Graph Neural Networks for Graphs with Heterophily: A Survey

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Abstract—Recent years have witnessed fast developments of graph neural networks (GNNs) that have benefited myriads of graph analytic tasks and applications. In general, most GNNs depend on the homophily assumption that nodes belonging to the same class are more likely to be connected. However, as a ubiquitous graph property in numerous real-world scenarios, heterophily, *i.e.*, nodes with different labels tend to be linked, significantly limits the performance of tailor-made homophilic GNNs. Hence, *GNNs for heterophilic graphs* are gaining increasing research attention to enhance graph learning with heterophily. In this paper, we provide a comprehensive review of GNNs for heterophilic graphs. Specifically, we propose a systematic taxonomy that essentially governs existing heterophilic GNN models, along with a general summary and detailed analysis. Furthermore, we discuss the correlation between graph heterophily and various graph research domains, aiming to facilitate the development of more effective GNNs across a spectrum of practical applications and learning tasks in the graph research community. In the end, we point out the potential directions to advance and stimulate more future research and applications on heterophilic graph learning with GNNs.

Index Terms—Graph neural networks, heterophily, graph representation learning, message passing.

✦

1 INTRODUCTION

GRAPHS are pervasively structured data and have been widely used in many real-world scenarios, such as social networks [1], [2], knowledge bases [3], traffic networks [4], and recommendation systems [5], [6]. Recently, graph neural networks (GNNs) have achieved remarkable success with powerful learning ability and become prevalent models to tackle various graph analytical tasks, such as node classification, link prediction, and graph classification [3], [7]–[9].

While a large number of GNNs with diverse architectures have been designed [10]–[15], the majority of them follow the homophily assumption, *i.e.*, nodes with similar features or same class labels are linked together. For example, in citation networks, a study usually cites reference papers from the same research area [16]. However, real-world graphs do not always obey the

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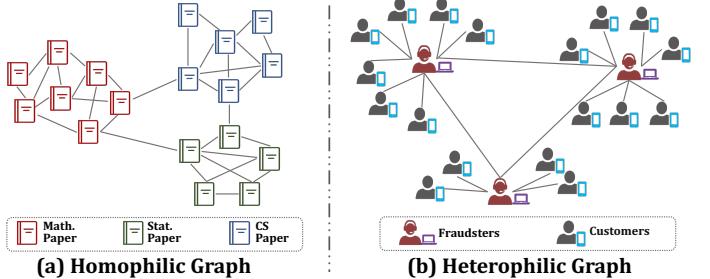- *Corresponding Author: Shirui Pan.*

Fig. 1: Examples of homophilic and heterophilic graphs (Left: (a) a citation network; Right: (b) an online transaction network).

homophily assumption but show an opposite property, *i.e.*, *heterophily* that linked nodes have dissimilar features and different class labels [17]–[21]. For instance, in online transaction networks, fraudsters are more likely to build connections with customers instead of other fraudsters [22]; in dating networks, most people prefer to date with people of the opposite gender [23]; in molecular networks, protein structures are more likely composed of different types of amino acids that are linked together [24]. The examples of homophilic and heterophilic graphs are provided in Fig. 1 to illustrate their difference visually. Importantly, such heterophily restricts the learning ability of existing homophilic GNNs on general graph-structural data, resulting in significant performance degradation on heterophilic graphs [23]–[25].

Core Challenges of GNNs for Heterophily. We attribute the performance degradation to the uniform message passing framework under the homophily setting. The procedure of this framework can be summarized as: first aggregating the messages extracted from local neighbor nodes, then updating the final ego node (the current central node itself) representations with aggregated neighbor messages. Nevertheless, due to the heterophily property of graphs, this mechanism poses significant challenges

for the development of heterophilic GNNs, primarily manifesting in two aspects:

- **Challenge-1: Undiscovered Non-local Neighbors.** Guided by homophily, neighbor aggregation in homophilic GNNs restricts information extraction to the proximal local topology of graphs. When applied to graphs with heterophily, it fails to explore non-local topology, where heterophilic nodes of the same class are typically situated at long-term distances. This poses a significant challenge in identifying and learning informative nodes with high structural and semantic similarities on heterophilic graphs.
- **Challenge-2: Indistinguishable Node Representation Learning.** Homophilic GNNs employ uniform local neighbor aggregation and update the central node representation when they are typically similar and share the same labels. Consequently, on heterophilic graphs, the discrepancy between similar non-local neighbors and dissimilar local neighbors can not be effectively captured. This results in critical challenges in learning discriminative node representations with distinguishable heterophily information through diverse customized message passing.

In light of these challenges, recently, an increasing number of researchers have started turning their attention to the study of GNNs with heterophily. The research focus is sufficiently broad, from heterophilic graph data exploration [26]–[28] to various technical algorithm development [17], [19], [21], [25], [29]–[31].

Importance of Developing Heterophilic GNNs. Heterophilic graph learning with GNNs is becoming an upward trending research topic and it shows closely tied connections with diverse domains in graph research. The compelling significance of GNN development for heterophilic graphs is underscored by the following aspects:

- *Enhancing the understanding of complex and diverse heterophily graphs.* Graph-structure data with the heterophilic property presents great complexity and diversity, and it is prevalent across various real-world application scenarios, ranging from daily-life personal relationships to scientific chemical molecular study. A thorough and ongoing exploration of heterophily graph data would significantly enhance the understanding of complex and diverse heterophily graphs, thereby providing valuable guidance for the development of GNN models and advancements in heterophily graph learning.
- *Advancing heterophilic graph analysis and learning.* Heterophilic graph analysis and learning tasks are still open and promising research topics in development, while numerous challenges need to be tackled for designing heterophilic GNN models with expressive performance, robustness, and generalization ability. The advancement of heterophilic GNNs is pivotal for unlocking the full potential of heterophilic graph analysis in addressing various practical graph learning tasks covering both heterophilic node representations and graph structures.
- *Adapting with versatility in heterophilic GNN development.* As heterophilic graphs exist prevalently and show close connections with various graph research domains, *e.g.*, over-smoothing and anomaly detection. Hence, developing specialized heterophilic GNN architectures and learning techniques would be pivotal in expanding the versatility and adaptability of GNN models, unleashing power

of heterophilic GNNs in cross graph research domains and applications.

In this paper, we present a comprehensive and systematic review of GNNs for heterophilic graphs, aiming to provide a general blueprint of heterophilic graph research. It can be beneficial to establish connections and make comparisons among different heterophilic GNN methods, leading to an in-depth understanding of how different methods tackle the challenges of heterophily learning. We are expecting that our survey will significantly inspire and facilitate the development of heterophilic graphs [1]. The contributions of our work are summarized as follows:

- **Comprehensive Overview**: We provide a comprehensive overview of current heterophilic GNNs in terms of data, algorithms, and applications. We provide detailed descriptions of each model type, along with the necessary comparison and the gist summary.
- **Systematic Taxonomy**: We provide a systematic taxonomy of heterophilic GNNs and categorize existing methods into three classes, *i.e.*, non-local neighbor extension methods, GNN architecture refinement methods, and hybrid methods.
- **Thorough Discussion**: We provide a thorough discussion of the correlation between graph heterophily and various graph research domains, including the relation between graph heterophily and model robustness, over-smoothing, and graph anomaly detection.
- **Future Directions**: We suggest promising future research directions and discuss the limitations of existing heterophilic GNNs from multiple perspectives, namely interpretability, robustness, scalability, and heterophilic graph data exploration.

The remainder of this article is organized as follows. Section 2 defines the related concepts and provides notations used in this survey. Section 3 describes the framework of heterophilic GNNs and provides the taxonomy. Section 4-6 review three categories of heterophilic GNNs methods respectively. Section 7 discusses heterophily GNNs on diverse graphs and the correlation between heterophily and diverse graph research domains. Section 8 analyzes the unexplored challenges and potential future directions. Section 9 concludes this article in the end. More details of real-world heterophilic graph dataset benchmarks, open-source codes, and the overall development timeline of heterophilic GNNs can be found in the appendix.

2 PRELIMINARY

2.1 Notations

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be an undirected, unweighted graph where $\mathcal{V} = \{v_1, \cdots, v_{|\mathcal{V}|}\}$ is the node set and $\mathcal{E} \in \mathcal{V} \times \mathcal{V}$ is the edge set. The neighbor set of node v is denoted as $\mathcal{N}(v) = \{u : (v, u) \in \mathcal{E}\}$. The node features are represented by a feature matrix $\mathbf{X} \in \mathbb{R}^{|\mathcal{V}| \times d}$, where the i-th row $\mathbf{x}_i \in \mathbb{R}^d$ is the feature vector of node v_i and d is the number of feature dimensions. Connectivity is represented by the adjacency matrix $\mathbf{A} \in \{0, 1\}^{n \times n}$. For any matrix $\mathbf{A}$, we use $\mathbf{A}_{uv}$ to refer to the scalar value at the (u, v) location. The graph Laplacian is defined as $\mathbf{L} = \mathbf{D} - \mathbf{A}$, where $\mathbf{D} \in \mathbb{R}^{n \times n}$ is the diagonal degree matrix.

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1. Our preprint of this article [32] has attracted 110+ citations, showing a strong uptrend of this research topic.

Due to its generalization ability [33], the symmetric normalized Laplacian is often used, which is defined as $\tilde{\mathbf{L}} = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$. Another option is random walk normalization: $\tilde{\mathbf{L}} = \mathbf{D}^{-1}\mathbf{L}$. Note that normalization could also be applied to the adjacency matrix. Their relationship can be derived as $\tilde{\mathbf{L}} = \mathbf{I} - \tilde{\mathbf{A}}$, where $\mathbf{I}$ is the identity matrix. Through eigendecomposition, $\mathbf{L}$ can be expressed as $\tilde{\mathbf{L}} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\top}$, where each column of $\mathbf{U} \in \mathbb{R}^{n \times n}$ represents an eigenvector of $\mathbf{L}$, $\mathbf{\Lambda}$ is the diagonal matrix whose diagonal elements are the corresponding eigenvalues (*i.e.*, $\mathbf{\Lambda}_{ii} = \lambda_i$).

2.2 Graph Neural Networks

Generally, GNNs adopt the message passing mechanism, where each node representation is updated by aggregating the messages from local neighbor representations, and then combining the aggregated messages with its ego representation [10]. The updating process of the l-th GNN layer for each node $v \in \mathcal{V}$ can be described as:

$$
\begin{aligned}
\mathbf{m}_v^{(l)} &= \text{AGGREGATE}^{(l)}(\{\mathbf{h}_u^{(l-1)} : u \in \mathcal{N}(v)\}), \\
\mathbf{h}_v^{(l)} &= \text{UPDATE}^{(l)}(\mathbf{h}_v^{(l-1)}, \mathbf{m}_v^{(l)}),
\end{aligned}
\tag{1}
$$

where $\mathbf{m}_v^{(l)}$ and $\mathbf{h}_v^{(l)}$ stand for the message vector and the representation vector of node v at the l-th layer, respectively. And AGGREGATE$(\cdot)$ and UPDATE$(\cdot)$ are aggregation function (*e.g.*, mean, LSTM, and max pooling) and update function (*e.g.*, linear-layer combination) [8], respectively. Given the input of the first layer as $\mathbf{H}^{(0)} = \mathbf{X}$, the learned node representations at each layer of L-layer GNN can be denoted as $\mathbf{H}^{(l)} = \left[\mathbf{h}_v^{(l)}\right]$ for $v = (1, \cdots, |\mathcal{V}|)$ and $l = (1, \cdots, L)$. For node classification task, the final node representation $\mathbf{H}^{(L)}$ would be fed into a classifier network (*e.g.*, a fully-connected layer) to generate the predictions for classes.

2.3 Spectral Graph Convolution

A graph convolution operation is defined in the Fourier domain such that

$$
f_1 * f_2 = \mathbf{U}[(\mathbf{U}^{\top}f_1) \odot (\mathbf{U}^{\top}f_2)],
\tag{2}
$$

where $\odot$ is the element-wise product, and f_1/f_2 are two signals defined on nodes. It follows that a node signal $f_2 = \mathbf{X}$ is filtered by spectral signal $\hat{f}_1 = \mathbf{U}^{\top}f_1 = \mathbf{g}$ as

$$
\mathbf{h}_v^{(l)} = \mathbf{g}(\tilde{\mathbf{L}})\mathbf{h}_v^{(l-1)} = \mathbf{U}[\mathbf{g}(\mathbf{\Lambda}) \odot (\mathbf{U}^{\top}\mathbf{h}_v^{(l-1)})] = \mathbf{U}\mathbf{g}(\mathbf{\Lambda})\mathbf{U}^{\top}\mathbf{h}_v^{(l-1)},
\tag{3}
$$

where $\mathbf{g}$ is known as frequency response function. Therefore, the objective of spectral methods is to learn a function $\mathbf{g}(\cdot)$. In simpler terms, $\mathbf{g}(\cdot)$ can be seen as a way to re-weight signals of different frequencies (or eigenvalues). Eigenvalues represent the smoothness or frequency of the corresponding eigenvectors. Consequently, assigning greater weight to smaller eigenvalues retains more low-frequency information, while assigning greater weight to larger eigenvalues retains more high-frequency information. In general, $F_{LP} = \epsilon\mathbf{I} + \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2} = (\epsilon + 1)\mathbf{I} - \mathbf{L}$ is a low-pass filter, while $F_{HP} = \epsilon\mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2} = (\epsilon - 1)\mathbf{I} + \mathbf{L}$ denotes high-pass filter.

2.4 Measure of Heterophily & Homophily

In general, heterophily and homophily of a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ can be measured by following metrics: node homophily [34], edge homophily [24], class homophily [27], label informativeness (LI) [35], and adjusted homophily [35].

Node homophily and edge homophily are two essential measures. Concretely, the node homophily $\mathcal{H}_{node}$ is the average proportion of the neighbors with the same class of each node:

$$
\mathcal{H}_{node} = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \frac{|\{u \in \mathcal{N}(v) : y_v = y_u\}|}{|\mathcal{N}(v)|}.
\tag{4}
$$

The edge homophily $\mathcal{H}_{edge}$ is the proportion of edges connecting two nodes with the same class:

$$
\mathcal{H}_{edge} = \frac{|\{(v, u) \in \mathcal{E} : y_v = y_u\}|}{|\mathcal{E}|}.
\tag{5}
$$

To alleviate the sensitivity issue of node homophily $\mathcal{H}_{node}$ and edge homophily $\mathcal{H}_{edge}$ on the node class number and balance, the class homophily measures the average proportion of neighbors with the same class across all nodes of each class while taking into account the constraint of class proportions, that is

$$
\mathcal{H}_{class} = \frac{1}{C-1} \sum_{c=1}^{C} \left[\frac{\sum_{v:y_v=c} |\{u \in \mathcal{N}(v) : y_v = y_u\}|}{\sum_{v:y_v=c} |\mathcal{N}(v)|} - \frac{n_c}{|\mathcal{V}|} \right]_{+},
\tag{6}
$$

where $n_c = |\{u : y_u = c\}|$ denotes the node number of class c.

Ensuring that the homophily measure satisfies essential properties is crucial for enhancing reliability, with a particular focus on maximum consistency and maintaining a constant baseline. To establish the constant baseline property, the adjusted homophily measure $\mathcal{H}_{adj}$ subtracts the expected value of the measure from $\mathcal{H}_{edge}$. Furthermore, to enable the obtained quantity comparisons across different datasets, label informativeness (LI) quantifies the informativeness of a neighbor's label for a node's label. These measures are respectively defined as

$$
\mathcal{H}_{adj} = \frac{\mathcal{H}_{edge} - \sum_{c=1}^{C}\left(\sum_{v:y_v=c} |\mathcal{N}(v)|/(2|\mathcal{E}|)\right)^2}{1 - \sum_{c=1}^{C}\left(\sum_{v:y_v=c} |\mathcal{N}(v)|/(2|\mathcal{E}|)\right)^2},
\tag{7}
$$

and

$$
\text{LI} = (H(y_u) - H(y_u|y_v))/H(y_u),
\tag{8}
$$

where $H(y_u)$ measures the "hardness" of predicting the label of u without knowing y_v. $H(y_u|y_v)$ is the conditional entropy.

Note that the range of $\mathcal{H}_{node}$, $\mathcal{H}_{edge}$, $\mathcal{H}_{class}$ and LI is $[0, 1]$. Graphs with strong homophily have higher $\mathcal{H}_{node}$, $\mathcal{H}_{edge}$, $\mathcal{H}_{class}$ and LI (closer to 1); whereas graphs with strong heterophily have smaller $\mathcal{H}_{node}$, $\mathcal{H}_{edge}$, $\mathcal{H}_{class}$ and LI (closer to 0). The measure $\mathcal{H}_{adj}$ is appropriately adjusted based on $\mathcal{H}_{edge}$, and it can occasionally have a negative value when $\mathcal{H}_{edge}$ is smaller than $\sum_{c=1}^{C}\left(\sum_{v:y_v=c} |\mathcal{N}(v)|/(2|\mathcal{E}|)\right)^2$. Nevertheless, the overall trend of $\mathcal{H}_{adj}$ aligns with the previous four measures: larger values indicate stronger homophily, while smaller values suggest stronger heterophily. Besides, we would like to emphasise that various metrics of homophily and heterophily are suited to specific

TABLE 1: Summary of existing measure methods of heterophily and homophily.

Measure Methods	Definition	Description
Node Homophily	$\mathcal{H}_{node} = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \frac{|\{u \in \mathcal{N}(v): y_v = y_u\}|}{|\mathcal{N}(v)|}$	Both $\mathcal{H}_{node}$ and $\mathcal{H}_{edge}$ are within the range of $[0, 1]$. These two measures are intuitive, but they are relatively sensitive to the number of classes and the balance between these classes.
Edge Homophily	$\mathcal{H}_{edge} = \frac{|\{(v,u) \in \mathcal{E}: y_v = y_u\}|}{|\mathcal{E}|}$	
Class Homophily	$\mathcal{H}_{class} = \frac{1}{C-1} \sum_{c=1}^{C} \left[\frac{\sum_{v:y_v=c} |\{u \in \mathcal{N}(v): y_v = y_u\}|}{\sum_{v:y_v=c} |\mathcal{N}(v)|} - \frac{n_c}{|\mathcal{V}|} \right]_{+}$	$\mathcal{H}_{class}$ avoids the class sensitivity issue of $\mathcal{H}_{node}$ and $\mathcal{H}_{edge}$ and falls within the range $[0, 1]$. However, it doesn't consider certain desirable properties of a reasonable homophily measure, such as variations in node degrees.
Adjusted Homophily	$\mathcal{H}_{adj} = \frac{\mathcal{H}_{edge} - \sum_{c=1}^{C} \left(\sum_{v:y_v=c} |\mathcal{N}(v)|/(2|\mathcal{E}|) \right)^2}{1 - \sum_{c=1}^{C} \left(\sum_{v:y_v=c} |\mathcal{N}(v)|/(2|\mathcal{E}|) \right)^2}$	$\mathcal{H}_{adj}$ is comparable across different datasets with varying numbers of classes and class size balances. In general, $\mathcal{H}_{adj} < \mathcal{H}_{edge}$ holds, and $\mathcal{H}_{adj}$ sometimes take on negative values.
Label Informativeness (LI)	$\text{LI} = \frac{H(y_u) - H(y_u|y_v)}{H(y_u)}$	LI is a straightforward graph characteristic that is suitable for comparing different datasets.

use cases, and we aim to discuss several characteristics of these metrics.

For one thing, although the node homophily $\mathcal{H}_{node}$ and edge homophily $\mathcal{H}_{edge}$ are intuitive, they are relatively sensitive to the number of classes and the balance between these classes. This can make them difficult to interpret and render them incomparable across different datasets. For example, suppose that each node in a graph is connected to one node of each class. Then, both edge homophily and node homophily for this graph will be equal to $1/C$. As a result, these metrics will produce widely different values for graphs with different numbers of classes, despite these graphs being similar in exhibiting no homophily.

For another thing, class homophily does not account for variations in node degrees when correcting the fraction of intra-class edges by its expected value. Specifically, if nodes of class c have, on average, larger degrees than $2|\mathcal{E}|/|\mathcal{V}|$, then the probability that a random edge goes to that class can be significantly larger than $n_c/|\mathcal{V}|$. Secondly, class homophily only considers positive deviations from $n_c/|\mathcal{V}|$, meaning that it doesn't take into account classes with heterophilic connectivity patterns.

As advised by [35], $\mathcal{H}_{adj}$ is a better alternative to the commonly used measures, as it satisfies most of the desirable properties. Additionally, this research also suggests another measure called "label informativeness (LI)", which allows one to further distinguish different types of heterophily.

Remark. Node homophily $\mathcal{H}_{node}$ and edge homophily $\mathcal{H}_{edge}$ are still popular measurement methods among recent works.

2.5 Mainstream Heterophily Learning Task

The main objective learning task of heterophily GNNs is *semi-supervised node classification*. In this task, we have a training graph $\mathcal{G} = (\mathbf{X}, \mathbf{A}, \mathbf{Y})$, where $\mathbf{X} \in \mathbb{R}^{N \times d}$ denotes N nodes with d-dimensional features, and $\mathbf{A} \in \mathbb{R}^{N \times N}$ denotes the adjacency matrix indicating the edge connection. Assuming each node v belongs to one out of C classes, only a part of nodes are provided with labels as $y_v \in \mathcal{Y}_L = \{1, \cdots, C\}$ in the training node set. The goal of the task is to predict the classes of nodes whose labels are not given.

Concretely, given a heterophily GNN model parameterized by $\boldsymbol{\theta}$, denoting as $\text{GNN}_{\boldsymbol{\theta}}(\cdot)$. For semi-supervised node class classification task, the cross-entropy loss is minimized to learn the optimal GNN parameters $\boldsymbol{\theta}$ over all labeled nodes as:

$$\min_{\boldsymbol{\theta}} \mathcal{L}_{\text{cross-entropy}} \left(\hat{\mathbf{Y}}, \mathbf{Y} \right), \text{ where } \hat{\mathbf{Y}} = \text{GNN}_{\boldsymbol{\theta}}(\mathbf{X}, \mathbf{A}). \quad (9)$$

where $\hat{\mathbf{Y}} \in \mathcal{Y}_L = \{1, \cdots, C\}$ denotes GNN predicted node labels and $\mathbf{Y}$ is the ground-truth node labels.

3 GNNs WITH HETEROPHILY: FRAMEWORK AND TAXONOMY

In this section, we provide a unified framework of heterophilic GNNs, and further categorize it from the lens of the message passing mechanism.

3.1 Framework of heterophilic GNNs

Following the general message passing principle for GNN model design, heterophilic GNNs focus on customizing the neighborhood aggregation and feature update schemes that specifically model the heterophily property. In contrast to homophilic GNNs, heterophilic GNNs exhibit distinct characteristics in three key design principles:

P1: Non-locality of Neighbor Sets: Incorporating information from non-local neighbors that may share the same class label as the central node;

P2: Class Distinguishability: Ensuring the aggregation process to effectively distinguish the class labels from both local and non-local neighbors;

P3: Depth Fusion of Multi-layer Information: Integrating hierarchical messages from different inter layers of GNNs for capturing comprehensive heterophily property.

3.2 Taxonomy of GNNs with Heterophily

According to the above three-fold design principles in heterophily instructed neighbor aggregation and feature updating, heterophilic GNNs can be categorized into three groups, including:

(1) Non-local neighbor extension methods ← **P1**.

(2) GNN architecture refinement methods ← **P2 & P3**.

(3) Hybrid methods ← **P1, P2 & P3**.

More fine-grained categorizations of these methods are briefly discussed below and shown in Fig. 2.

Non-Local Neighbor Extension Methods attempt to improve node representation by incorporating higher-order neighbor nodes that share labels during the message-passing process. This kind of methods break the locality limitations of $\mathcal{N}(v)$ in Eq. (1) by reconstructing the non-local neighbor set from two perspectives: high-order neighbor mixing and potential neighbor discovery. Specifically, these methods focus on discovering appropriate neighbors from multi-hops nodes and redefining neighbor sets as
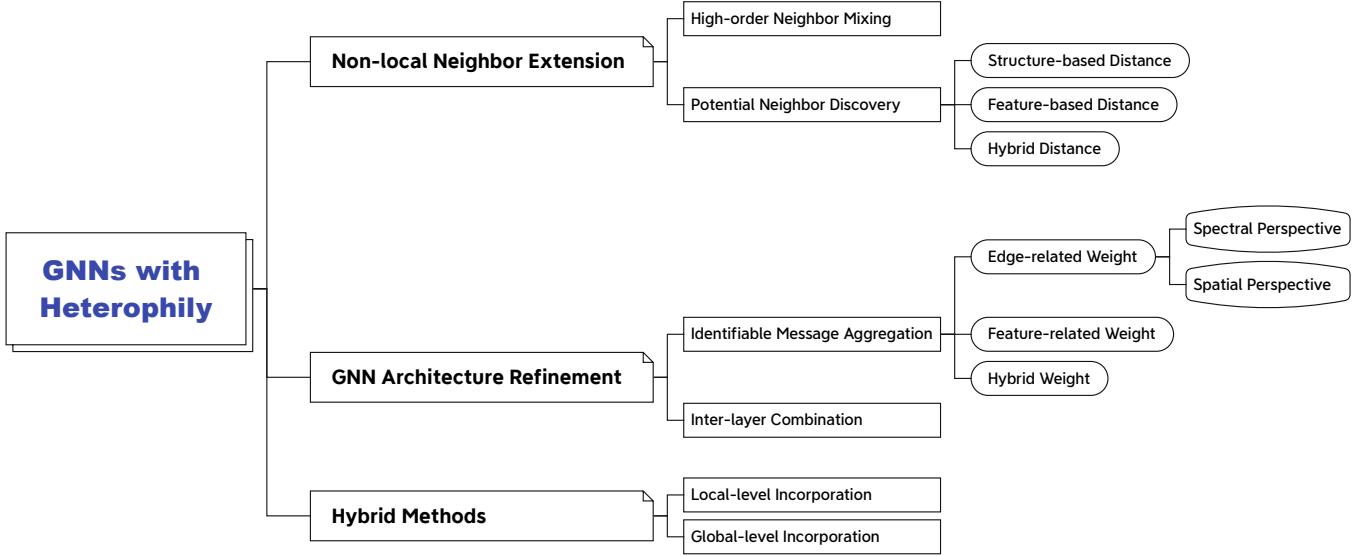
Fig. 2: Categorization of Heterophily GNNs.

$\mathcal{N}_p(v) = \{u : \mathrm{dist}(u, v) \leq p\}$ in the message aggregation stage in Eq. (1), where $\mathrm{dist}(u, v)$ denotes the distance method to measure the distance between nodes u and v. p is a threshold to limit the number of neighbors. In particular, $\mathcal{N}_p(v)$ can be degenerated into $\mathcal{N}(v)$ when the metric function $\mathrm{dist}(\cdot)$ is the shortest distance and $p = 1$.

GNN Architecture Refinement Methods boost the expressive ability of GNNs by facilitating message passing that distinguishes between similar and dissimilar neighbors or by deeply fusing multi-layer information. Specifically, focusing on the crafted architecture design of message aggregation and feature updates, these methods are categorized into identifiable message aggregation methods and inter-layer combination methods. Among these, identifiable message aggregation methods have gained significant attention. Their objective is to allocate appropriate weights in the message aggregation process, aiming to strengthen the fusion of homophilic information while mitigating the fusion of heterophilic information. With a focus on weight assignment schemes from various perspectives, existing methods can be further classified into three types: edge-related weight, feature-related weight, and hybrid weight.

Hybrid Methods can be taken as the combination of non-local neighbor extension methods and GNNs architecture refinement methods. Typically, hybrid methods first construct an appropriate neighbor set through non-local neighbor extension, and then refine the GNN architectures from two perspectives: (1) local-level incorporation, that focuses on intra-layer heterophily-guided message passing, and (2) global-level incorporation, that enhances effective inter-layer heterophily information transfer throughout the entire GNN architecture.

Discussion. Different heterophilic GNNs exhibit distinct properties. The fundamental concept of non-local neighbor extension methods is quite straightforward and simple to implement, as it directly models and captures the similarity relationships between nodes to enhance the homophily of local neighborhoods; however, for large-scale graphs, it can be memory-intensive to traverse the entire graph in order to model the similarity between each pair of nodes. GNN architecture refinement methods focus on mitigating

the impact of local heterophilic information during the message passing process. This primarily involves further refinement of message aggregation and feature updates for the heterophilic design. However, the challenge lies in how to customize the heterophilic message passing mechanism with only a limited number of observable homophilic or heterophilic relationships. Hybrid methods combine the advantages of both non-local neighbor extension and GNN architecture refinement. Nevertheless, a major challenge is devising a strategy for seamlessly integrating these approaches into the message-passing process.

4 HETEROPHILIC GNNS WITH NON-LOCAL NEIGHBOR EXTENSION

Under the uniform message passing framework of homophilic GNNs, the neighborhood is usually defined as the set of all neighbors one-hop away (*e.g.*, GCN), which means only messages from proximal nodes in a graph are aggregated. However, such a local neighborhood definition might not be appropriate for heterophilic graphs, where nodes belonging to the same class exhibit high structural similarity but can be farther away from each other. In light of these, current heterophilic GNNs attempt to extend the local neighbors to non-local ones primarily through two schemes: *high-order neighbor mixing* and *potential neighbor discovery*. As a result, the representation ability of heterophilic GNNs can be improved significantly by capturing the important features from distant and informative nodes. The pipelines of two example methods are given in Fig. 3, and a summary of the non-local neighbor extension works is illustrated in Table 2.

4.1 High-order Neighbor Mixing

Higher-order neighbor mixing allows the ego node to receive latent representations from their local one-hop neighbors and from further k-hop neighbors, so that the heterophilic GNNs can mix latent information from neighbors at various distances. Formally, the k-hop neighbor set is defined as

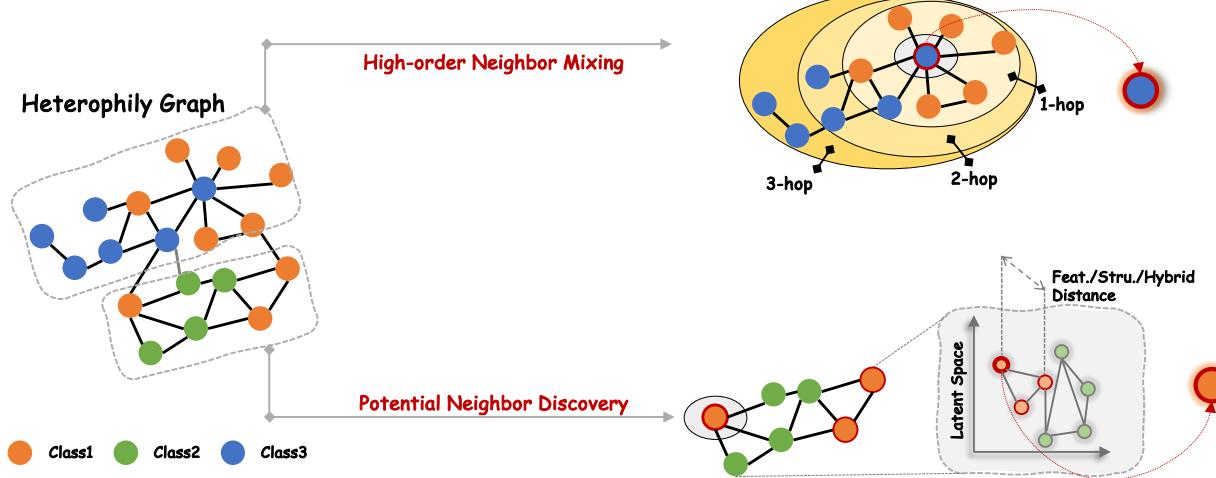$$\mathcal{N}_k(v) = \{u : \mathrm{dist}(u, v) = k\}, \tag{10}$$

Fig. 3: Schematic diagram of high-order neighbor mixing method and potential neighbor discovery method.

where $\mathrm{dist}(u,v)$ measures the shortest distance between nodes u and v. In addition, how to mix the information from the different k-hop neighbor sets is an important research point of higher-order neighbor mixing methods.

Typically, MixHop [36] is a representative method that aggregates messages from multi-hop neighbors. Apart from one-hop neighbors, MixHop also considers two-hop neighbors for message propagation. After that, the messages acquired from different hops are encoded by different linear transformations and then mixed by concatenation. The l-th layer MixHop for each node $v \in \mathcal{V}$ can be described as

$$
\begin{aligned}
\mathbf{m}_{v,k}^{(l)} &= \mathrm{AGGREGATE}^{(l)}(\{\mathbf{h}_u^{(l-1)} : u \in \mathcal{N}_k(v)\}), \\
\mathbf{h}_{v,k}^{(l)} &= \mathrm{UPDATE}^{(l)}(\mathbf{h}_v^{(l-1)}, \mathbf{m}_{v,k}^{(l)}), \\
\mathbf{h}_v^{(l)} &= \|_{k=2}\mathbf{h}_{v,k}^{(l)},
\end{aligned}
\tag{11}
$$

where $\|$ means column-wise combination. It can be noted that cross-level information fusion of MixHop is performed after the feature aggregation and updating among the same hop neighbors.

Another perspective for cross-level information fusion is to merge cross-hop neighbors before the feature aggregation stage, and then aggregate and update multi-hop neighbors' features simultaneously. The most representative method is TDGNN [37], which uses a tree decomposition method to disentangle neighborhood information in different layers and focus on adjusting the aggregation stage in Eq. (1) to promote information fusion among different layers, modeled as

$$
\mathbf{m}_v^{(l)} = \mathrm{AGGREGATE}^{(l)}(\{\mathbf{h}_u^{(l-1)} : u \in \bigcup_{k=1}^{K} \mathcal{N}_k(v)\}), \tag{12}
$$

where K is the highest-hop setting the collection neighbor sets.

Recently, Ordered GNN [38] proposes to order the messages passing into the node representation, with specific blocks of neurons targeted for message passing within specific hops. This is achieved by aligning the hierarchy of the rooted-tree of a central node with the ordered neurons in its node representation. Based on simple design in the spectral domain, EvenNet [39] discards messages from odd-order neighbors inspired by balance theory, deriving a graph filter with only even-order terms, which can be generalized to graphs of different homophily.

In summary, the high-order neighbor mixing methods straightforwardly include higher-order neighbors in local neighbor sets and devise an appropriate combination scheme to effectively integrate multi-order neighborhood information. Its objective is to alleviate the impact of local heterophily by incorporating richer homophilic information from higher-order neighborhoods.

4.2 Potential Neighbor Discovery

Compared to high-order neighbor mixing methods directly utilizing the inherent structural information from graphs, potential neighbor discovery methods reconsider the definition of neighbors in heterophilic graphs and build innovative structural neighbors through the entire topology exploration with heterophily. Apart from the original neighbor set, these methods construct a new potential neighbor set that can be further formalized as

$$
\mathcal{N}_\rho(v) = \{u : \mathrm{dist}(v,u) < \rho\}, \tag{13}
$$

where $\mathrm{dist}(u,v)$ is a metric function that measures the distance between nodes u and v in a specifically defined latent space and ρ is a threshold to limit the number of neighbors. It is evident that distance measurement plays a pivotal role in identifying suitable potential neighbors. Current methods can be categorized into three main types based on the focal variables of distance measurement: structure-based distance, feature-based distance, and hybrid distance.

4.2.1 Structure-based Distance

Structure-based distance methods typically search for potential neighbors that meet measurement criteria within the geometric relationship latent space, which is defined by prior information about the graph topology. Typically, Geom-GCN [34] maps the input graph to a continuous latent space and defines the geometric relationships, *i.e.*, split 2D Euclidean geometry locations, as the criteria to discover potential neighbors. Apart from inherent neighbors in original input graphs, neighbors that conform to the defined geometric relationships also participate in the message aggregation of GCN. Specifically, based on the graph and latent space, a structural neighborhood is built as $(\{\mathcal{N}(v), \mathcal{N}_\rho(v)\}, \tau)$ underlying the relational operator τ, where $\mathcal{N}(v)$ is the set of adjacent nodes of v in the graph, $\mathcal{N}_\rho(v)$ is the set of potential

TABLE 2: Summary of non-local neighbor extension methods. 'Structure-based Distance', 'Feature-based Distance', and 'Hybrid Distance' take the structure-based scheme, feature-based scheme, and hybrid scheme as the distance metric for potential neighbor discovery, respectively.

Publication Year and Venue	Method	Neighbor Range	Distance Measurement
High-Order Neighbors Mixing			
[2019 ICML]	MixHop [36]	2-Hops	Shortest Distance
[2021 CIKM]	TDGNN [37]	Multi-Hops	Shortest Distance
[2022 NeurIPS]	EvenNet [39]	Odd-Hops	Shortest Distance
[2023 ICLR]	Ordered GNN [38]	Multi-Hops	Shortest Distance
[2024 ICLR]	MPformer [43]	Multi-Hops	Shortest Distance
Potential Neighbors Discovery			
[2020 ICLR]	Geom-GCN [34]	Multi-Hops	Structure-based Distance
[2021 WSDM]	SimP-GCN [41]	Multi-Hops	Feature-based Distance
[2022 AAAI]	HOG-GNN [44]	2-Hops	Hybrid Distance
[2022 ICML]	GloGNN [45]	Multi-Hops	Hybrid Distance
[2022 NeurIPS]	Diag-NSD [46]	Multi-Hops	Feature-based Distance
[2023 TNNLS]	HES-GSL [42]	Multi-Hops	Feature-based Distance
[2023 WWW]	SE-GSL [47]	Multi-Hops	Hybrid Distance
[2023 ICML]	GOAL [21]	Multi-Hops	Hybrid Distance
[2023 ICASSP]	GraphTU [48]	Multi-Hops	Hybrid Distance
[2023 CVPR]	HopGNN [49]	Multi-Hops	Feature-based Distance
High-Order Neighbors Mixing & Potential Neighbors Discovery			
[2021 NeurIPS]	U-GCN [40]	2-Hops	Feature-based Distance

neighbors from which the distance to v is less than a pre-given parameter ρ in the latent space, described as

$$\mathcal{N}_\rho(v) = \{u : \|\mathbf{h}_u - \mathbf{h}_v\|_2 < \rho\}, \tag{14}$$

where $\mathbf{h}_u$ and $\mathbf{h}_v$ are the representations for nodes u and v. $\|\cdot\|_2$ is the Euclidean norm to measure relative positions between two nodes. ρ is determined from zero until the average cardinality of $\mathcal{N}_s(v)$ equals that of $\mathcal{N}(v)$, $\forall v \in \mathcal{V}$, that is, when the average neighborhood sizes in the graph and latent spaces are the same.

4.2.2 Feature-based Distance

Different from the structure-based distance methods that use structural information to determine potential neighbor nodes, feature-based distance methods determine connection relationships based on feature similarity. For instance, U-GCN [40] and SimP-GCN [41] choose top k similar node pairs in terms of feature-level cosine similarity for each ego node to construct the neighbor set through the kNN algorithm. The potential neighbor set for this method can be built as

$$\mathcal{N}_K(v) = \{u : \text{TopK}(\text{Cos}(\mathbf{h}_u, \mathbf{h}_v), K)\}, \tag{15}$$

where $\text{Cos}(\cdot, \cdot)$ is usually defined the cosine similarity function, K is the number of nearest neighbors set manually, $\text{TopK}(\cdot)$ denotes a pooling operation for discovering potential neighbors with K highest similarity. The recent work HES-GSL [42] still determines relationships of node pairs through cosine similarity, and further designs homophily-enhanced self-supervision to provide more supervision for similarity learning.

4.2.3 Hybrid Distance

Recent works increasingly emphasize the comprehensive consideration of structural and node feature information in potential neighbor discovery. These methods focus more on the potential message passing among global homophily neighbors in the graph.

Typically, HOG-GCN [44] and GloGNN [45] design similarity calculation modules to capture the correlations between global nodes through both topological and attribute information. Specifically, HOG-GCN constructs a homophily degree matrix with the label propagation technique to explore the extent to which a pair of nodes belong to the same class in the entire heterophilic graph from the perspective of topology space. By involving the class-aware information during the propagation process, intra-class nodes with higher heterophily (i.e., lower homophily degree) would contribute more to the neighbor aggregation than underlying inter-class nodes. More simplified than HOG-GCN, GloGNN directly measures potential correlations between global nodes in terms of both feature attribute similarity and topology similarity by further regularizing node representations with nodes' multi-hop reachabilities. In general, the potential neighbors set can be defined as

$$\mathcal{N}(v) = \mathcal{N}_T(v) \cap \mathcal{N}_S(v), \tag{16}$$

where $\mathcal{N}_T(v) = \{u : \tilde{\mathbf{h}}_u \tilde{\mathbf{h}}_v^\mathsf{T} \neq 0\}$ and $\mathcal{N}_S(v) = \{u : \hat{\mathbf{h}}_u \hat{\mathbf{h}}_v^\mathsf{T} < \rho\}$ are potential neighbor sets defined by measuring node correlations in terms of topology similarity and feature similarity, $\cap$ is the intersection operation, and $\tilde{\mathbf{h}}_u$ and $\hat{\mathbf{h}}_u$ are representations of node u through topology structure information (i.e., $\mathbf{A}$) and node attribute information (i.e., $\mathbf{X}$), respectively.

Furthermore, SE-GSL [47] offers an effective measure of the information embedded in an arbitrary graph and structural diversity (where $\mathcal{N}_T(v)$ is characterized by both the kNN structure and the original topology structure) and presents a novel sampling-based mechanism for restoring the graph structure via node structural entropy distribution. It increases the connectivity among nodes with larger uncertainty in lower-level communities. GraphTU [48] offers a probabilistic approach to exploring potential neighbors. A key observation in this research is that the statistical variances based features and topology information within local neighborhoods can be effectively harnessed to extend the

TABLE 3: Summary of GNN architecture refinement methods. 'Feature-Related', 'Edge-Related' and 'Hybrid' respectively represent weight assignment schemes that work on node feature, edges, and both of them for adaptive message aggregation. '✓' and '✗' indicate whether to include the according schemes, respectively.

Publication Year and Venue	Method	Weight Assignment	Ego-Neighbor Separation	Combination Function
Identifiable Message Aggregation				
[2021 AAAI]	FAGCN [25]	Edge-Related	✗	✗
[2021 NeurIPS]	DMP [29]	Edge-Related	✗	✗
[2021 AAAI]	CPGNN [23]	Feature-Related	✗	✗
[2021 ICDM]	CGCN [28]	Feature-Related	✓	✗
[2022 ICLR]	ACM [50]	Edge-Related	✗	✗
[2022 WWW]	GBK-GNN [51]	Feature-Related	✗	✗
[2022 WWW]	F2GNN [52]	Edge-Related	✗	✗
[2022 WWW]	MWGNN [53]	Hybrid	✗	✗
[2022 ICASSP]	MMP [54]	Feature-Related	✓	✗
[2022 ICML]	GIND [55]	Feature-Related	✓	✗
[2022 NeurIPS]	ASGC [56]	Edge-Related	✗	✗
[2022 LoG]	GESN [57]	✗	✓	✗
[2022 TNNLS]	NCGNN [58]	Feature-Related	✗	✗
[2022 TNNLS]	GDAMN [59]	Edge-Related	✗	✗
[2023 TNNLS]	CGP [60]	Edge-Related	✗	✗
[2023 TNNLS]	RFA-GNN [61]	Edge-Related	✗	✗
[2023 TKDE]	AutoGCN [62]	Edge-Related	✗	✗
[2023 ICML]	GOAT [63]	Edge-Related	✗	✗
[2023 WWW]	Mid-GCN [64]	Edge-Related	✗	✗
[2023 NeurIPS]	TEDGCN [65]	Edge-Related	✗	✗
[2023 NeurIPS]	LRGNN [66]	Edge-Related	✗	✗
Inter-Layer Combination				
[2018 ICML]	JK-Net [67]	✗	✗	Skip Connections
[2020 ICLR]	GPR-GNN [30]	✗	✗	Adaptive Connections
[2022 NeurIPS]	PowerEmbed [68]	✗	✗	Skip Connections
Identifiable Message Aggregation & Inter-Layer Combination				
[2022 LoG]	LW-GCN [69]	Hybrid	✓	Adaptive Connections
[2023 TNNLS]	CAGNNs [70]	✗	✓	Adaptive Connections

training distribution, creating novel potential neighbor sets through a non-parametric method. This approach is particularly valuable for addressing heterophily within the entire graph, especially in the case of minor class nodes. To reveal attribute relationships among nodes in the entire graph, GOAL [21] augments the existing graph by constructing a fully connected graph through a graph completion process. This augmentation considers two modes: homophilic connections and heterophilic connections. An important aspect involves developing a method to distinguish between connections that reflect a tendency for homophily and those that indicate heterophily. This distinction is made based on the Connected Structure Difference (CSD) computed between connected node pairs and randomly selected node pairs, ultimately facilitating the optimization of the complemented graph.

In summary, potential neighbor discovery methods focus on identifying homophilic neighbors among high-order neighbors and incorporating them into local neighbor sets to enhance homophilic message-passing. By measuring the similarity of node features with different distance calculation schemes, potential neighbor discovery methods are able to effectively identify potential homophilic neighbors that share the same class labels.

5 HETEROPHILIC GNN ARCHITECTURE REFINEMENT

General GNN architectures in Eq. (1) contain two essential components: the aggregation function AGGREGATE(·) to integrate

information from the discovered neighbors, and the update function UPDATE(·) to combine the learned neighbor messages with the initial ego representation. Given the original local neighbors and the extended non-local neighbors on heterophilic graphs, existing GNN architecture refinement methods contribute to fully exploiting the neighbor information from the following aspects by accordingly revising AGGREGATE(·) and UPDATE(·): (1) *Identifiable message aggregation* discriminates and enhances the messages of similar neighbors from dissimilar ones; (2) *Inter-layer combination* emphasizes the effect of different propagation ranges (*i.e.*, the number of GNN layers) on node representation learning. All these two aspects come to the same destination: boosting the expressive ability of GNNs for heterophilic graphs by encouraging distinguishable and discriminative node representations.

5.1 Identifiable Message Aggregation

Given the neighbors to be aggregated, the key of integrating beneficial messages on heterophilic graphs is distinguishing the information of similar neighbors (likely in the same class) from that of dissimilar neighbors (likely in different classes). To make node representations on heterophilic graphs more discriminative, identifiable message aggregation methods alter the aggregation operation AGGREGATE(·) by imposing adaptive edge-aware weights $a_{uv}^{(l)}$ for node pair (u, v) at the l-th layer as:

$$\mathbf{m}_v^{(l)} = \text{AGGREGATE}^{(l)}(\{a_{uv}^{(l)} \mathbf{h}_u^{(l-1)} : u \in \mathcal{N}(v)\}). \quad (17)$$
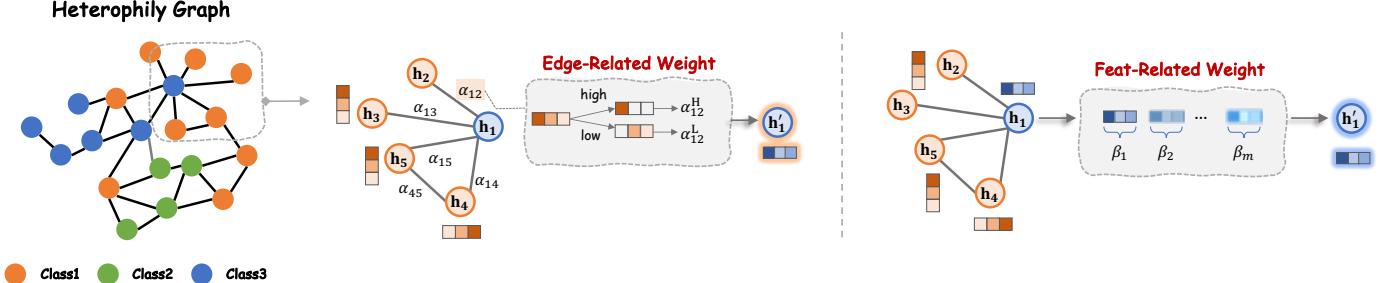
Fig. 4: Illustration of identifiable message passing with edge-related weight and feature-related weight assignment schemes in GNN architecture refinement methods.

In this way, different methods develop various weight assignment schemes for $a_{uv}^{(l)}$ to model the importance of similar and dissimilar neighbors during aggregation. In the following, we provide the details of weight assignment schemes adopted by existing methods, which respectively work on node *feature* and *edge* related weights. Fig. 4 provides the pipelines of two weight assignment schemes.

5.1.1 Edge-Related Weight

In general, edge-related methods simultaneously focus on *spectral* domain and the *spatial* domain. To be concrete, spectral GNNs leverage the theory of graph signal processing to design graph filters, and spatial GNNs focus on the graph structural topology to develop aggregation strategies.

Spectral Perspective. In contrast to Laplacian smoothing [71] and low-pass filtering [72] to approximate graph Fourier transformation on homophilic graphs, spectral GNNs on heterophilic graphs involve both low-pass and high-pass filters to adaptively extract low-frequency and high-frequency graph signals. The essential intuition behind this lies in that low-pass filters mainly retain the commonality of node features, while high-pass filters capture the difference between nodes.

Typically, FAGCN [25] adopts a self-gating attention mechanism to learn the proportion of low-frequency and high-frequency signals by splitting the $a_{uv}^{(l)}$ into two components, *i.e.*, $a_{uv}^{(l,LP)}$ and $a_{uv}^{(l,HP)}$, corresponding to low-pass and high-pass filters, respectively. Through adaptive frequency signal learning, FAGCN could achieve expressive performance on different types of graphs with homophily and heterophily. Formally, adaptive edge-aware weights $a_{uv}^{(l)}$ are defined in FAGCN as

$$a_{uv}^{(l)} = \frac{a_{uv}^{(l,LP)} - a_{uv}^{(l,HP)}}{\sqrt{d_u d_v}}, \tag{18}$$

where d_u and d_v respectively denote the degree of node u and v, $a_{uv}^{(l,LP)} - a_{uv}^{(l,HP)}$ is the coefficient learned through a shared self-gating mechanism $\tanh\left(\mathbf{q}^{\mathsf{T}}[\mathbf{h}_u; \mathbf{h}_v]\right)$, from which $[;]$ denotes the concatenation operation, $\mathbf{g}$ can be seen as a shared convolutional kernel, $\tanh(\cdot)$ is the hyperbolic tangent function, which can naturally limits the value of $a_{uv}^{(l,LP)} - a_{uv}^{(l,HP)}$ in $[-1, 1]$. In a similar fashion, RFA-GNN [61] captures edge-aware weights using a relation-based frequency adaptive mechanism. This mechanism takes into account higher-order contextual information compared to FAGCN. It precisely defines edge-aware weights for a specific relation. Specifically, the edge-aware weight of $(l + 1)$-order information between nodes u and v for relation k is described as $a_{uvk}^{(l)} = \tanh(\mathbf{q}_{lk}^{\mathsf{T}}[\mathbf{h}_{uk}^{(l)}; \mathbf{h}_{vk}^{(l)}])$, where $\mathbf{q}_{lk}$ is the attention coefficient for relation k in the l-th iteration.

Apart from low-pass and high-pass filters, ACM [50] further involve the identity filter, which is the linear combination of low-pass and high-pass filters, i.e.,

$$a_{uv}^{(l)} = \text{Softmax}\left(([a_{uv}^{(l,LP)}, a_{uv}^{(l,IP)}, a_{uv}^{(l,HP)}]/\tau)\mathbf{W}_{uv}^{(l)}\right), \tag{19}$$

where τ indicates a temperature parameter and $\mathbf{W}_{uv}^{(l)} \in \mathbb{R}^{1\times 3}$ is used to learn which filters is important or not for each node. $a_{uv}^{(l,LP)}$, $a_{uv}^{(l,IP)}$ and $a_{uv}^{(l,HP)}$ respectively denotes low-pass, identity and high-pass edge-aware weights, which learn from 3 channels features. AutoGCN [62] captures the full spectrum of graph signals and automatically update the bandwidth of graph convolutional filters. In addition, Mid-GCN [64] contains a mid-pass filter determined by both low-pass and high-pass filters. The robustness of signals passing through this mid-pass filter is theoretically guaranteed by their analyses.

In this way, ACM, AutoGCN and Mid-GCN could adaptively exploit beneficial neighbor information from different filter channels for each node; Meanwhile, their identity or mid-pass filters could guarantee less information loss of the input signal.

Spatial Perspective. Heterophilic GNNs in the spatial domain require the diverse topology-based aggregation of neighbors from the same or different classes guided by the heterophily. Therefore, the edge-aware weights of neighbors should be assigned according to the spatial graph topology and node labels. Taking node attributes as weak labels, DMP method [29] considers node attribute heterophily for diverse message passing and specifies every attribute propagation weight on each edge. Furthermore, instead of the scalar weight $a_{uv}^{(l)}$ that aggregates all the node attributes with the same weight at the node level, DMP extends the weight to a vector $\mathbf{a}_{uv}^{(l)}$ through operating in the attribute dimension, and this vector can be calculated by either relaxing GAT [9] weights to real values or allowing an element-wise average of neighbor weights.

Moreover, certain methods learn edge-aware weights based on node labels. For instance, Chen et al. [59] introduce the concept of graph decoupling attention Markov networks (GDAMNs). This approach incorporates variational inference to model edge uncertainty and employs both hard and soft attention mechanisms on node labels to improve the learning of edge-aware weights, represented as

$$a_{uv}^{(l)} = \frac{a_{uv}^{\text{hard}} \exp \delta_{uv}^{(l-1)}}{\sum_{v=1}^{N} a_{uv}^{\text{hard}} \exp \delta_{uv}^{(l-1)}}, \tag{20}$$

where $a_{uv}^{\text{hard}} = \mathbf{A}_{uv} \cdot \tilde{\mathbf{y}}^{\mathsf{T}} w_{uv} \tilde{\mathbf{y}}$ is the hard attention with label similarity and $\delta_{uv}^{(l-1)} = -\text{Cos}(\mathbf{h}_u^{(l-1)}, \mathbf{h}_v^{(l-1)})$ denotes the soft

attention with feature dissimilarity. In general, the hard attention is learned on labels for a refined graph structure with fewer inter-class edges so that the aggregation's negative disturbance can be reduced. The soft attention aims to learn the aggregation weights based on features over the refined graph structure to enhance information gains during message passing.

Recent research has shown a growing interest in the efficiency of computing edge-aware weights for large-scale graphs. CGP [60] introduces a graph pruning paradigm during training, enabling the discovery of high-performing sparse GNNs within a single training process. Additionally, a global graph transformer model has been proposed for large-scale heterophilic node classification tasks, known as GOAT [63]. GOAT samples potential neighbors for each node from its k-hop neighbors. To distinguish between neighbors based on topology information during the propagation process, GOAT further incorporates a global attention module designed to learn attention scores between potential neighbors and source nodes.

5.1.2   Feature-Related Weight

Apart from the adaptive edge-aware weight learning, there is another solution working on the neighbor representation learning by revising $\mathbf{h}_u^{(l-1)}$ in $\mathrm{AGGREGATE}^{(l)}(\{a_{uv}^{(l)}\mathbf{h}_u^{(l-1)} : u \in \mathcal{N}(v)\})$. Conventionally, the above-mentioned methods mainly utilize the contextual node representations of neighbors; In contrast, this solution transforms contextual node embeddings $\mathbf{h}_u^{(l-1)}$ to other node-level properties that reflect the heterophily. In this way, heterophilic GNNs learn node-level attention $\beta_v^{(l)}$, which is shared with each $u \in \mathcal{N}(v)$, to capture the beneficial information of heterophily for distinguishable node representation learning. As a result, the aggregation progress can be redefined as $\mathrm{AGGREGATE}^{(l)}(\{\beta_v^{(l)}\mathbf{h}_u^{(l-1)} : u \in \mathcal{N}(v)\})$. Existing methods mainly learn $\beta_v^{(l)}$ through two schemes based on homophily/heterophily prior knowledge and homophily attributes attention.

Prior-Based. The prior-based method considers the incorporation of homophily/heterophily prior knowledge in the process of feature transformation, primarily estimating the assignment weight $\beta_v^{(l)}$ through class information. Typically, instead of propagating original node feature representations, CPGNN [23] propagates a prior belief estimation based on a compatibility matrix, so that it can capture both heterophily and homophily by modeling the likelihood of connections between nodes in different classes. The feature-aware weight of embeddings $\mathbf{h}_v^{(l-1)}$ with prior belief is defined as

$$\beta_v^{(l)} = \text{Sinkhorn-Knopp}(y_v, \mathbf{A}_v, \mathbf{B}_v), \qquad (21)$$

where Sinkhorn-Knopp denotes the Sinkhorn-Knopp algorithm proposed in [73], which is to ensure that $\beta_v^{(l)}$ is doubly stochastic. $\mathbf{B}_v$ denotes an enhanced belief matrix for node v, depending on a training mask matrix and a prior belief. Going beyond the uniform GCN aggregation, NLGNN [74] and GPNN [75] consider the sequential aggregation where the neighbors are ranked based on the class similarity (*i.e.*, a homophily/heterophily prior belief) in order. A regular 1D-convolution layer is applied to extract the affinities between the sequential nodes whether the nodes are close or distant in heterophilic graphs. GIND [55] extends the linear isotropic diffusion to a more expressive nonlinear diffusion mechanism, which learns nonlinear flux features between node pairs before aggregation. This design of the nonlinear diffusion

ensures that more information can be aggregated from similar neighbors and less from dissimilar neighbors by learning $\beta_v^{(l)}$, making node features less likely to over-smooth.

Attention-Based. The majority of research focuses on developing diverse attention mechanisms for learning $\beta_v^{(l)}$. A straightforward approach involves learning attribute similarity and utilizing this similarity to determine attention on node features. CGCN [28] uses the cosine similarity to send signed neighbor features under certain constraints of relative node degrees. In this way, the messages are allowed to be optionally multiplied by a negative sign or a positive sign, *i.e.*, for node v, its message is described as

$$\begin{aligned}
\mathbf{h}_v^{(l+1)} = \sigma \Big(&\beta_0^{(l)}\tilde{\mathbf{h}}_v^{(l)} + \beta_1^{(l)}(\mathbf{s}_{\mathsf{v,pos}}^{(l)} \odot \mathbf{A}_v^{(l)})\tilde{\mathbf{h}}_v^{(l)} \\
&+ \beta_2^{(l)}(\mathbf{s}_{\mathsf{v,neg}}^{(l)} \odot \mathbf{A}_v^{(l)})\tilde{\mathbf{h}}_v^{(l)} \Big),
\end{aligned} \qquad (22)$$

where $\beta_0^{(l)}$, $\beta_1^{(l)}$, and $\beta_2^{(l)}$ are the l-th layer learned scalars. $\mathbf{s}_{\mathsf{u,pos}}^{(l)}$ and $\mathbf{s}_{\mathsf{u,neg}}^{(l)}$ respectively indicate positive matrix and negative matrix, which are split from the matrix with sign information. Intuitively, signed messages consist of the negated messages sent by neighbors of the opposing classes, and the positive messages sent by neighbors of the same class. Similarly, Du et al. [51] propose a method for defining positive and negative correlation weights when modeling the similarity and dissimilarity between node features. They introduce a novel GNN model called GBK-GNN, which is based on a bi-kernel feature transformation and a selection gate. The two kernels capture homophily and heterophily information, and the gate is used to determine which kernel should be applied to a specific pair of nodes. Formally, the gate signal is described as $\beta_v^{(l)} = \sum_{u \in \mathcal{N}(v)} \text{Sigmoid}\left(\text{MLP}(\mathbf{h}_v^{(l-1)}, \mathbf{h}_u^{(l-1)}; \mathbf{W}_v^{(l-1)})\right)$, where $\text{MLP}(\cdot)$ is a multilayer perceptron. MMP [54] decouples the messages into two parts, i.e., memory for propagation and self-embedding for discrimination. The memory for propagation aims to endow each node with a memory cell and sends messages from the memory cell instead of hidden self-embedding. After propagation, each node can leverage a learnable control mechanism to adaptively update its self-embedding and memory cell according to their recent states. CAGNNs [70] investigates the feature aggregation of inter-class edges from an entire neighbor identifiable perspective by a new metric based on von Neumann entropy. Using an importance score $\beta_v^{(l)}$ obtained by a mixer combines discriminant feature and neighbor information, which are decoupled from embedding $\mathbf{h}_v^{(l-1)}$. To overcome the limitations of traditional messaging methods, NCGNN [58] represents nodes as collections of node-level capsules. Each capsule is responsible for extracting distinct features from its associated node. For each node-level capsule, a novel dynamic routing procedure is implemented to intelligently select the most suitable capsules for aggregation from a subgraph identified by the designed graph filter. NCGNN exclusively aggregates advantageous capsules while constraining irrelevant messages to prevent excessive feature mixing among interacting nodes. As a result, this approach mitigates the problem of oversmoothing and enables the learning of effective node representations in graphs characterized by either homophily or heterophily.

5.1.3   Hybrid Weight

Hybrid methods aim to calculate edge weights guided by node features and edge information simultaneously. A typical method
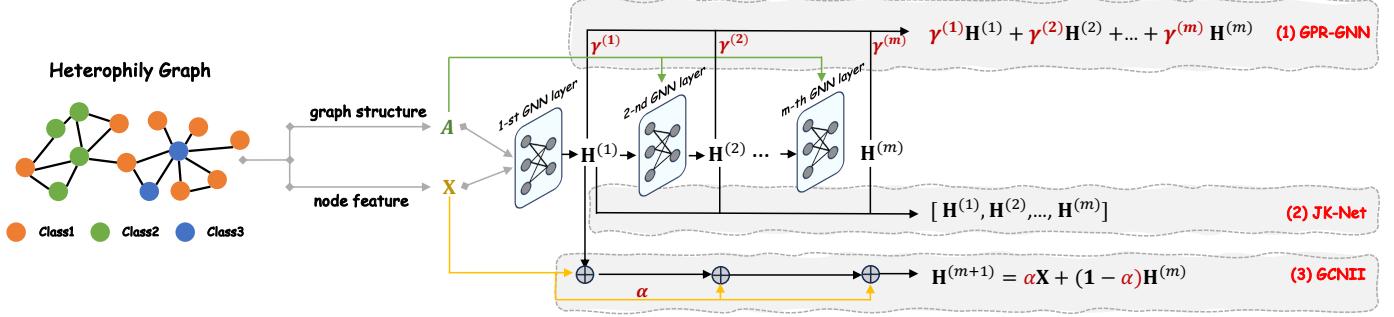
Fig. 5: Illustration of typical inter-layer combination methods: (1) GPR-GNN [30]; (2) JK-Net [67]; and (3) GCNII [76].

is MWGNN [53], which models the node local distribution from node feature, topological structure, and positional identity aspects with the meta-weight. Then, based on the meta-weight, an adaptive graph convolution is derived to conduct node-specific weighted aggregation for boosted node representation learning.

Remark. On heterophilic graphs, an ego node is likely to be dissimilar with its neighbors in terms of class labels. Hence, encoding ego-node representations separately from the aggregated representations of neighbor nodes would benefit distinguishable node embedding learning. In detail, ego-neighbor separation methods detach self-loop connections of the ego nodes in $\mathrm{AGGREGATE}(\cdot)$. Meanwhile, they alter the $\mathrm{UPDATE}(\cdot)$ as the non-mixing operations, *e.g.*, concatenation, instead of the mixing operation, *e.g.*, "average" in vanilla GCN. H2GCN [24] first proposes to exclude the self-loop connection and points out that the non-mixing operations in the update function ensure that expressive node representations would survive over multiple rounds of propagation without becoming prohibitively similar. Besides, WRGNN [77] imposes different mapping functions on the ego-node embedding and its neighbor aggregated messages, while GGCN [28] simplifies the mapping functions to learnable scalar parameters to separately learn ego-neighbor representations. Moreover, ACM [50] adopts the identity filter to separate the ego embedding and then conducts the channel-level combination with its neighbor information in the update function.

5.2 Inter-Layer Combination

Different from identifiable message aggregation methods focusing on the fine-grained intra-layer design of GNN architectures with heterophily, inter-layer combination methods consider layer-wise operations to boost the representation power of heterophilic GNNs. The intuition behind this strategy is that in the shallow layers of GNNs, they collect local information, *e.g.*, one-hop neighbor locality in two-layer vanilla GCN, when the layers go deeper, GNNs gradually capture global information implicitly via multiple rounds of neighbor propagation. Due to the heterophily characteristic, neighbors with similar information, *i.e.*, class labels, might locate in both local geometry and long-term global topology. Hence, combining intermediate representations from each layer contributes to leveraging different neighbor ranges with the consideration of both local and global structural properties, resulting in powerful heterophilic GNNs. Fig. 5 shows the formulation and illustrations of the closely related methods.

The prior idea first comes from JK-Net [67] which flexibly captures better structure-aware representation with different neigh-

borhood ranges. The combination of features among different layers is described as

$$\hat{\mathbf{h}}_v = \mathrm{LA}(\mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \dots, \mathbf{h}^{(L)}), \qquad (23)$$

where $\mathrm{LA}(\cdot)$ denotes the layer aggregation, such as column-wise combination, max pooling, attention with LSTM, etc.

Compared with the methods using all previous intermediate representations, GCNII [76] only integrates the first layer's node embedding at each layer with the initial residual connection, defined as

$$\mathbf{h}_v^{(l)} = \alpha \mathbf{h}_v^{(0)} + \mathrm{AGGREGATE}^{(l)}(\{(1-\alpha)\mathbf{h}_v^{(l-1)} : u \in \mathcal{N}(v)\}), \qquad (24)$$

where α is a hyperparameter that maintains a balance between the node embedding of the first layer and the representation of the current layer.

Instead of using the simple concatenation operation, GPR-GNN [30] further assigns learnable weights to combine the representations of each layer adaptively via the Generalized PageRank (GPR) technique. PowerEmbed [68] employs an inception network to learn the rich representations that interpolate from local message-passing features to global spectral information. Hence, inter-layer combination methods are able to conduct topological feature exploration and benefit from informative multi-round propagation, making node features of heterophilic graphs distinguishable.

6 HYBRID METHODS

Recently, researchers have recognized that simultaneously expanding the non-local neighbor set and refining heterophily-guided GNN architectures, can significantly facilitate heterophilic graph representation learning. Generally, existing hybrid methods can be categorized into two groups: (1) local-level incorporation, which designs intra-layer heterophilic GNN message passing with the neighbor extension; and (2) global-level incorporation, which enhances effective inter-layer information transfer of heterophilic GNNs with the neighbor extension. The diagram of two types of hybrid methods is presented in Fig. 6.

The majority of methods fall into the category of local-level incorporation, typically following a two-step process. First, they establish a graph topology that emphasizes local homophily, and then they design a message aggregation method based on this homophilic topology. For instance, WRGNN [77] employs the degree sequence of neighbor nodes as a metric for measuring structural similarity between ego nodes. This is used to reconstruct a multi-relational graph that captures homophily in relational edges, followed by relational aggregation with explicit
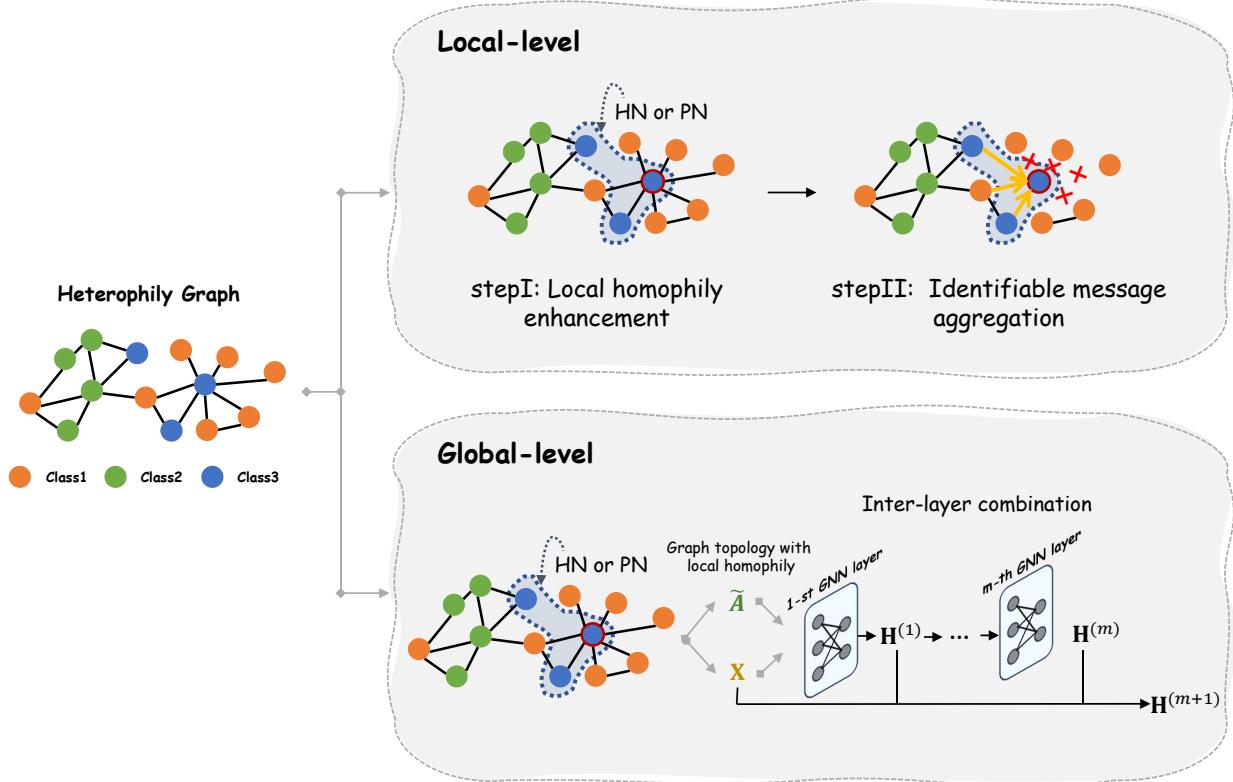
Fig. 6: A diagram of two types of hybrid methods: Local-level incorporation and global-level incorporation.

TABLE 4: Summary of hybrid extension methods. 'HN' and 'PN' mean 'High-Order Neighbors Mixing' and 'Potential Neighbors Discovery', respectively. 'IA' and 'IC' mean 'Identifiable Message Aggregation' and 'Inter-Layer Combination', respectively. 'Local-Level' and 'Global-Level' indicate whether the GNN architecture refinement method, incorporating neighbor extension technology, primarily focuses on heterophilic design within the message-passing layer or enhances effective inter-layer information transfer throughout the entire network architecture, respectively.

Publication Year and Venue	Method	Category	Hybrid Mode
[2020 NeurIPS]	H2GCN [24]	HN & IC & IA	Global-Level
[2021 KDD]	WRGNN [77]	PN & IA	Local-Level
[2022 IJCAI]	RAW-GNN [78]	HN & IA	Local-Level
[2022 TPAMI]	NLGNN [74]	PN & IA	Global-Level
[2022 AAAI]	BM-GCN [79]	PN & IA	Local-Level
[2022 AAAI]	Deformable GCN [80]	PN & IA	Local-Level
[2022 AAAI]	GPNN [75]	PN & IC	Local-Level

link weights. Additionally, BM-GCN [79] constructs a novel network topology using a block similarity matrix. This approach allows it to explore block-guided neighbors and perform classified aggregation with distinct aggregation rules for homophilic and heterophilic nodes. RAW-GNN [78] employs breadth-first random walk searches to capture homophily information and depth-first searches to gather heterophily information. Instead of traditional neighborhoods, it utilizes path-based neighborhoods and introduces a new path-based aggregator based on Recurrent Neural Networks. GPNN [75] leverages a pointer network to rank the potential neighbor nodes according to the attention scores or the relevant relationships to the ego node. In this way, potential neighbors that are most similar to the ego node in heterophilic graphs can be discovered and selected. Deformable GCN, as presented in the recent work by Park et al. [80], dynamically conducts convolution in multiple latent spaces, enabling it to capture both short and long-range dependencies between nodes. In this approach, the model also learns the positional embeddings

(coordinates) of nodes to infer the relationships between nodes in an end-to-end manner. Depending on the position of a node, the convolution kernels are deformed using deformation vectors and make distinct transformations being applied to neighbors.

The global-level incorporation method, which is intended to establish effective homophilic guidance within the graph network framework. A typical example of such a method is H2GNN [24], which incorporates a set of crucial design elements. These include the separation of ego- and neighbor-embedding separation, higher-order neighborhoods, and incorporation of intermediate representations into a graph neural network. These design choices collectively enhance the model's capacity to learn from the graph structure, especially when dealing with heterophilic relationships. Furthermore, NLGNN [74] employs the attention mechanism to guide the sorting of non-local neighbors based on their importance. The entire architecture achieves efficient node classification on a heterogeneous graph using only two steps: straightforward attention-guided sorting and non-local aggregation.

7 DISCUSSION

7.1 Heterophily GNNs on Diverse Graph Types

While most current research primarily addresses the challenge of heterophilic problems in single relational static graphs, numerous real-world applications are related to diverse and complex graph types. For instance, in a traffic controlling system, the traffic flows are typically presented with dynamic graphs that change along with temporal information; Besides, graph data involving user-item co-purchasing relationships [81], paper co-citation relationships [82], film co-occurrence relationships [83], etc., is usually determined by hypergraphs.

Recent studies [84], [85] have started to acknowledge this gap and introduced concepts like the heterophilic dynamic graph and the heterophilic hypergraph. These advancements prompt a closer examination of the definition and design of heterophily solutions tailored to specific graph types. However, this expansion also brings forth a set of unique challenges for heterophilic GNNs to address.

7.1.1 Heterophily GNNs on Dynamic Graphs

As a typical dynamic graph instantiation, spatial-temporal graph data is often inherently heterophilic. Zhou et al. [84] recently aimed to validate this assertion by exploring spatial-temporal graphs in various real-world scenarios, such as traffic control, climate early-warning, and social networks. As depicted in Fig. 7(a), observations in these scenarios tend to change over time, leading to dynamic and time-varying characteristics in the correlation between nodes. The challenge posed by these dynamic and time-varying characteristics is termed "topology-task discordance" in [84]. This challenge arises when employing homophilic graph neural networks for node-level regression tasks on spatial-temporal graphs. It refers to the utilization of a pre-defined fixed topology for message passing on spatial-temporal graphs with diverse node-wise relations, resulting in the aggregation of neighbors that deviate from the intended target.

To formally measure spatial-temporal heterophily, two types of homophily measurements are introduced: "intra-graph spatial homophily", capturing node correlations within the same graph frames, and "inter-graph transition homophily" which extracts temporal evolution between adjacent temporal frames. The study further investigates the average homophily ratios for four real-world dynamic graphs: Metr-LA [86], PeMS-Bay [86], KnowAir [87], and Temperature [87]. The homophily ratios within intra-graph frames and across temporally adjacent frames are observed to be low. This suggests that physically connected nodes may not necessarily share similar observations or exhibit the same directional variations.

Furthermore, adapting existing homophily theories to address the topology-task discordance based on the spatial-temporal characteristics of node-wise relationships remains a challenging endeavor. The primary hurdles can be summarized as follows:

- Determining which pairs of nodes belong to homophily components in the absence of categorical labels.
- Incorporating target information to reconstruct node-wise correlations, thereby enabling improved and target-oriented aggregations.
- Leveraging dynamic local neighborhood environments for personalized high-order propagation.

These three aspects are expected to be key challenges in the study of heterophilic GNNs on dynamic graphs. This research
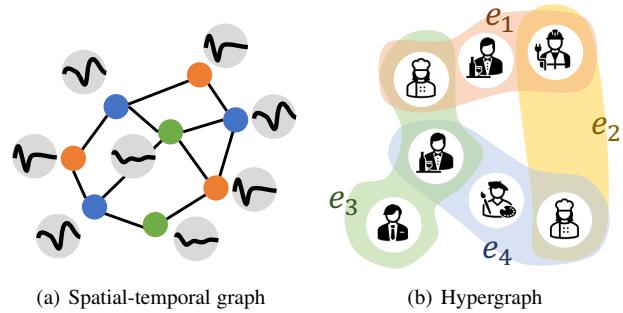

(a) Spatial-temporal graph   (b) Hypergraph

Fig. 7: Examples of (a) heterophilic dynamic graph and (b) heterophilic hypergraph.

direction will continue to demand the dedicated efforts of a significant number of researchers.

7.1.2 Heterophily GNNs on Hypergraphs

Fig. 7(b) illustrates a heterophilic hypergraph using a social network as an example. Each node represents a social user, and the hyperedge connects all users in the same community. It is common for users within the same community to have different identity backgrounds but be connected by attributes such as interests and hobbies, resembling the concept of heterophily in graphs. Recently, heterophily has been demonstrated in [88] to be a more prevalent phenomenon in hypergraphs compared to graphs. This is due to the challenge of expecting all nodes within a large hyperedge to share a common label. Consequently, recent research on hypergraph neural network methods has shifted its focus towards highlighting their exceptional performance on heterophilic hypergraphs.

Inspired by hypergraph diffusion algorithms, ED-HNN [85] has been developed as a novel hypergraph neural network (HNN) architecture that can effectively approximate any continuous equivariant hypergraph diffusion operators. These operators have the capability to model a wide array of higher-order relations. In this research, it is asserted that predicting node labels in heterophilic hypergraphs is more intricate than in graphs since a hyperedge may consist of nodes from multiple categories. Therefore, the research further analyzes its learnable equivariant diffusion operator and demonstrates its superiority in predicting heterophilic node labels on four hypergraphs: Congress [89], Senate [89], Walmart [90], and House [91].

However, based on our review of related works, there is currently no established characterization or algorithmic design for specific heterophilic hypergraphs. The primary challenges revolve around accurately describing the heterophily of hypergraphs and developing architecture refinement methods that capture the local homophily of hypergraphs. This research direction is still promising but in its early stages of development.

7.2 Unveiling the Correlation Between Graph Heterophily and Other Research Problems

7.2.1 Relation between Graph Heterophily and Adversarial Robustness

Adversarial robustness is a critical aspect of GNN models, concerning the safety and trustworthiness of modern systems. It pertains to the vulnerability or extreme non-robustness of a GNN
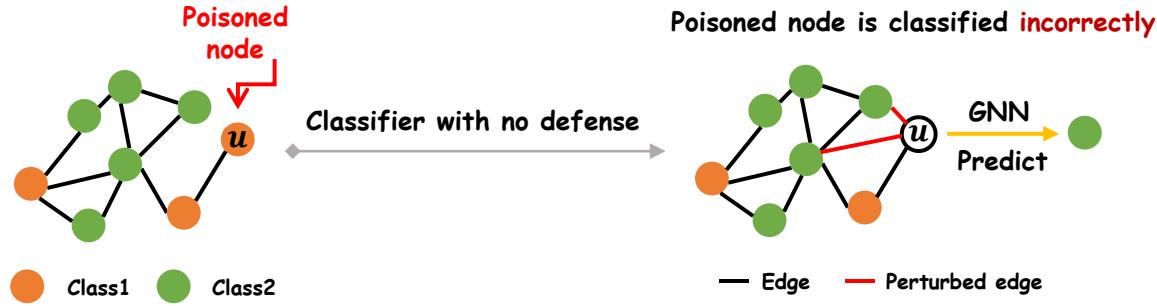
Fig. 8: Small, adversarial perturbations of the graph structure and node features lead GNN to misclassify target u.
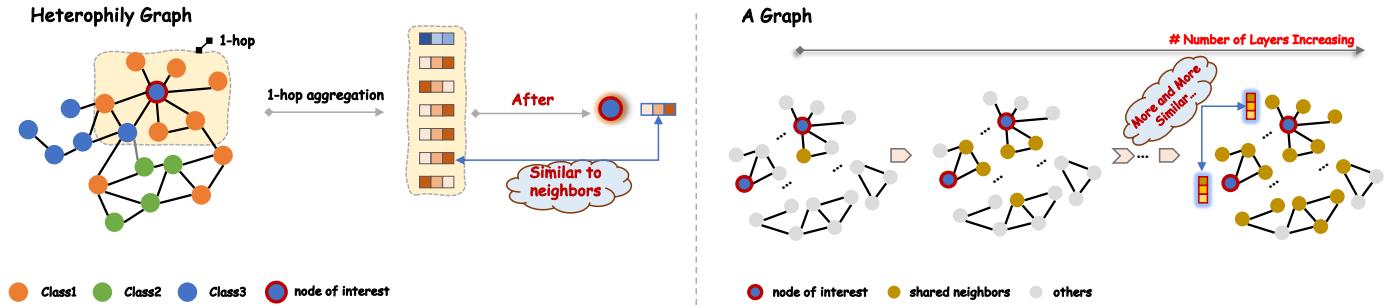

Fig. 9: Illustration of the connection between the heterophily property (Left) and the over-smoothing issue (Right) on GNNs.

model when confronted with an input that has been adversarially perturbed. These perturbations are often imperceptible or indiscernible to humans, posing a significant challenge to the robustness and reliability of the model. Early studies [92]–[95] primarily focused on robustness in the context of homophilic GNNs. Only recently has there been a growing recognition of the necessity to analyze heterophilic problems to design robust GNNs. The intuition behind this recognition is that structural attacks are predominantly heterophilic in nature, as shown in Fig. 8. The current researches [96]–[99] are centered around the design of defense GNNs, which refer to a class of methods or techniques used to protect or defend GNN from different types of adversarial attacks. Focusing on heterophilic connections as structural attacks on graphs, GNNGUARD [96] stands out as the first technique that shows a successful defense on heterophilic graphs. Specifically, GNNGUARD detects and quantifies the relationship between graph structure and node features, if such a relationship exists, then leverages this relationship to mitigate the adverse effects of these attacks. Consequently, GNNGUARD allows for robust propagation of neural messages within the underlying GNN. Similarly, GARNET [98] and ATDGIA [97] also treat heterophilic edges as adversarial edges and concentrate on designing defensive GNNs with anti-interference mechanisms for these adversarial edges. In recent research, Zhu et al. [99] take an additional statement by providing theoretical insights into the relation between adversarial structural attacks and changes in the homophily level of the underlying graphs. As an implication of this relation, it is further discussed that incorporating graph heterophily considerations into GNN designs can also contribute to enhancing model robustness. The key findings from this study are as follows:

- Through empirical validation on several strongly homophilic graphs, including Cora, Pubmed, and Citeseer, it is observed that all changes introduced by effective

attacks in the graph structure align with the conclusion that **structural attacks are primarily heterophilic** in nature.
- A comprehensive benchmark study of GNN models is conducted to validate that the incorporation of **heterophilic design leads to improved empirical robustness**.
- Through empirical validation, **models that incorporate identified heterophilic design demonstrate significantly enhanced certifiable robustness** compared to models lacking this design.

Robustness and the interplay between homophily and heterophily in structural attacks on GNNs are key areas of investigation in these studies, with implications for improving robust GNN model designs.

7.2.2 Relation between Graph Heterophily and Over-Smoothing

Heterophily and over-smoothing are two critical aspects that limit the performance of modern GNNs, where the former violates the general homophilic topological assumption, and the latter prevents most GNNs from going deeper when the performance drops with the increasing number of layers. Surprisingly, some studies show that GNNs for heterophilic graphs could be empirically utilized to address the over-smoothing problem [25], [29], [74], and vice versa [76]. We illustrate the connection between the heterophily property of graphs and the over-smoothing issue in GNN learning in Fig. 9.

While previous work has proposed empirical designs that simultaneously address both of these issues, Yan et al. [28] took the first step in explaining the connections between these two aspects. They suggested that these issues could be attributed to a common underlying cause from a unified theoretical perspective: Discriminative node representations are challenging to learn under over-smoothing/heterophily problems. More recently, Bodnar et
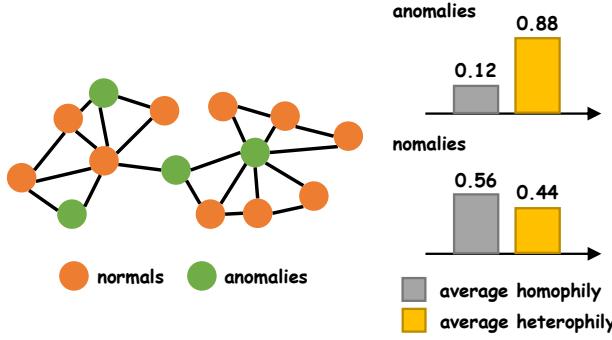
Fig. 10: A toy graph for anomaly detection. The average homophily and heterophily for anomalies and normals are presented.

Fig. 11: Illustration of the uncertainty of connections in a graph.

al. [46] utilized cellular sheaf theory to provide a novel topological perspective on heterophily and oversmoothing in GNNs. Their analysis demonstrated that the underlying sheaf structure of the graph is intimately linked with both of these critical factors that influence the performance of GNNs. Interestingly, both of these studies found evidence supporting the benefits of negatively signed edges in GNNs, albeit with different mathematical justifications. These theoretical findings also provide support for the effectiveness of technologies represented by FAGCN [25].

In summary, these observations and analyses have yielded promising results in quest to comprehensively explore and understand the relationship between heterophily and oversmoothing. This opens up significant opportunities for researchers to delve deeper into the solid foundations and evidence supporting these concepts and collectively work towards overcoming them.

7.2.3 Relation between Graph Heterophily and Graph Anomaly Detection

Fraud detection is a well-studied area within anomaly detection, which is primarily focused on identifying anomalies or abnormal behaviors within datasets. Recent studies [100]–[103], referring to these anomalies as abnormal nodes within a graph, have emphasized that in fraud networks, these abnormal nodes often display significant heterophily. As shown in Fig. 10, this heterophily is a consequence of the fact that these abnormal nodes tend to be clustered in minority subgroups while being surrounded by normal nodes, resulting in higher levels of heterophily compared to their normal counterparts.

Most graph-based anomaly detection (GAD) methods tend to emphasize how to obtain homophilic representations and often ignore the impact of heterophilic attributes of abnormal nodes during message aggregation [104]–[106]. This poses challenges in the context of fraud detection. Gao et al. [100] acknowledge these challenges and investigate structural distribution shift (SDS) across anomaly and normal data. They observed discrepancies in SDS between anomaly and normal nodes and argued that this discrepancy is exacerbated by the class imbalance nature of GAD. Additionally, Gong et al. [102] hold a similar viewpoint by calculating the average homophily ratios of normal nodes and abnormal nodes in various fraud graphs and discovering that abnormal nodes consistently demonstrate high heterophily. Therefore, they adopted a strategy to sparsify the structures of target graphs to effectively reduce heterophilic connections and collaboratively learn node representations. This approach robustly detects anomalies by uncovering the underlying dependency among node pairs in
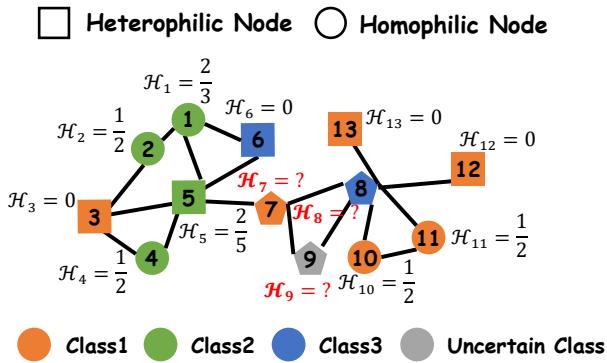
terms of homophily and heterophily. Similarly, researchers like Shi et al. [101], Gao et al. [107], and Chai et al. [108] also recognize the significance of addressing heterophily problems in fraud detection tasks. They argued that relying solely on low-pass properties during GNN aggregation introduces noise containing heterophilic attributes into normal node representation learning, consequently impairing fraud detection performance. As a solution, various strategies have been devised in these studies to enable models to dynamically select low-frequency, high-frequency, or a combination of both components to differentiate abnormal nodes. This adaptive approach effectively captures both low-frequency and high-frequency graph signals to enhance fraud detection performance.

7.2.4 Relation between Graph Heterophily and Uncertainty Modeling

The modeling of uncertainty involves capturing and comprehending inherent uncertainties in data, a subject that has garnered significant attention in the development of reliable decision-making systems [48], [109]–[111]. Within the context of graph heterophily, where nodes can exhibit diverse connections, uncertainty emerges as a pivotal factor. The varied degrees of heterophilic relationships between nodes contribute to the complex information flow, introducing uncertainties regarding the nature and impact of these connections. As depicted in Fig. 11, a toy graph illustrates the uncertainty of connections.

An examination of graph structures from a node-level perspective reveals a mixture of homophily and heterophily in uncertain real-world scenarios, signifying the coexistence of both homophilic and heterophilic nodes. In the presence of such a mixture, GNNs exhibit a notable bias towards homophilic nodes, resulting in a substantial performance decline on heterophilic nodes. Liu et al. [110] underscore this bias issue of GNNs and advocate for model predictions to maintain high accuracy while minimizing model bias. Model bias refers to the phenomenon where GNNs trained on semi-homophilic graphs perform worse on a heterophilic set than the same model exclusively trained on the heterophilic segment of the graph. This leads to a more pronounced performance bias, emphasizing the need for GNNs to effectively address heterophily to ensure robust and unbiased predictions across diverse nodes.

To mitigate the bias issue, Liu et al. [110] explore an Uncertainty-aware Debiasing (UD) framework, which retains the knowledge of the biased model on certain nodes and compensates for the nodes with high uncertainty. In particular, UD estimates

the uncertainty of the GNN output to recognize heterophilic nodes. Additionally, a probabilistic solution named Graph Topology Uncertainty (GraphTU) is innovatively proposed in [48], which enables the synthetic nodes to better catch the informative characteristics from the topology space. For each source minor node, Gao et al. [48] not only consider the feature but also the valuable information from their crucial neighbors. Interestingly, they observe that statistical variances in local neighborhoods can be fully exploited to extend the training distribution for the minor class in a non-parametric manner.

In conclusion, the relation between graph heterophily and uncertainty modeling provides a rich landscape for exploration. By delving into this connection, researchers can enhance their understanding of how network structures influence uncertainty, paving the way for improved models and strategies in various applications, from social networks to biological systems.

Other Promising Heterophily Explorations. Recently, researchers have sought to extend the design of heterophilic GNNs beyond the semi-supervised paradigm, focusing on self-supervised heterophilic GNNs [31], [112], [113]. It is noteworthy that He et al. [112] identified commonalities between the establishment of the Graph Contrastive Learning (GCL) framework and the design of heterophilic GNNs. In the GCL framework, the task involves identifying additional positive samples belonging to the same class, while in the design of heterophilic GNNs, the objective is to identify other intra-class neighbors for each node. Recognizing this similarity, they integrated the GCL sampling strategy with homophily discrimination, creating a novel contrastive learning framework to address these crucial challenges. This framework draws inspiration from homophily, breaking traditional data enhancement strategies and providing a fresh perspective on establishing a GCL framework. Furthermore, it executes contrastive learning by sampling homophily neighbors as positive examples, offering innovative insights for the design of heterophilic GNNs. To address the limitations imposed by the strong homophily assumption and label dependency, Li et al. [113] introduced a novel multi-task model named PairE with a contrastive learning method. This model is designed to preserve information pertaining to both homophily and heterophily by transcending the localized node view. It achieves this by harnessing higher-level entities with more expressive power, enabling the representation of feature signals beyond homophily. In a similar vein and motivated by comparable considerations, Liu et al. [31] propose an innovative self-supervised Graph Representation Learning method called Edge Heterophily Discriminating (GREET). By discriminating edges, GREET obtains contrastive views with both homophilic and heterophilic edges, leveraging them to learn expressive representations.

8 FUTURE DIRECTIONS

GNNs for heterophilic graphs are fast developing in the past few years. Beyond current research, there still remain several open challenges and opportunities worthy of further attention and exploration. In this section, we discuss the following directions to stimulate future research.

Interpretable Heterophilic GNNs. Interpretability is a crucial aspect of GNN models in risk-sensitive or privacy-related application fields, *e.g.*, healthcare and cybersecurity. Although there are several studies on the interpretability [114]–[116] for homophily GNNs, how to explain the predictions of heterophilic GNNs is still under-explored. Heterophily makes interpretability more challenging than homophily: since most local neighbor nodes are not in the same class as the ego nodes, extracting explainable subgraphs from highly heterophilic graph data is much harder, where both proximal and distant topological structures are required to be discovered and exploited. For instance, ShapeGGen [116] typically proposed a dataset generator that can automatically generate a variety of benchmark datasets (*e.g.*, varying graph sizes, degree distributions, homophilic and heterophilic graphs), accompanied by ground-truth explanations From the data-centric view of heterophilic graphs, how to extract explainable subgraphs under complex similarity relationships between ego nodes and their potential neighbors on heterophilic graphs for interpretability is an open question. Moreover, from the model-centric view of heterophilic GNNs, how to explain the model's predictions on graphs with different degrees of heterophily also deserves further exploration.

Scalable Heterophilic GNNs. Current heterophilic GNNs are generally trained on relatively small graphs, which significantly limits their ability to model large-scale data and explore more complicated heterophilic patterns. Although possible solutions to tackle scalability can be borrowed from the mainstream graph sampling strategies [117], [118] for homophilic GNNs, the connections and relationships of heterophilic nodes would be undermined by sampling only mini-batches, especially when similar and dissimilar neighbors contribute differently to learning the ego-node representations. LINKX [27] recently verifies that even a simple MLP-based model could outperform GNNs for mini-batch training on large-scale heterophilic graphs. Moreover, HopGNN [49] introduces a hop interaction paradigm to address the scalability and over-smoothing problem of GNNs simultaneously, where its core idea is to convert the interaction target among nodes to pre-processed multi-hop features inside each node. Hence, addressing the scalability problem of heterophilic graphs requires exploring more relationships between ego-neighbor node features and multi-hop information. How to keep the inherent heterophily unchanged when conducting sampling on heterophilic graphs is still an open question.

Theoretical Heterophily Exploration. Despite the notable achievements of heterophilic GNNs across diverse tasks and datasets, their efficacy lacks a solid theoretical foundation to substantiate their impact on enhancing graph representation learning. Presently, many methods are predominantly designed based on intuition and evaluated through empirical experiments. Notably, a recent breakthrough by Ma et al. [119] has unveiled that, under specific conditions, GCN can exhibit remarkable performance on heterophilic graphs. This discovery has been supported by comprehensive theoretical validation, outlining the distinctive characteristics and conditions under which heterophilic graphs can excel with GCN. The elucidation of these theoretical findings poses a significant challenge to the current rationale underlying the design of heterophilic GNNs. Consequently, there arises a critical need for intensified theoretical exploration in the future. This exploration should delve into aspects such as the impact of heterophily on altering the trends of generalization bounds. Bridging this explanatory gap is crucial for comprehending the extent to which heterophily influences the performance constraints of homophilic GNNs.

Diverse Heterophily Learning Tasks. The research on heterophilic GNNs has primarily demonstrated success in node-

level tasks, covering both semi-supervised [36], [51], [63] and unsupervised scenarios [31], [112], [120]. A recent study by Zhou et al. [121] introduces a novel heterophilic framework named DisenLink, specifically designed for addressing link-level tasks on heterophilic graphs. In heterophilic graphs, DisenLink reveals that link formation is influenced by numerous latent factors, causing linked nodes to share similarity in certain factors while being dissimilar in others. This results in an overall low similarity between linked nodes. Many existing link prediction approaches operate under the homophily assumption, using similarity-based heuristics or representation learning methods to predict links. Therefore, accurately predicting links with heterophilic attributes, determined by specific potential similar factors, poses a significant challenge. DisenLink identifies the challenges of link-level tasks on heterophilic graphs, but there are still significant open questions in this domain. These include the development of reasonable heterophilic benchmark datasets and the refinement of GNN architectures for link-level tasks. Additionally, similar open questions exist for graph-level tasks, indicating that further exploration is needed in these areas.

Broader Scope of Practical Applications. In the real world, heterophilic relationships are pervasive and exist widely in various graph-structured data [122]–[126]. However, current research on heterophilic GNNs predominantly focuses on specific strong heterophilic graphs, such as social networks [122] and web page networks [123]. Other fields, such as biomedicine [124] and chemistry [125], [126], which also naturally exhibit the heterophilic property, deserve more explorations. For instance, in protein-protein interaction networks, proteins with interactions often belong to different gene ontologies. Moreover, in the field of drug discovery, DCMGCN [127] verifies the heterophily property of the drug-drug networks and proposed a combination of intermediate representations, and high-similarity neighborhoods, to boost GCN learning on the heterophily and sparse drug-drug networks. Besides, in the field of fraud detection, fraudsters tend to be more connected to regular users represented by fraud networks. And some existing research, *e.g.*, DRAG [128] and GAGA [103], solved the problem by conducting the binary heterophilic graph classification task. This highlights the untapped potential of heterophilic GNNs in a broader range of application areas. There is an expectation to extend the use of heterophilic GNNs to various fields, including financial networks, network security, community detection, biomedicine, and chemistry.

9 CONCLUSION

In this paper, we conducted a comprehensive overview of graph neural networks for heterophilic graphs. To achieve this, we proposed a novel and systematic taxonomy of existing heterophilic GNNs, categorizing them into non-local neighbor extension methods, GNN architecture refinement methods, and hybrid methods. Our contribution includes a thorough introduction and analysis of the current research progress and challenges in the field of heterophilic graph learning. To highlight the significance of heterophilic GNNs, we delved into a thorough discussion of their applications on diverse graphs, revealing the correlation between graph heterophily and various problem domains, such as model robustness, over-smoothing, and graph anomaly detection. In the end, we shared our insights into future research opportunities and directions that can contribute to the advancement of heterophilic GNNs.

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APPENDIX A
REAL-WORLD BENCHMARKS

To provide the data support for the development of heterophilic graph learning, we collect and list current real-world benchmarks of heterophilic graph datasets with detailed statistics, as shown in Tables 5 - 7. All datasets can be divided in three categories: standard datasets, large-scale datasets and high-quality datasets.

A.1 Standard Datasets

Most current works conduct experiments for empirical evaluations on the first 6 datasets in Table 5, which are originally presented by the work [34]. Specifically, Cornell, Texas, and Wisconsin are three subdatasets from WebKB web-page dataset [129], where nodes are the web pages from computer science departments of different universities, and edges are mutual links between pages. Chameleon and Squirrel are two web page datasets collected from Wikipedia [130], where nodes are web pages on specific topics and edges are hyperlinks between them. Actor is an actor co-occurrence network [1], where nodes are actors and edges mean two actors are co-occurred on the same Wikipedia page.

A.2 Large-Scale Datasets

Subsequently, a series of new benchmark datasets with larger scales from diverse areas are collected and released by [27] and [26], including a Wikipedia web page dataset (Wiki), two citation network datasets (ArXiv-Year and Snap-Patents), five

online social network datasets (Penn94, Pokec, Genius, Deezer-Europe, and Twitch-Gamers), as well as a web-page hotel and restaurant review dataset (YelpChi).

A.3 High-Quality Datasets

Recent research [135] has highlighted significant issues with standard datasets used to evaluate heterophily-specific models. These issues make results obtained using such datasets unreliable. One of the most notable drawbacks is the presence of a large number of duplicate nodes in datasets like squirrel and chameleon, which results in train-test data leakage. Removing these duplicate nodes has a strong impact on GNN performance in these datasets. To address these challenges, a set of reliable heterophilic graphs with diverse properties has been proposed. These graphs include Roman-Empire, Amazon-Ratings, Minesweeper, Tolokers, and Questions. This effort aims to create a collection of trustworthy heterophilic benchmarks that can support and advance research and applications of GNNs on heterophilic graphs. It is expected that more publicly available benchmarks for heterophily will be developed to further facilitate research in this area.

B OPEN-SOURCE IMPLEMENTATIONS

We have gathered the implementations of heterophilic GNN approaches discussed in this survey if open-source code for these methods is available. You can find the hyperlinks to the source codes in Table 8.

TABLE 5: Statistics of standard heterophilic graph benchmarks.

Types	Datasets	# Nodes	# Edges	# Features	# Classes	$\mathcal{H}_{node}$	$\mathcal{H}_{edge}$	$\mathcal{H}_{class}$
WebKB Webpage	Cornell	183	295	1,703	5	0.11	0.30	0.05
	Texas	183	309	1,703	5	0.06	0.11	0.00
	Wisconsin	251	499	1,703	5	0.16	0.21	0.09
Author Co-occurrence	Actor	7,600	33,544	931	5	0.24	0.22	0.01
Wikipedia Webpage	Chameleon	2,277	36,101	2,325	5	0.25	0.23	0.06
	Squirrel	5,201	217,073	2,089	5	0.22	0.22	0.03

TABLE 6: Statistics of large-scale heterophilic graph benchmarks.

Types	Datasets	# Nodes	# Edges	# Features	# Classes	$\mathcal{H}_{node}$	$\mathcal{H}_{edge}$	$\mathcal{H}_{class}$	$\mathcal{H}_{adj}$	LI
Wikipedia Webpage	Wiki	1,925,342	303,434,860	600	5	-	0.39	-	-	-
Citation	ArXiv-Year	169,343	1,166,243	128	5	0.29	0.22	0.07	0.01	0.04
	Snap-Patents	2,923,922	13,975,788	269	5	-	0.07	-	-	-
Social Networks	Deezer-Europe	28,281	92,752	31,241	2	0.53	0.53	0.03	0.03	0.00
	Penn94	41,554	1,362,229	5	2	-	0.47	-	-	-
	Twitch-Gamers	168,114	6,797,557	7	2	0.56	0.55	0.09	0.09	0.01
	Genius	421,961	984,979	12	2	-	0.62	-	-	-
	Pokec	1,632,803	30,622,564	65	2	-	0.45	-	-	-
Webpage Review	YelpChi	45,954	3,846,979	32	2	0.77	0.77	-	-	-

TABLE 7: Statistics of high-quality heterophilic graph benchmarks.

Types	Datasets	# Nodes	# Edges	# Features	# Classes	$\mathcal{H}_{node}$	$\mathcal{H}_{edge}$	$\mathcal{H}_{class}$	$\mathcal{H}_{adj}$	LI
Wikipedia Webpage	Roman-Empire	22,662	32,927	300	18	0.05	0.05	0.02	-0.05	0.11
Product Co-Purchasing	Amazon-Ratings	24,492	93,050	300	5	0.38	0.38	0.13	0.14	0.04
Game	Minesweeper	10,000	39,402	7	2	0.68	0.68	0.01	0.01	0.00
Social Networks	Tolokers	11,758	519,000	10	2	0.63	0.59	0.18	0.09	0.01
	Questions	48,921	153,540	301	2	0.90	0.84	0.08	0.02	0.00

TABLE 8: A summary of open-source implementations.

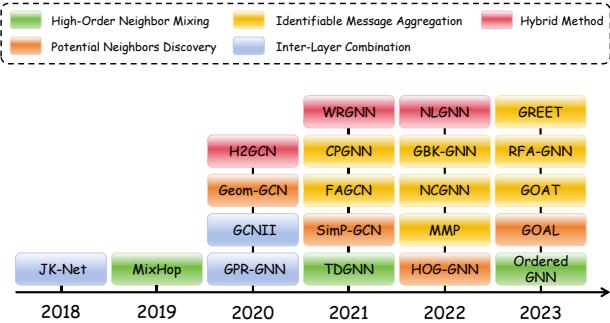| Method	Framework	Github Link
JK-Net (2018) [67]	TensorFlow	https://github.com/ShinKyuY/Representation_Learning_on_Graphs_with_Jumping_Knowledge_Networks
	PyTorch	https://github.com/xnuohz/JKNet-dgl
MixHop (2019) [36]	PyTorch	https://github.com/samihaija/mixhop
GCNII (2020) [76]	PyTorch	https://github.com/chennnM/GCNII
Geom-GCN (2020) [34]	PyTorch	https://github.com/alexfanjn/GeomGCN_PyG
GPR-GNN (2020) [30]	PyTorch	https://github.com/jianhao2016/GPRGNN
H2GCN (2020) [24]	PyTorch	https://github.com/GemsLab/H2GCN
TDGNN (2021) [37]	PyTorch	https://github.com/Leo-Q-316/TDGNN
SimP-GCN (2021) [41]	PyTorch	https://github.com/ChandlerBang/SimP-GCN
U-GCN (2021) [40]	PyTorch	https://github.com/jindi-tju/U-GCN
FAGCN (2021) [25]	PyTorch	https://github.com/bdy9527/FAGCN
CPGNN (2021) [23]	TensorFlow	https://github.com/GemsLab/CPGNN
CGCN (2021) [28]	PyTorch	https://github.com/Yujun-Yan/Heterophily_and_oversmoothing
EvenNet (2022) [39]	PyTorch	https://github.com/Leirunlin/EvenNet
Diag-NSD (2022) [46]	PyTorch	https://github.com/twitter-research/neural-sheaf-diffusion
MPNN (2022) [68]	PyTorch	https://github.com/nhuang37/spectral-inspired-gnn
GARNET (2022) [98]	PyTorch	https://github.com/cornell-zhang/GARNET
LW-GNN (2022) [69]	PyTorch	https://github.com/EnyanDai/LWGCN
GBK-GNN (2022) [51]	PyTorch	https://github.com/Xzh0u/GBK-GNN
F2GNN (2022) [52]	PyTorch	https://github.com/LARS-research/F2GNN
GloGNN (2022) [45]	PyTorch	https://github.com/RecklessRonan/GloGNN
GIND (2022) [55]	PyTorch	https://github.com/7qchen/GIND
BM-GCN (2022) [79]	PyTorch	https://github.com/hedongxiao-tju/BM-GCN
Deformable GCN (2022) [80]	PyTorch	https://github.com/mlvlab/DeformableGCN
GIA-HAO (2022) [131]	PyTorch	https://github.com/LFhase/GIA-HAO
HeteRobust (2022) [23]	PyTorch	https://github.com/GemsLab/HeteRobust
GREET (2023) [31]	PyTorch	https://github.com/yixinliu233/GREET
HopGNN (2023) [49]	PyTorch	https://github.com/JC-202/HopGNN
ED-HNN (2023) [85]	PyTorch	https://github.com/Graph-COM/ED-HNN
Ordered GNN (2023) [38]	PyTorch	https://github.com/LUMIA-Group/OrderedGNN
GReTo (2023) [84]	PyTorch	https://github.com/zzyy0929/ICLR23-GReTo
SNGNN (2023) [132]	PyTorch	https://github.com/MinhZou/SNGNN
CAGNNs (2023) [70]	PyTorch	https://github.com/JC-202/CAGNN
CGP (2023) [60]	PyTorch	https://github.com/LiuChuang0059/CGP
RFA-GNN (2023) [61]	PyTorch	https://github.com/LirongWu/RFA-GNN
HES-GSL (2023) [42]	PyTorch	https://github.com/LirongWu/Homophily-Enhanced-Self-supervision
GDN (2023) [100]	PyTorch	https://github.com/blacksingular/wsdm_GDN
SE-GSL (2023) [47]	PyTorch	https://github.com/RingBDStack/SE-GSL
GHRN (2023) [107]	PyTorch	https://github.com/blacksingular/GHRN
AutoGCN (2023) [62]	PyTorch	https://github.com/nnzhan/AutoGCN
GOAL (2023) [21]	PyTorch	https://github.com/zyzisastudyreallyhardguy/GOAL-Graph-Complementary-Learning
L2A (2023) [133]	PyTorch	https://github.com/LirongWu/L2A
GPRGNN-L (2023) [134]	PyTorch	https://github.com/lucio-win/PKDD2023

Fig. 12: A timeline of heterophilic GNNs development.

include straightforward layer-inter combination methods like JK-Net [67], GPR-GNN [30], and GCNII [76]. Another category of early works explores non-local neighbor mixing and discovery intuitively, exemplified by MixHop [36] and Geom-GCN [34]. H2GCN [24] represents an early exploration into hybrid methods. In 2021, the introduction of FAGCN [25] marked a significant development by incorporating adaptive edge-aware weighted techniques, which arises the flourishing exploration of adaptive message aggregation. Subsequent in 2022 and 2023, witnessed the integration of more advanced techniques with heterophilic GNNs, including dynamic routing (NCGNN [58]), self-supervised learning (GREET [31]), and attention mechanisms with memory (MMP [54]).

C   TIMELINE OF HETEROPHILY GNNS

Fig. 12 illustrates a timeline featuring some of the most notable heterophilic GNNs developed since 2018. Early works in the field