central node features and the information of their neighbors for node classification on heterophilic graphs. LW-GNN also outperforms other GNNs for heterophilic graphs by a large margin. This further demonstrates the effectiveness of label-wise aggregation.

Performance on Homophilic Graphs. We report the average results of 5 runs in Table 3. Similarly, the model selection weight for f_C is also presented. From the table, we can observe that existing GNNs for heterophilic graphs generally perform worse than state-of-the-art GNNs on homophilic graphs such as GCNII. In contrast, LW-GNN achieves comparable results with the best model on homophilic graphs. This is because LW-GNN combines the GNN using label-wise message passing and a state-of-the-art GNN for homophilic graph. And it can automatically select the right model for the given homophilic graph.

5.3 Analysis of Node Representations

To answer RQ2, we compare the representation similarity of intra-class node pairs and inter-class node pairs. Results
of GCN is also reported as the reference. For both GCN and LW-GNN, representations learned by the last layer are used for analysis. Since we have similar observations on other heterophilic graphs, we only show the results on Texas in Fig. 3. From this figure, we can observe that the learned representations of GCN are very similar for both intra-class pairs and inter-class pairs. This verifies that simply aggregating the neighbors will make the node representations less discriminative. With label-wise aggregation, the similarity scores of intra-class pairs are significantly higher than inter-class node pairs. This demonstrates that the representations learned by label-wise message passing can well preserve the target nodes’ features and their contextual information.

### 5.4 Ablation Study

To answer RQ3, we conduct ablation studies to understand the contributions of each component to LW-GNN. To investigate how the quality of pseudo labels can affect LW-GNN, we train a variant LW-GNN\(\text{\textbackslash}P\) by replacing the MLP-based label predictor with a GCN model. To show the importance of the automatic model selection, we train a variant LW-GNN\(\text{\textbackslash}G\) which removes the GNN for homophilic graphs and only uses label-wise aggregation GNN. Finally, we replace the GCNII backbone of \(f_G\) to GCN to show LW-GNN is flexible to adopt various GNNs for \(f_G\). Experiments are conducted on both homophilic and heterophilic graphs. The results are shown in Table 4. We can observe that:

- On homophilic graphs, LW-GNN\(\text{\textbackslash}P\) shows comparable results with LW-GNN, because GCNII will be selected given a homophilic graph. On the heterophilic graph Texas, the performance of LW-GNN\(\text{\textbackslash}P\) is significantly worse than LW-GNN. This is because GNNs can produce poor pseudo labels on heterophilic graph, which degrades the label-wise message passing.

- Compared with MLP, LW-GNN\(\text{\textbackslash}G\) performs much better. This shows label-wise aggregation can capture structure information. However, LW-GNN\(\text{\textbackslash}G\) performs worse than GCNII and LW-GNN on homophilic graphs. This indicates the necessity of combining GNN for homophilic graphs with label-wise aggregation.

- LW-GNN\(\mathcal{G}_{\text{GCN}}\) achieves comparable results with GCN on homophilic graphs. On heterophilic graphs, LW-GNN\(\mathcal{G}_{\text{GCN}}\) performs similarly with LW-GNN. This shows the flexibility of LW-GNN in adopting traditional GNN models designed for homophilic graphs.

### 5.5 Impacts of Label-Wise Aggregation Layers

In this subsection, we explore the sensitivity of LW-GNN on the depth of \(f_C\), i.e., the number of layers of label-wise message passing. Since LW-GNN will not select \(f_C\) for homophilic graphs. We only conduct the sensitivity analysis on two heterophilic graphs, i.e., Chameleon and Squirrel. We vary the depth of \(f_C\) as \(\{2, 3, \ldots, 6\}\). The other experimental settings are the same as that described in Sec. 5.1. The average results and standard deviations are shown in Fig. 4. From the figure, we find that our LW-GNN is insensitive to the number of layers, while the performance of GCN will drop with the increase of depth. This is because (i) aggregation of LW-GNN is performed label-wisely. Embeddings of nodes in different classes will not be similar even after many iterations; and (ii) the intermediate representations for different hops of neighbors are combined together to give the final prediction, which further reduces the potential risk brought by poor representations in deep model.

### 6 Conclusion and Future Work

In this paper, we develop a novel label-wise message-passing mechanism to learn representations that preserve the node features and their neighbors’ information for heterophilic graphs. An automatic model selection module is applied to ensure the performance of the proposed framework on graphs with any homophily ratio. Extensive experiments show that our proposed LW-GNN can achieve state-of-the-art results on both homophilic and heterophilic graphs. There are several interesting directions need further investigation. First, since better pseudo labels will benefit the label-wise message passing, it is promising to incorporate the predictions of LW-GNN in label-wise message passing. Second, in some applications such as link prediction, labels are not available. Therefore, we will investigate how to generate useful pseudo labels for label-wise aggregation for applications where no labeled nodes are provided.
References

Abu-El-Haija, S.; Perozzi, B.; Kapoor, A.; Alipourfard, N.; Lerman, K.; Harutyunyan, H.; Ver Steeg, G.; and Galstyan, A. 2019. Mixhop: Higher-order graph convolutional architectures via sparsified neighborhood mixing. In international conference on machine learning, 21–29. PMLR.

Bo, D.; Wang, X.; Shi, C.; and Shen, H. 2021. Beyond low-frequency information in graph convolutional networks. arXiv preprint arXiv:2101.00797.

Bongini, P.; Bianchini, M.; and Scarselli, F. 2021. Molecuar generative Graph Neural Networks for Drug Discovery. Neurcomputing, 450: 242–252.

Bruna, J.; Zaremba, W.; Szlam, A.; and LeCun, Y. 2014. Spectral networks and locally connected networks on graphs. ICLR.

Chen, J.; Ma, T.; and Xiao, C. 2018. Fastgcn: fast learning with graph convolutional networks via importance sampling. ICLR.

Chen, M.; Wei, Z.; Huang, Z.; Ding, B.; and Li, Y . 2020. ICML with graph convolutional networks via importance sampling.

Chen, J.; Ma, T.; and Xiao, C. 2018. Fastgcn: fast learning with graph convolutional networks via importance sampling. ICLR.

Cayleynets: Graph convolutional neural networks with complex rational spectral filters. IEEE Transactions on Signal Processing, 67(1): 97–109.

Li, G.; Muller, M.; Thabet, A.; and Ghanem, B. 2019. Deepgcn: Can gcns go as deep as cnns? In Proceedings of the IEEE/CVF International Conference on Computer Vision, 9267–9276.

Li, Q.; Han, Z.; and Wu, X.-M. 2018. Deeper insights into graph convolutional networks for semi-supervised learning. AAAI.

McPherson, M.; Smith-Lovin, L.; and Cook, J. M. 2001. Birds of a feather: Homophily in social networks. Annual review of sociology, 27(1): 415–444.

Niepert, M.; Ahmed, M.; and Kutzkov, K. 2016. Learning convolutional neural networks for graphs. In ICML, 2014–2023.

Pandit, S.; Chau, D. H.; Wang, S.; and Faloutsos, C. 2007. Netprobe: a fast and scalable system for fraud detection in online auction networks. In Proceedings of the 16th international conference on World Wide Web, 201–210.

Pei, H.; Wei, B.; Chang, K. C.-C.; Lei, Y.; and Yang, B. 2020. Geom-gen: Geometric graph convolutional networks. arXiv preprint arXiv:2002.05287.

Qiu, J.; Chen, Q.; Dong, Y.; Zhang, J.; Yang, H.; Ding, M.; Wang, K.; and Tang, J. 2020. Gcc: Graph contrastive coding for graph neural network pre-training. In Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, 1150–1160.

Rozemberczki, B.; Allen, C.; and Sarkar, R. 2021. Multiscale attributed node embedding. Journal of Complex Networks, 9(2): cnab014.

Sun, K.; Zhu, Z.; and Lin, Z. 2020. Multi-stage self-supervised learning for graph convolutional networks. AAAI.

Veličković, P.; Cucurull, G.; Casanova, A.; Romero, A.; Lio, P.; and Bengio, Y. 2018. Graph attention networks. ICLR.

Wang, D.; Lin, J.; Cui, P.; Jia, Q.; Wang, Z.; Fang, Y.; Yu, Q.; Zhou, J.; Yang, S.; and Qi, Y. 2019. A semi-supervised graph attentive network for financial fraud detection. ICDM.

Wu, Z.; Pan, S.; Chen, F.; Long, G.; Zhang, C.; and Philip, S. Y. 2020. A comprehensive survey on graph neural networks. IEEE transactions on neural networks and learning systems.

Xu, K.; Hu, W.; Leskovec, J.; and Jegelka, S. 2018a. How powerful are graph neural networks? arXiv preprint arXiv:1810.00826.

Xu, K.; Li, C.; Tian, Y.; Sonobe, T.; Kawarabayashi, K.-i.; and Jegelka, S. 2018b. Representation learning on graphs with jumping knowledge networks. In International Conference on Machine Learning, 5453–5462. PMLR.

You, Y.; Chen, T.; Sui, Y.; Chen, T.; Wang, Z.; and Shen, Y. 2020. Graph contrastive learning with augmentations. Advances in Neural Information Processing Systems, 33.

Yu, B.; Yin, H.; and Zhu, Z. 2017. Spatio-temporal graph convolutional networks: A deep learning framework for traffic forecasting. arXiv preprint arXiv:1709.04875.
Zhao, T.; Tang, X.; Zhang, X.; and Wang, S. 2020. Semi-Supervised Graph-to-Graph Translation. In CIKM, 1863–1872.

Zhu, J.; Yan, Y.; Zhao, L.; Heimann, M.; Akoglu, L.; and Koutra, D. 2020. Beyond homophily in graph neural networks: Current limitations and effective designs. arXiv preprint arXiv:2006.11468.

Zhu, Q.; Du, B.; and Yan, P. 2020. Self-supervised Training of Graph Convolutional Networks. arXiv preprint arXiv:2006.02380.