
Is Heterophily A Real Nightmare For Graph Neural Networks To Do Node Classification?

Anonymous Author(s)

Affiliation

Address

email

Abstract

1 Graph Neural Networks (GNNs) extend basic Neural Networks (NNs) by using
2 the graph structures based on the relational inductive bias (homophily assumption).
3 Though GNNs are believed to outperform NNs in real-world tasks, performance
4 advantages of GNNs over graph-agnostic NNs seem not generally satisfactory.
5 Heterophily has been considered as a main cause and numerous works have been
6 put forward to address it. In this paper, we first show that not all cases of heterophily
7 are harmful for GNNs with aggregation operation. Then, we propose new metrics
8 based on a similarity matrix which considers the influence of graph structure and
9 input features on GNNs. The metrics demonstrate advantages over the commonly
10 used homophily metrics by tests on synthetic graphs. From the metrics and the
11 observations, we find some cases of harmful heterophily can be addressed by
12 diversification operation. With this fact and knowledge of filterbanks, we propose
13 the Adaptive Channel Mixing (ACM) framework to adaptively exploit aggregation,
14 diversification and identity operations in each GNN layer to address harmful
15 heterophily. We validate the ACM-augmented baselines with 11 real-world node
16 classification tasks. They consistently achieve significant performance gain and
17 exceed the state-of-the-art GNNs on most of the tasks without incurring significant
18 computational burden.

19 1 Introduction

20 Deep Neural Networks (NNs) [18] have revolutionized many machine learning areas, including
21 image recognition [17], speech recognition [10] and natural language processing [2], *etc.* One major
22 strength is their capacity and effectiveness of learning latent representation from Euclidean data.
23 Recently, the focus has been put on its applications on non-Euclidean data [4], *e.g.*, relational data
24 or graphs. Combining graph signal processing and convolutional neural networks [19], numerous
25 Graph Neural Networks (GNNs) [29, 7, 12, 30, 15, 24] have been proposed which empirically out-
26 perform traditional neural networks on graph-based machine learning tasks, *e.g.*, node classification,
27 graph classification, link prediction and graph generation, *etc.* GNNs are built on the homophily
28 assumption [26], *i.e.*, connected nodes tend to share similar attributes with each other [11], which
29 offers additional information besides node features. Such relational inductive bias [3] is believed to
30 be a key factor leading to GNNs' superior performance over NNs' in many tasks.

31 Nevertheless, growing evidence shows that GNNs do not always gain advantages over traditional NNs
32 when dealing with relational data. In some cases, even simple Multi-Layer Perceptrons (MLPs) can
33 outperform GNNs by a large margin [35, 22, 5]. An important reason for the performance degradation
34 is believed to be the heterophily problem, *i.e.*, connected nodes tend to have different labels which
35 makes the homophily assumption fail. Heterophily challenge has received attention recently and
36 there are increasing number of models being put forward to address this problem [35, 22, 5, 34, 33].

37 **Contributions** In this paper, we first demonstrate that not all heterophilous graphs are harmful for
 38 aggregation-based GNNs and the existing metrics of homophily are insufficient to decide whether the
 39 aggregation operation will make nodes less distinguishable or not. By constructing a similarity matrix
 40 from backpropagation analysis, we derive new metrics to depict how much GNNs are influenced by
 41 the graph structure and node features. We show the advantage of our metrics over the existing metrics
 42 by comparing the ability of characterizing the performance of two baseline GNNs on synthetic graphs
 43 of different levels of homophily. From the similarity matrix, we find that diversification operation
 44 is able to address some harmful heterophily cases, and then based on which we propose Adaptive
 45 Channel Mixing (ACM) GNN framework. The experiments on the synthetic datasets, real-world
 46 datasets and the ablation studies consistently show that baseline GNN augmented by ACM framework
 47 is able to obtain significant performance boost on node classification tasks on heterophilous graphs.

48 The rest of this paper is mainly organized as follows: In section 2 we introduce the notation and the
 49 background knowledge. In section 3 we conduct node-wise heterophily analysis, derive new metrics
 50 based on a similarity matrix and conduct experiments to show their advantage. In section 4.3 we
 51 propose the ACM-GNN framework to adaptively utilize the information from different filterbank
 52 channels to address heterophily problem. In section 5 we discuss the related works and clarify
 53 the differences to our method. In section 6 we provide empirical evaluations on ACM framework,
 54 including ablation study and tests on 11 real-world node classification tasks.

55 2 Preliminaries

56 We introduce the related notation and background knowledge. We use **bold** fonts for vectors (*e.g.*,
 57 \mathbf{v}). Suppose we have an undirected connected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, A)$, where \mathcal{V} is the node set with
 58 $|\mathcal{V}| = N$; \mathcal{E} is the edge set without self-loop; $A \in \mathbb{R}^{N \times N}$ is the symmetric adjacency matrix with
 59 $A_{i,j} = 1$ iff $e_{ij} \in \mathcal{E}$, otherwise $A_{i,j} = 0$. We use D to denote the diagonal degree matrix of \mathcal{G} , *i.e.*,
 60 $D_{i,i} = d_i = \sum_j A_{i,j}$ and use \mathcal{N}_i to denote the neighborhood set of node i , *i.e.*, $\mathcal{N}_i = \{j : e_{ij} \in \mathcal{E}\}$.
 61 A graph signal is a vector $\mathbf{x} \in \mathbb{R}^N$ defined on \mathcal{V} , where x_i is defined on the node i . We also have a
 62 feature matrix $X \in \mathbb{R}^{N \times F}$, whose columns are graph signals and whose i -th row $X_{i,:}$ is a feature
 63 vector of node i . We use $Z \in \mathbb{R}^{N \times C}$ to denote the label encoding matrix, whose i -th row $Z_{i,:}$ is the
 64 one-hot encoding of the label of node i . The i -th column of the identity matrix I is denoted by \mathbf{e}_i .

65 2.1 Graph Laplacian, Affinity Matrix and Their Variants

66 The (combinatorial) graph Laplacian is defined as $L = D - A$, which is Symmetric Positive
 67 Semi-Definite (SPSD) [6]. Its eigendecomposition gives $L = U\Lambda U^T$, where the columns \mathbf{u}_i of
 68 $U \in \mathbb{R}^{N \times N}$ are orthonormal eigenvectors, namely the *graph Fourier basis*, $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_N)$
 69 with $\lambda_1 \leq \dots \leq \lambda_N$, and these eigenvalues are also called *frequencies*. The graph Fourier transform
 70 of the graph signal \mathbf{x} is defined as $\mathbf{x}_{\mathcal{F}} = U^{-1}\mathbf{x} = U^T\mathbf{x} = [\mathbf{u}_1^T\mathbf{x}, \dots, \mathbf{u}_N^T\mathbf{x}]^T$, where $\mathbf{u}_i^T\mathbf{x}$ is the
 71 component of \mathbf{x} in the direction of \mathbf{u}_i .

72 In addition to L , some variants are also commonly used, *e.g.*, the symmetric normalized Laplacian
 73 $L_{\text{sym}} = D^{-1/2}LD^{-1/2} = I - D^{-1/2}AD^{-1/2}$ and the random walk normalized Laplacian $L_{\text{rw}} =$
 74 $D^{-1}L = I - D^{-1}A$. The affinity (transition) matrices can be derived from the Laplacians, *e.g.*,
 75 $A_{\text{rw}} = I - L_{\text{rw}} = D^{-1}A$, $A_{\text{sym}} = I - L_{\text{sym}} = D^{-1/2}AD^{-1/2}$ and are considered to be low-pass
 76 filters [25]. Their eigenvalues satisfy $\lambda_i(A_{\text{rw}}) = \lambda_i(A_{\text{sym}}) = 1 - \lambda_i(L_{\text{sym}}) = 1 - \lambda_i(L_{\text{rw}}) \in (-1, 1]$.
 77 Applying the renormalization trick [15] to affinity and Laplacian matrices respectively leads to
 78 $\hat{A}_{\text{sym}} = \tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2}$ and $\hat{L}_{\text{sym}} = I - \hat{A}_{\text{sym}}$, where $\tilde{A} \equiv A + I$ and $\tilde{D} \equiv D + I$. The renormalized
 79 affinity matrix essentially adds a self-loop to each node in the graph, and is widely used in Graph
 80 Convolutional Network (GCN) [15] as follows,

$$Y = \text{softmax}(\hat{A}_{\text{sym}} \text{ReLU}(\hat{A}_{\text{sym}} X W_0) W_1) \quad (1)$$

81 where $W_0 \in \mathbb{R}^{F \times F_1}$ and $W_1 \in \mathbb{R}^{F_1 \times O}$ are learnable parameter matrices. GCN can be trained by
 82 minimizing the following cross entropy loss

$$\mathcal{L} = -\text{trace}(Z^T \log Y) \quad (2)$$

83 where $\log(\cdot)$ is a component-wise logarithm operation. The random walk renormalized matrix
 84 $\hat{A}_{\text{rw}} = \tilde{D}^{-1}\tilde{A}$, which shares the same eigenvalues as \hat{A}_{sym} , can also be applied in GCN. The

85 corresponding Laplacian is defined as $\hat{L}_{rw} = I - \hat{A}_{rw}$. \hat{A}_{rw} is essentially a random walk matrix and
 86 behaves as a mean aggregator that is applied in spatial-based GNNs [12, 11]. To bridge the spectral
 87 and spatial methods, we use \hat{A}_{rw} in the paper.

88 2.2 Metrics of Homophily

89 The metrics of homophily are defined by considering different relations between node labels and
 90 graph structures defined by adjacency matrix. There are three commonly used homophilies: edge
 91 homophily [1, 35], node homophily [28], and class homophily [21] defined as follows:

$$H_{\text{edge}}(\mathcal{G}) = \frac{|\{e_{uv} \mid e_{uv} \in \mathcal{E}, Z_{u,:} = Z_{v,:}\}|}{|\mathcal{E}|}, \quad H_{\text{node}}(\mathcal{G}) = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \frac{|\{u \mid u \in \mathcal{N}_v, Z_{u,:} = Z_{v,:}\}|}{d_v},$$

$$H_{\text{class}}(\mathcal{G}) = \frac{1}{C-1} \sum_{k=1}^C \left[h_k - \frac{|\{v \mid Z_{v,k} = 1\}|}{N} \right]_+, \quad h_k = \frac{\sum_{v \in \mathcal{V}} |\{u \mid Z_{v,k} = 1, u \in \mathcal{N}_v, Z_{u,:} = Z_{v,:}\}|}{\sum_{v \in \{v \mid Z_{v,k} = 1\}} d_v} \quad (3)$$

92 where $[a]_+ = \max(a, 0)$; h_k is the class-wise homophily metric [21]. They are all in the range
 93 of $[0, 1]$ and a value close to 1 corresponds to strong homophily while a value close to 0 indicates
 94 strong heterophily. $H_{\text{edge}}(\mathcal{G})$ measures the proportion of edges that connect two nodes in the same
 95 class; $H_{\text{node}}(\mathcal{G})$ evaluates the average proportion of edge-label consistency of all nodes; $H_{\text{class}}(\mathcal{G})$
 96 tries to avoid the sensitivity to imbalanced class, which can cause H_{edge} misleadingly large. The
 97 above definitions are all based on the graph-label consistency and imply that the inconsistency will
 98 cause harmful effect to GNNs. With this in mind, we will show a counter example to illustrate the
 99 insufficiency of the above metrics and propose new metrics.

100 3 Analysis of Heterophily

101 3.1 Motivation and Aggregation Homophily

102 Heterophily is believed to be harmful for
 103 message-passing based GNNs [35, 28, 5] be-
 104 cause intuitively features of nodes in different
 105 classes will be falsely mixed and this will lead
 106 nodes indistinguishable [35]. Nevertheless, it
 107 is not always the case, *e.g.*, the bipartite graph
 108 shown in Figure 1 is highly heterophilous accord-
 109 ing to the homophily metrics in (3), but
 110 after mean aggregation, the nodes in classes 1
 111 and 2 only exchange colors and are still distin-
 112 guishable. Authors in [5] also point out the
 113 insufficiency of H_{node} by examples to show that
 114 different graph typologies with the same H_{node}
 115 can carry different label information.

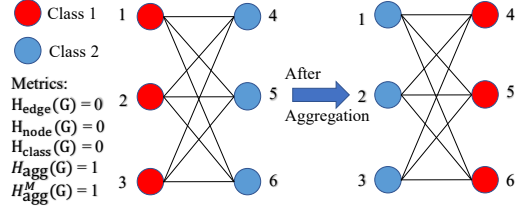


Figure 1: Example of harmless heterophily

116 To analyze to what extent the graph structure can affect the output of a GNN, we first simplify the
 117 GCN by removing its non-linearity as [31]. Let $\hat{A} \in \mathbb{R}^{N \times N}$ denote a general aggregation operator.
 118 Then, equation (1) can be simplified as,

$$Y = \text{softmax}(\hat{A}XW) = \text{softmax}(Y') \quad (4)$$

119 After each gradient decent step $\Delta W = \gamma \frac{\partial \mathcal{L}}{\partial W}$, where γ is the learning rate, and the update of Y' will
 120 be (see Appendix B for derivation),

$$\Delta Y' = \hat{A}X \Delta W = \gamma \hat{A}X \frac{\partial \mathcal{L}}{\partial W} \propto \hat{A}X \frac{\partial \mathcal{L}}{\partial W} = \hat{A}X X^T \hat{A}^T (Z - Y) = S(\hat{A}, X)(Z - Y) \quad (5)$$

121 where $S(\hat{A}, X) \equiv \hat{A}X(\hat{A}X)^T$ is a node similarity matrix after aggregation, $Z - Y$ is the prediction
 122 error matrix. The update direction of node i is essentially a weighted sum of the prediction error, *i.e.*,
 123 $\Delta(Y')_{i,:} = \sum_{j \in \mathcal{V}} [S(\hat{A}, X)]_{i,j} (Z - Y)_{j,:}$

¹The authors in [21] did not name this homophily metric. We name it class homophily based on its definition.

124 To study the effect of heterophily, we define the *aggregation similarity score*.

125 **Definition 1.** *Aggregation similarity score*

$$S_{\text{agg}}(S(\hat{A}, X)) = \frac{\left| \left\{ v \mid \text{Mean}_u(\{S(\hat{A}, X)_{v,u} \mid Z_{u,:} = Z_{v,:}\}) \geq \text{Mean}_u(\{S(\hat{A}, X)_{v,u} \mid Z_{u,:} \neq Z_{v,:}\}) \right\} \right|}{|\mathcal{V}|} \quad (6)$$

126 where $\text{Mean}_u(\{\cdot\})$ takes the average over u of a given multiset of values or variables.

127 $S_{\text{agg}}(S(\hat{A}, X))$ is the proportion of nodes $v \in \mathcal{V}$ that will put relatively larger similarity weights on
 128 nodes in the same class than in other classes after aggregation. It is easy to see that $S_{\text{agg}}(S(\hat{A}, X)) \in$
 129 $[0, 1]$. But in practice, we observe that in most datasets, we will have $S_{\text{agg}}(S(\hat{A}, X)) \geq 0.5$. Based on
 130 this observation, we rescale (6) to the following modified aggregation similarity for practical usage,

$$S_{\text{agg}}^M(S(\hat{A}, X)) = \left[2S_{\text{agg}}(S(\hat{A}, X)) - 1 \right]_+ \quad (7)$$

131 In order to measure the consistency between labels and graph structures without considering node
 132 features and make a fair comparison with the existing homophily metrics in (3), we define the graph
 133 (\mathcal{G}) aggregation (\hat{A}) homophily and its modified version as

$$H_{\text{agg}}(\mathcal{G}) = S_{\text{agg}}(S(\hat{A}, Z)), \quad H_{\text{agg}}^M(\mathcal{G}) = S_{\text{agg}}^M(S(\hat{A}, Z)) \quad (8)$$

134 In practice, we will only check $H_{\text{agg}}(\mathcal{G})$ when $H_{\text{agg}}^M(\mathcal{G}) = 0$. As Figure 1 shows, when $\hat{A} = \hat{A}_{\text{rw}}$,
 135 $H_{\text{agg}}(\mathcal{G}) = H_{\text{agg}}^M(\mathcal{G}) = 1$. Thus, this new metric reflects the fact that nodes in classes 1 and 2 are still
 136 highly distinguishable after aggregation, while other metrics mentioned before fail to capture the
 137 information and misleadingly give value 0. This shows the advantage of $H_{\text{agg}}(\mathcal{G})$ and $H_{\text{agg}}^M(\mathcal{G})$ by
 138 additionally considering information from aggregation operator \hat{A} and the similarity matrix.

139 To comprehensively compare $H_{\text{agg}}^M(\mathcal{G})$ and the metrics in (3) in terms of how they reveal the influence
 140 of graph structure on the GNN performance, we generate synthetic graphs and evaluate SGC (31)
 141 and GCN (15) on them in the next subsection.

142 3.2 Evaluation and Comparison on Synthetic Graphs

143 **Data Generation & Experimental Setup** For one dataset, we generate 95 graphs in total with 19
 144 edge homophily levels varied from 0.05 to 0.95, each corresponding to 5 graphs. For every generated
 145 graph, we have 5 classes with 400 nodes in each class. In each class, there are randomly generated
 146 800 intra-class edges and $[(800 - 800H_{\text{edge}}(\mathcal{G})) / H_{\text{edge}}(\mathcal{G})]^2$ inter-class edges. The features of nodes
 147 in each class are sampled from node features in the corresponding class of the base dataset. Nodes
 148 are randomly split into 60%/20%/20% for train/validation/test. We train 1-hop SGC (*sgc-1* (31)) and
 149 GCN (15) on synthetic data (see appendix A.1 for hyperparameter searching range). For each value
 150 of $H_{\text{edge}}(\mathcal{G})$, we take the average test accuracy and standard deviation of runs over 5 generated graphs.
 151 For each generated graph, we also calculate its $H_{\text{node}}(\mathcal{G})$, $H_{\text{class}}(\mathcal{G})$ and $H_{\text{agg}}^M(\mathcal{G})$. Model performance
 with respect to different homophily values are shown in Figure 2

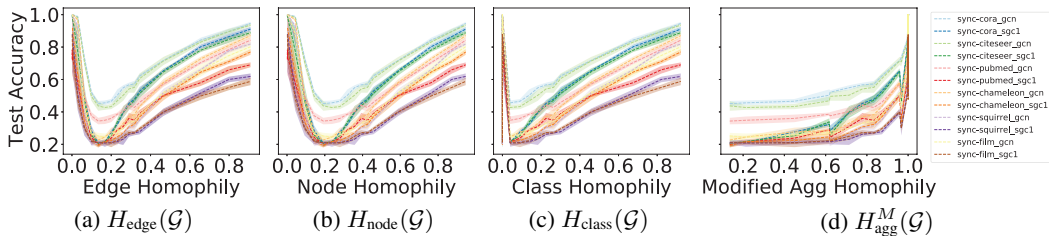


Figure 2: Comparison of baseline performance under different homophily metrics.

152

²According to (3), $H_{\text{edge}}(\mathcal{G}) = \# \text{intra-class edges} / (\# \text{intra-class edges} + \# \text{inter-class edges})$

153 **Comparison of Homophily Metrics** The performance of SGC-1 and GCN are expected to be
 154 monotonically increasing with a proper and informative homophily metric. However, Figure 2(a)(b)(c)
 155 show that the performance curves under $H_{\text{edge}}(\mathcal{G})$, $H_{\text{node}}(\mathcal{G})$ and $H_{\text{class}}(\mathcal{G})$ are U-shaped³, while
 156 Figure 2(d) reveals a nearly monotonic curve with a little perturbation around 1. This indicates that
 157 $H_{\text{agg}}^M(\mathcal{G})$ can describe how the graph structure affects the performance of SGC-1 and GCN.

158 In addition, we notice that in Figure 2(a), both SGC-1 and GCN get the worst performance on all
 159 datasets when $H_{\text{edge}}(\mathcal{G})$ is around somewhere between 0.1 and 0.2. This interesting phenomenon can
 160 be explained by the following theorem.

161 **Theorem 1.** (See Appendix C for proof). Suppose there are C classes in the graph \mathcal{G} , edges for each
 162 node are *i.i.d.* generated such that each edge of any node has probability h of connecting with nodes in
 163 the same class and probability $1 - h$ of connecting with nodes in different classes, and $\mathbb{E}(d_v) = d$ for
 164 all nodes. Let the aggregation operator $\hat{A} = \hat{A}_{\text{rw}}$. Then, for nodes v , u_1 and u_2 , where $Z_{u_1,:} = Z_{v,:}$
 165 and $Z_{u_2,:} \neq Z_{v,:}$, we have

$$g(h) \equiv \mathbb{E} \left(S(\hat{A}, Z)_{v,u_1} \right) - \mathbb{E} \left(S(\hat{A}, Z)_{v,u_2} \right) = \left(\frac{(C-1)(hd+1) - (1-h)d}{(C-1)(d+1)} \right)^2 \quad (9)$$

and the minimum of $g(h)$ is reached at

$$h = \frac{d+1-C}{Cd} = \frac{d_{\text{intra}}/h + 1 - C}{C(d_{\text{intra}}/h)} \Rightarrow h = \frac{d_{\text{intra}}}{Cd_{\text{intra}} + C - 1}$$

166 where $d_{\text{intra}} = dh$, which is the expectation of the number of neighbors of a node that have the same
 167 label as the node.

168 The value of $g(h)$ in (9) is the expected differences of the similarity values between nodes in the
 169 same class as v and nodes in other classes. $g(h)$ is strongly related to the definition of aggregation
 170 homophily and its minimum potentially implies the worst value of $H_{\text{agg}}(\mathcal{G})$. In the synthetic experi-
 171 ments, we have $d_{\text{intra}} = 2$, $C = 5$ and the minimum of $g(h)$ is reached at $h = 1/7 \approx 0.14$, which
 172 corresponds to the lowest point in the performance curve in Figure 2(a). In other words, the h where
 173 SGC-1 and GCN perform worst is where $g(h)$ gets the smallest value, instead of the point with the
 174 smallest edge homophily value. This again shows the advantage of $H_{\text{agg}}(\mathcal{G})$ over $H_{\text{edge}}(\mathcal{G})$ by taking
 175 use of the similarity matrix.

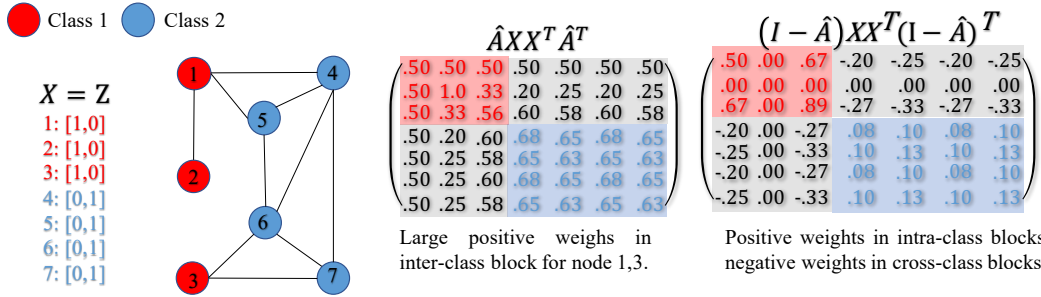


Figure 3: Example of how HP filter addresses harmful heterophily

176 4 Adaptive Channel Mixing (ACM) Framework

177 4.1 How Diversification Operation Helps with Harmful Heterophily

178 We first consider the example shown in Figure 3. From $S(\hat{A}, X)$, nodes 1,3 assign relatively large
 179 positive weights to nodes in class 2, which will negatively affect information aggregation. Despite
 180 the fact, we can still distinguish between nodes 1,3 and 4,5,6,7 by considering their neighborhood

³A similar J-shaped curve is found in [35], though using different data generation processes. It does not mention the insufficiency of edge homophily.

181 difference: nodes 1,3 are distinguishable from their neighbors while nodes 4,5,6,7 are homogeneous to
 182 their neighbors. This indicates, in some cases, although some nodes become similar after aggregation,
 183 they are still distinguishable via surrounding dissimilarities. This suggests the possibility of using
 184 *diversification operation to address harmful heterophily i.e.*, high-pass (HP) filter $I - \hat{A}$ [8] (will be
 185 introduced in next subsection). As $S(I - \hat{A}, Z)$ in Figure 3 shows, nodes 1,3 assign negative weights
 186 to nodes 4,5,6,7, i.e., nodes 1,3 treat nodes 4,5,6,7 as negative samples and will move away from
 187 them. Base on this example, we propose diversification distinguishability as follows,

188 **Definition 2.** *Diversification Distinguishability (DD) based on $S(I - \hat{A}, X)$.*

189 *Given $S(I - \hat{A}, X)$, a node v is diversification distinguishable if the following two conditions are*
 190 *satisfied at the same time,*

$$\begin{aligned} 1. & \text{Mean}_u \left(\{S(I - \hat{A}, X)_{v,u} | u \in \mathcal{V} \wedge Z_{u,:} = Z_{v,:}\} \right) \geq 0; \\ 2. & \text{Mean}_u \left(\{S(I - \hat{A}, X)_{v,u} | u \in \mathcal{V} \wedge Z_{u,:} \neq Z_{v,:}\} \right) \leq 0 \end{aligned} \quad (10)$$

191 *Then, graph diversification distinguishability value is defined as*

$$\text{DD}_{\hat{A},X}(\mathcal{G}) = \frac{1}{|\mathcal{V}|} \left| \{v | v \text{ is diversification distinguishable} \} \right| \quad (11)$$

192 $\text{DD}_{\hat{A},X}(\mathcal{G}) \in [0, 1]$ measures the proportion of nodes that HP filter is helpful for. Its effectiveness
 193 can be proved for binary classification problems under certain conditions, leading us to:

194 **Theorem 2.** (See Appendix E for proof). Suppose $X = Z, \hat{A} = \hat{A}_{\text{rw}}$. Then, for a binary classifica-
 195 tion problem, i.e., $C = 2$, all nodes are diversification distinguishable and $\text{DD}_{\hat{A},Z}(\mathcal{G}) = 1$.

196 Conducting both aggregation and diversification operations to distinctively extract the low- and high-
 197 frequency information from graph signals is the same as using filterbanks in graph signal processing.
 198 We introduce filterbanks in next subsection.

199 4.2 Filterbank in Spectral and Spatial Forms

200 **Filterbank** For the graph signal \mathbf{x} defined on \mathcal{G} , a 2-channel linear (analysis) filterbank [8] ⁴
 201 includes a pair of filters $H_{\text{LP}}, H_{\text{HP}}$, where H_{LP} and H_{HP} retain the low-frequency and high-frequency
 202 content of \mathbf{x} , respectively.

203 Most existing GNNs are under uni-channel filtering architecture [15, 30, 12] with either H_{LP} or
 204 H_{HP} channel that only partially preserves the input information. Unlike the uni-channel architecture,
 205 filterbanks with $H_{\text{LP}} + H_{\text{HP}} = I$ will not lose any information of the input signal, i.e., perfect
 206 reconstruction property [8, 27].

207 Generally, the Laplacian matrices ($L_{\text{sym}}, L_{\text{rw}}, \hat{L}_{\text{sym}}, \hat{L}_{\text{rw}}$) can be regarded as HP filters [8] and affinity
 208 matrices ($A_{\text{sym}}, A_{\text{rw}}, \hat{A}_{\text{sym}}, \hat{A}_{\text{rw}}$) can be treated as LP filters [25, 11]. Moreover, MLPs can be
 209 considered as owing a special identity filterbank with matrix I that satisfies $H_{\text{LP}} + H_{\text{HP}} = I + 0 = I$.

210 **Filterbank in Spatial Form** Filterbank methods can also be extended to spatial GNNs. Formally,
 211 on the node level, left multiplying H_{LP} and H_{HP} on \mathbf{x} performs as aggregation and diversification
 212 operations, respectively. For example, suppose $H_{\text{LP}} = \hat{A}$ and $H_{\text{HP}} = I - \hat{A}$, then for node i we have

$$(H_{\text{LP}}\mathbf{x})_i = \sum_{j \in \{\mathcal{N}_i \cup i\}} \hat{A}_{i,j} \mathbf{x}_j, (H_{\text{HP}}\mathbf{x})_i = \mathbf{x}_i - \sum_{j \in \{\mathcal{N}_i \cup i\}} \hat{A}_{i,j} \mathbf{x}_j \quad (12)$$

213 where $\hat{A}_{i,j}$ is the connection weight between two nodes. To leverage HP and identity channels in
 214 GNNs, we propose the Adaptive Channel Mixing (ACM) architecture in the following subsection.

⁴In graph signal processing, an additional synthesis filter [8] is required to form the 2-channel filterbank. But synthesis filter is not needed in our framework, so we do not introduce it in our paper.

215 **4.3 Adaptive Channel Mixing(ACM) GNN Framework**

216 ACM framework can be applied in lots of baseline GNNs and in this subsection, we use GCN as an
 217 example and introduce ACM framework in matrix form. We use H_{LP} and H_{HP} to represent general
 218 LP and HP filters. The ACM framework includes 3 steps as follows,

Step 1. Feature Extraction for Each Channel:

$$H_L^l = H_{LP} \text{ReLU}(H^{l-1}W_L^{l-1}), H_H^l = H_{HP} \text{ReLU}(H^{l-1}W_H^{l-1}), H_I^l = I \text{ReLU}(H^{l-1}W_I^{l-1}),$$

$$W_L^{l-1}, W_H^{l-1}, W_I^{l-1} \in \mathbb{R}^{F_{l-1} \times F_l};$$

Step 2. Feature-based Weight Learning with Row Normalization (RN):

$$\tilde{H}_L^l = \text{RN}(H_L^l), \tilde{H}_H^l = \text{RN}(H_H^l), \tilde{H}_I^l = \text{RN}(H_I^l);$$

$$\alpha_L^l = \sigma(\text{ELU}(\tilde{H}_L^l \tilde{W}_L^l)), \alpha_H^l = \sigma(\text{ELU}(\tilde{H}_H^l \tilde{W}_H^l)), \alpha_I^l = \sigma(\text{ELU}(\tilde{H}_I^l \tilde{W}_I^l)),$$

$$\tilde{W}_L^{l-1}, \tilde{W}_H^{l-1}, \tilde{W}_I^{l-1} \in \mathbb{R}^{F_l \times 1};$$

Step 3. Channel Mixing:

$$H^l = (\text{diag}(\alpha_L^l)H_L^l + \text{diag}(\alpha_H^l)H_H^l + \text{diag}(\alpha_I^l)H_I^l). \tag{13}$$

219 ACM-GCN first implements distinct non-linear feature extractions for 3 channels, respectively. After
 220 processed by a set of filterbanks, 3 filtered components H_L^l, H_H^l, H_I^l are obtained. Different nodes
 221 may have different needs for the information in the 3 channels, *e.g.*, in Figure 3, nodes 1,3 demand
 222 high-frequency information while node 2 only needs low-frequency information. To adaptively exploit
 223 information from different channels, ACM-GCN learns rowwise (nodewise) feature-conditioned
 224 (un-normalized) weights to combine the 3 channels. ACM can be easily plugged into spatial GNNs by
 225 replacing H_{LP} and H_{HP} by aggregation and diversification operations as shown in (12). See Appendix
 226 F for a detailed discussion of model comparison on synthetic datasets.

227 **Complexity** Number of learnable parameters in layer l of ACM-GCN is $3F_{l-1}(F_l + 1)$, while it is
 228 $F_{l-1}F_l$ in GCN. The computation of step 1-3 takes $NF_l(20 + F_{l-1}) + 2F_l(\text{nnz}(H_{LP}) + \text{nnz}(H_{HP}))$
 229 flops, while GCN layer takes $2NF_{l-1}F_l + 2F_l(\text{nnz}(H_{LP}))$ flops, where $\text{nnz}(\cdot)$ is the number of
 230 non-zero elements. A detailed experiments on running time is conducted in section 6.1

231 **Limitations** Diversification operation does not work well in all harmful heterophily cases. For
 232 example, consider an imbalanced dataset where several small clusters with distinctive labels are
 233 densely connected to a large cluster. In this case, the surrounding differences of nodes in small
 234 clusters are similar, *i.e.*, the neighborhood differences are mainly from their connection to the same
 235 large cluster, and this possibly makes diversification operation fail to discriminate them. See a more
 236 detailed demonstration and discussion in Appendix G

237 **5 Prior Work**

238 **GNNs on Addressing Heterophily** We discuss relevant work of GNNs on addressing heterophily
 239 challenge in this part. [1] acknowledges the difficulty of learning on graphs with weak homophily
 240 and propose MixHop to extract features from multi-hop neighborhood to get more information.
 241 Geom-GCN [28] precomputes unsupervised node embeddings and uses graph structure defined by
 242 geometric relationships in the embedding space to define the bi-level aggregation process. [13]
 243 proposes measurements based on feature smoothness and label smoothness that are potentially
 244 helpful to guide GNNs on dealing with heterophilous graphs. H₂GCN [35] combines 3 key designs
 245 to address heterophily: (1) ego- and neighbor-embedding separation; (2) higher-order neighborhoods;
 246 (3) combination of intermediate representations. CPGNN [34] models label correlations by the
 247 compatibility matrix, which is beneficial for heterophily settings, and propagates a prior belief
 248 estimation into GNNs by the compatibility matrix. GPRGNN [5] uses learnable weights that can be
 249 both positive and negative for feature propagation, it allows GRPGNN to adapt heterophily structure
 250 of graph and is able to handle both high and low frequency parts of the graph signals.

251 **GNNs with Filterbanks** Previously, there are geometric scattering networks [9, 27] that apply
 252 filterbanks to address over-smoothing [20] problem. The scattering construction captures different
 253 channels of variation from node features or labels. In geometric learning and graph signal processing,
 254 the band-pass filtering operations extract geometric information beyond smooth signals, thus it is
 255 believed that filterbanks can alleviate over-smoothing in GNNs. In ACM framework, we aim to

design a framework with the help of filterbanks to adaptively utilize different channels to address the challenge of learning on heterophilous graph. We deal with different problem as in [9, 27].

6 Experiments on Real-World Datasets

In this section, we evaluate ACM framework on real-world datasets. We first conduct ablation studies in subsection 6.1 to validate different components. Then, we compare with the state-of-the-arts models in subsection 6.2.

6.1 Ablation Study & Efficiency

Ablation Study on Different Components in ACM-SGC and ACM-GCN (%)										
Baseline	Model Components	Cornell	Wisconsin	Texas	Film	Chameleon	Squirrel	Cora	CiteSeer	PubMed
Models	LP HP Identity Mixing	Acc ± Std	Acc ± Std	Acc ± Std	Acc ± Std	Acc ± Std	Acc ± Std	Acc ± Std	Acc ± Std	Acc ± Std
SGC-1 w/	✓	74.43 ± 6.01	69.75 ± 5.02	84.1 ± 2.32	25.34 ± 2.41	64.55 ± 1.38	42.8 ± 1.1	85.24 ± 1.85	79.85 ± 1.04	84.44 ± 0.38
	✓ ✓	84.92 ± 4.59	91.75 ± 4.05	89.34 ± 3.67	36.94 ± 1.07	63.11 ± 1.64	44.8 ± 1.35	85.6 ± 1.33	80.33 ± 1.25	84.5 ± 0.42
	✓ ✓ ✓	92.3 ± 3.8	93 ± 2.11	91.64 ± 3.65	38.25 ± 1.6	57 ± 1.93	40.2 ± 2.18	85.98 ± 0.84	80.2 ± 2.01	84.37 ± 0.44
	✓ ✓ ✓ ✓	92.46 ± 2.10	93.38 ± 2.68	91.97 ± 3.23	38.71 ± 1.22	62.39 ± 2.45	45.65 ± 1.44	86.52 ± 1.55	80.79 ± 1.65	87.69 ± 0.6
GCN w/	✓	81.31 ± 3.13	70.25 ± 4.7	82.13 ± 4.05	34.45 ± 0.83	64.86 ± 1.56	45.11 ± 1.39	87.47 ± 0.82	81.3 ± 0.95	87.85 ± 0.44
	✓ ✓	82.95 ± 5.17	88.63 ± 2.51	88.03 ± 2.67	40.16 ± 1.06	68.12 ± 1.73	52.08 ± 1.47	88.44 ± 1.62	81.45 ± 0.9	90.09 ± 0.29
	✓ ✓ ✓	92.13 ± 2.65	94.37 ± 3.27	93.11 ± 2.48	40.3 ± 1.63	66.67 ± 2.16	49.45 ± 0.83	88.46 ± 1.31	81.42 ± 1.13	91.21 ± 1.17
	✓ ✓ ✓ ✓	92.62 ± 3.04	95.37 ± 2.1	94.75 ± 1.77	41.48 ± 0.78	67.79 ± 1.79	52.86 ± 1.96	89.11 ± 0.87	82.16 ± 0.84	90.72 ± 0.7
Average Running Time Per Epoch/Average Total Running Time Comparison										
SGC-1 w/	✓	2.70ms/0.59s	2.53ms/0.51s	2.63ms/0.55s	3.62ms/1.13s	4.96ms/3.99s	4.09ms/0.87s	5.34ms/8.22s	4.79ms/4.55s	5.58ms/7.70s
	✓ ✓	4.93ms/1.04s	5.03ms/1.04s	6.67ms/1.58s	6.68ms/1.37s	6.42ms/1.96s	7.41ms/1.93s	6.68ms/2.43s	6.69ms/1.96s	7.20ms/2.48s
	✓ ✓ ✓	4.73ms/0.98s	4.99ms/1.09s	4.79ms/1.02s	5.53ms/1.28s	5.89ms/1.50s	6.48ms/1.50s	6.50ms/2.09s	6.23ms/1.76s	6.73ms/2.24s
	✓ ✓ ✓ ✓	4.30ms/0.88s	4.51ms/0.91s	4.58ms/0.95s	5.86ms/1.19s	5.99ms/1.43s	6.84ms/1.63s	5.44ms/1.37s	5.72ms/1.44s	6.36ms/2.04s
GCN w/	✓	3.78ms/0.78s	3.91ms/0.79s	3.80ms/0.78s	4.42ms/0.89s	4.44ms/0.89s	6.85ms/1.48s	4.19ms/0.87s	5.22ms/1.13s	4.81ms/0.99s
	✓ ✓	7.63ms/1.54s	7.99ms/1.92s	7.26ms/1.48s	8.42ms/1.73s	9.74ms/2.76s	11.19ms/2.38s	7.74ms/1.61s	9.98ms/3.56s	9.10ms/1.85s
	✓ ✓ ✓	6.75ms/1.36s	6.83ms/1.41s	6.99ms/1.46s	7.62ms/1.54s	7.80ms/1.67s	9.76ms/2.02s	7.59ms/1.54s	7.43ms/1.54s	8.28ms/1.70s
	✓ ✓ ✓ ✓	7.33ms/1.49s	6.80ms/1.38s	6.99ms/1.41s	8.76ms/2.19s	7.81ms/1.59s	11.26ms/2.29s	7.77ms/1.59s	7.66ms/1.56s	8.36ms/1.70s
	✓ ✓ ✓ ✓	8.04ms/1.63s	8.98ms/1.83s	8.17ms/1.65s	9.29ms/2.00s	9.33ms/1.96s	12.15ms/2.53s	9.16ms/1.85s	9.48ms/1.95s	9.54ms/1.92s

Table 1: Ablation study on 9 real-world datasets [28]. Cell with ✓ means the component is applied to the baseline model. The best test results are highlighted.

We investigate the effectiveness and efficiency of adding HP, identity channels and the adaptive mixing mechanism in ACM framework by ablation study. Specifically, we apply the above components to SGC-1 and GCN separately, run 10 times on each dataset used in [28] with 60%/20%/20% random splits for train/validation/test and report the average test accuracy as well as the standard deviation. We also record the average running time per epoch (in milliseconds)/average total running time (in seconds) to compare the efficiency. (See Appendix A for hyperparameter searching space.)

From the results we can see that on most datasets, the additional HP and identity channels are helpful, even on strong homophily datasets, such as Cora, CiteSeer and PubMed. The adaptive mixing mechanism also shows its advantage over the method that directly adds the three channels together. This illustrates the necessity of learning to customize the channel usage adaptively for different nodes. As for efficiency, we can see that the running time is approximately doubled in ACM framework than the original model.

6.2 Comparison with State-of-the-art Models

Datasets & Experimental Setup In this section, we implement SGC [31] with 1 hop and 2 hop (SGC-1, SGC-2), GCN [15] and GraphSAGE and apply them [12] in ACM framework: we use \hat{A}_{rw} and mean aggregator as LP filter and the corresponding HP filter can be derived from [12]. We compare them with several baselines and state-of-the-art models: MLP with 2 layers (MLP-2), GAT [30], APPNP [16], GPRGNN [5], H₂GCN [35], MixHop [1], GCN+JK [15, 32, 21], GAT+JK [30, 32, 21] and Geom-GCN [28]. Besides the 9 benchmark datasets used in [28], we further tests the above models on 2 new benchmark datasets, *Deezer-Europe* and *YelpChi*, that are proposed in

	Cornell	Wisconsin	Texas	Film	Chameleon	Squirrel	Deezer-Europe	YelpChi	Cora	CiteSeer	PubMed	
#nodes	183	251	183	7,600	2,277	5,201	28,281	45,954	2,708	3,327	19,717	
#edges	295	499	309	33,544	36,101	217,073	92,752	3,846,979	5,429	4,732	44,338	
#features	1,703	1,703	1,703	931	2,325	2,089	31,241	32	1,433	3,703	500	
#classes	5	5	5	5	5	5	2	2	7	6	3	
$H_{edge}(\mathcal{G})$	0.5669	0.4480	0.4106	0.3750	0.2795	0.2416	0.5251	0.7730	0.8100	0.7362	0.8024	
$H_{node}(\mathcal{G})$	0.3855	0.1498	0.0968	0.2210	0.2470	0.2156	0.5299	0.7698	0.8252	0.7175	0.7924	
$H_{class}(\mathcal{G})$	0.0468	0.0941	0.0013	0.0110	0.0620	0.0254	0.0304	0.0520	0.7657	0.6270	0.6641	
$H_{agg}^M(\mathcal{G})$	0.8032	0.7768	0.694	0.6822	0.61	0.3566	0.5790	0.7206	0.9904	0.9826	0.9432	
Data Splits(%)	60/20/20	60/20/20	60/20/20	60/20/20	60/20/20	60/20/20	50/25/25	50/25/25	60/20/20	60/20/20	60/20/20	
Test Accuracy (%) of State-of-the-art Models, Baseline GNN Models and ACM-GNN models												Rank
MLP-2*	91.30 ± 0.70	93.87 ± 3.33	92.26 ± 0.71	38.58 ± 0.25	46.72 ± 0.46	31.28 ± 0.27	66.55 ± 0.72	87.94 ± 0.52	76.44 ± 0.30	76.25 ± 0.28	86.43 ± 0.13	9.00
GAT*	76.00 ± 1.01	71.01 ± 4.66	78.87 ± 0.86	35.98 ± 0.23	63.9 ± 0.46	42.72 ± 0.33	61.09 ± 0.77	81.42 ± 2.12	76.70 ± 0.42	67.20 ± 0.46	83.28 ± 0.12	11.73
APPNP*	91.80 ± 0.63	92.00 ± 3.59	91.18 ± 0.70	38.86 ± 0.24	51.91 ± 0.56	34.77 ± 0.34	67.21 ± 0.56	75.60 ± 0.48	79.41 ± 0.38	68.59 ± 0.30	85.02 ± 0.09	9.09
GPRGNN*	91.36 ± 0.70	93.75 ± 2.37	92.92 ± 0.61	39.30 ± 0.27	67.48 ± 0.40	49.93 ± 0.53	66.90 ± 0.50	71.59 ± 0.38	79.51 ± 0.36	67.63 ± 0.38	85.07 ± 0.09	6.64
H ₂ GCN	86.23 ± 4.71	87.5 ± 1.77	85.90 ± 3.53	38.85 ± 1.17	52.30 ± 0.48	30.39 ± 1.22	67.22 ± 0.90	88.48 ± 0.21	87.52 ± 0.61	79.97 ± 0.69	87.78 ± 0.28	7.27
MixHop	60.33 ± 28.53	77.25 ± 7.80	76.39 ± 7.66	33.13 ± 2.40	36.28 ± 10.22	24.55 ± 2.60	66.80 ± 0.58	87.02 ± 0.50	65.65 ± 11.31	49.52 ± 13.35	87.04 ± 4.10	13.09
GCN+JK	66.56 ± 13.82	62.50 ± 15.75	80.66 ± 1.91	32.72 ± 2.62	64.68 ± 2.85	53.40 ± 1.90	60.99 ± 0.14	64.35 ± 0.86	86.90 ± 1.51	73.77 ± 1.85	90.09 ± 0.68	10.09
GAT+JK	74.43 ± 10.24	69.50 ± 3.12	75.41 ± 7.18	35.41 ± 0.97	68.14 ± 1.18	52.28 ± 3.61	59.66 ± 0.92	90.04 ± 0.61	89.52 ± 0.43	74.49 ± 2.76	89.15 ± 0.87	8.27
Geom-GCN [†]	60.81	64.12	67.57	31.63	60.9	38.14	NA	NA	85.27	77.99	90.05	12.33
SGC-1	74.43 ± 6.01	69.75 ± 5.02	84.1 ± 2.42	25.34 ± 3.41	62.34 ± 1.92	42.8 ± 1.1	59.73 ± 0.12	58.62 ± 0.85	85.16 ± 0.82	79.93 ± 1.03	80.97 ± 0.91	12.18
SGC-2	77.7 ± 4.47	72.75 ± 3.91	81.48 ± 3.88	29.39 ± 0.20	63.02 ± 0.43	37.41 ± 1	61.56 ± 0.51	57.18 ± 0.75	86.58 ± 0.26	76.23 ± 0.29	81.14 ± 0.71	11.73
GCN	81.31 ± 3.13	70.25 ± 4.7	82.13 ± 4.05	34.45 ± 0.83	64.86 ± 1.56	45.11 ± 1.39	62.23 ± 0.53	63.62 ± 1.00	87.47 ± 0.82	81.3 ± 0.95	87.85 ± 0.44	8.18
GraphSAGE	71.41 ± 1.24	64.85 ± 5.14	79.03 ± 1.20	36.37 ± 0.21	62.15 ± 0.42	41.26 ± 0.26	62.55 ± 0.48	62.57 ± 1.12	86.58 ± 0.26	78.24 ± 0.30	86.85 ± 0.11	11.00
ACM-SGC-1	91.31 ± 2.94	93.38 ± 2.68	91.97 ± 3.23	38.71 ± 1.22	62.39 ± 2.45	45.65 ± 1.44	66.42 ± 0.96	85.83 ± 1.34	86.52 ± 1.55	80.79 ± 1.65	87.69 ± 0.6	6.27
ACM-SGC-2	90.66 ± 3.36	92.13 ± 5.06	90.66 ± 2.84	38.77 ± 1.74	58.51 ± 2.42	39.37 ± 1.41	66.98 ± 0.88	85.84 ± 1.17	87.44 ± 0.8	80.03 ± 1.26	88.01 ± 0.93	6.73
ACM-GCN	92.62 ± 3.04	95.37 ± 2.1	95.08 ± 1.8	41.48 ± 0.78	67.79 ± 1.79	52.86 ± 1.96	66.85 ± 0.95	89.91 ± 1.02	89.11 ± 0.87	82.16 ± 0.84	90.72 ± 0.7	1.73
ACM-SAGE	91.31 ± 2.94	90.13 ± 2.67	91.97 ± 3.15	36.68 ± 2.46	61.84 ± 2.71	44.63 ± 3.02	66.21 ± 0.89	88.73 ± 1.45	86.24 ± 1.25	80.87 ± 1.36	88.51 ± 0.9	6.45

Table 2: Experimental results: average test accuracy \pm standard deviation on 11 real-world benchmark datasets. The best results are highlighted. The "†" results are from [28] and NA means the reported results are not available. Results "*" are from [5, 21].

283 [21]⁵ We test these models 10 times on *Cornell*, *Wisconsin*, *Texas*, *Film*, *Chameleon*, *Squirrel*, *Cora*,
284 *Citeseer* and *Pubmed* following the same early stopping strategy, the same data splitting and Adam
285 [14] optimizer used in GPRGNN [5]. For *Deezer-Europe* and *YelpChi*, we test the above models
286 5 times with the same early stopping strategy, the same splits and AdamW [23] used in [21]. The
287 details of hyperparameter search are reported in appendix A.

288 The main results of this set of experiments with statistics of datasets are summarized in Table 2, where
289 we report the mean accuracy and standard deviation. We can see that after applied in ACM framework,
290 the performance of baseline models are boosted on almost all tasks. Especially, ACM-GCN performs
291 the best in terms of average rank (1.73) across all datasets and achieves SOTA performance on 6 out
292 of 11 datasets. Overall, It suggests that ACM framework can help GNNs to generalize better on node
293 classification tasks on heterophilous graphs.

294 7 Future Work

295 The similarity matrix and the new metrics defined in this paper mainly capture the linear relations
296 of the aggregated nodes. But this might be insufficient sometimes when nonlinearity information in
297 feature vectors are important for classification. In the future, similarity matrix that is able to capture
298 nonlinear relations between nodes can be proposed to define new homophily metrics.

299 From experimental results, the standard deviation of ACM-GNNs are relatively higher than GNNs on
300 some tasks and this is suspiciously caused by the feature-based weight learning mechanism. In the
301 future, a stabilizer or a more robust weight learning method can be proposed to reduce the variance.

302 8 Social Impact

303 We do not find any direct path of this work to any negative social impact.

⁵The authors proposed 8 new datasets. From the reported results, GCN only underperform MLP-2 on *Deezer-Europe* and *YelpChi*, which demonstrates the heterophily of these 2 datasets, therefore we choose them.

References

- 304
- 305 [1] S. Abu-El-Haija, B. Perozzi, A. Kapoor, N. Alipourfard, K. Lerman, H. Harutyunyan,
306 G. Ver Steeg, and A. Galstyan. Mixhop: Higher-order graph convolutional architectures
307 via sparsified neighborhood mixing. In *international conference on machine learning*, pages
308 21–29. PMLR, 2019.
- 309 [2] D. Bahdanau, K. Cho, and Y. Bengio. Neural machine translation by jointly learning to align
310 and translate. *arXiv preprint arXiv:1409.0473*, 2014.
- 311 [3] P. W. Battaglia, J. B. Hamrick, V. Bapst, A. Sanchez-Gonzalez, V. Zambaldi, M. Malinowski,
312 A. Tacchetti, D. Raposo, A. Santoro, R. Faulkner, et al. Relational inductive biases, deep
313 learning, and graph networks. *arXiv preprint arXiv:1806.01261*, 2018.
- 314 [4] M. M. Bronstein, J. Bruna, Y. LeCun, A. Szlam, and P. Vandergheynst. Geometric deep learning:
315 going beyond euclidean data. *arXiv*, abs/1611.08097, 2016.
- 316 [5] E. Chien, J. Peng, P. Li, and O. Milenkovic. Adaptive universal generalized pagerank graph
317 neural network. In *International Conference on Learning Representations*. [https://openreview.](https://openreview.net/forum)
318 *net/forum*, 2021.
- 319 [6] F. R. Chung and F. C. Graham. *Spectral graph theory*. Number 92. American Mathematical
320 Soc., 1997.
- 321 [7] M. Defferrard, X. Bresson, and P. Vandergheynst. Convolutional neural networks on graphs
322 with fast localized spectral filtering. *arXiv*, abs/1606.09375, 2016.
- 323 [8] V. N. Ekambaram. *Graph structured data viewed through a fourier lens*. University of California,
324 Berkeley, 2014.
- 325 [9] F. Gao, G. Wolf, and M. Hirn. Geometric scattering for graph data analysis. In *International*
326 *Conference on Machine Learning*, pages 2122–2131. PMLR, 2019.
- 327 [10] A. Graves, A.-r. Mohamed, and G. Hinton. Speech recognition with deep recurrent neural
328 networks. In *2013 IEEE international conference on acoustics, speech and signal processing*,
329 pages 6645–6649. Ieee, 2013.
- 330 [11] W. L. Hamilton. Graph representation learning. *Synthesis Lectures on Artificial Intelligence and*
331 *Machine Learning*, 14(3):1–159, 2020.
- 332 [12] W. L. Hamilton, R. Ying, and J. Leskovec. Inductive representation learning on large graphs.
333 *arXiv*, abs/1706.02216, 2017.
- 334 [13] Y. Hou, J. Zhang, J. Cheng, K. Ma, R. T. Ma, H. Chen, and M.-C. Yang. Measuring and
335 improving the use of graph information in graph neural networks. In *International Conference*
336 *on Learning Representations*, 2019.
- 337 [14] D. P. Kingma and J. Ba. Adam: A method for stochastic optimization. *arXiv preprint*
338 *arXiv:1412.6980*, 2014.
- 339 [15] T. N. Kipf and M. Welling. Semi-supervised classification with graph convolutional networks.
340 *arXiv*, abs/1609.02907, 2016.
- 341 [16] J. Klicpera, A. Bojchevski, and S. Günnemann. Predict then propagate: Graph neural networks
342 meet personalized pagerank. *arXiv preprint arXiv:1810.05997*, 2018.
- 343 [17] A. Krizhevsky, I. Sutskever, and G. E. Hinton. Imagenet classification with deep convolutional
344 neural networks. In *Advances in neural information processing systems*, pages 1097–1105,
345 2012.
- 346 [18] Y. LeCun, Y. Bengio, and G. Hinton. Deep learning. *nature*, 521(7553):436, 2015.
- 347 [19] Y. LeCun, L. Bottou, Y. Bengio, P. Haffner, et al. Gradient-based learning applied to document
348 recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.

- 349 [20] Q. Li, Z. Han, and X. Wu. Deeper insights into graph convolutional networks for semi-supervised
350 learning. *arXiv*, abs/1801.07606, 2018.
- 351 [21] D. Lim, X. Li, F. Hohne, and S.-N. Lim. New benchmarks for learning on non-homophilous
352 graphs. *arXiv preprint arXiv:2104.01404*, 2021.
- 353 [22] M. Liu, Z. Wang, and S. Ji. Non-local graph neural networks. *arXiv preprint arXiv:2005.14612*,
354 2020.
- 355 [23] I. Loshchilov and F. Hutter. Decoupled weight decay regularization. *arXiv preprint*
356 *arXiv:1711.05101*, 2017.
- 357 [24] S. Luan, M. Zhao, X.-W. Chang, and D. Precup. Break the ceiling: Stronger multi-scale deep
358 graph convolutional networks. *arXiv preprint arXiv:1906.02174*, 2019.
- 359 [25] T. Maehara. Revisiting graph neural networks: All we have is low-pass filters. *arXiv preprint*
360 *arXiv:1905.09550*, 2019.
- 361 [26] M. McPherson, L. Smith-Lovin, and J. M. Cook. Birds of a feather: Homophily in social
362 networks. *Annual review of sociology*, 27(1):415–444, 2001.
- 363 [27] Y. Min, F. Wenkel, and G. Wolf. Scattering gcn: Overcoming oversmoothness in graph
364 convolutional networks. *arXiv preprint arXiv:2003.08414*, 2020.
- 365 [28] H. Pei, B. Wei, K. C.-C. Chang, Y. Lei, and B. Yang. Geom-gcn: Geometric graph convolutional
366 networks. *arXiv preprint arXiv:2002.05287*, 2020.
- 367 [29] F. Scarselli, M. Gori, A. C. Tsoi, M. Hagenbuchner, and G. Monfardini. The graph neural
368 network model. *IEEE transactions on neural networks*, 20(1):61–80, 2008.
- 369 [30] P. Velickovic, G. Cucurull, A. Casanova, A. Romero, P. Lio, and Y. Bengio. Graph attention
370 networks. *arXiv*, abs/1710.10903, 2017.
- 371 [31] F. Wu, T. Zhang, A. H. d. Souza Jr, C. Fifty, T. Yu, and K. Q. Weinberger. Simplifying graph
372 convolutional networks. *arXiv preprint arXiv:1902.07153*, 2019.
- 373 [32] K. Xu, C. Li, Y. Tian, T. Sonobe, K.-i. Kawarabayashi, and S. Jegelka. Representation learning
374 on graphs with jumping knowledge networks. In J. Dy and A. Krause, editors, *Proceedings of*
375 *the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine*
376 *Learning Research*, pages 5453–5462. PMLR, 10–15 Jul 2018.
- 377 [33] Y. Yan, M. Hashemi, K. Swersky, Y. Yang, and D. Koutra. Two sides of the same coin:
378 Heterophily and oversmoothing in graph convolutional neural networks. *arXiv preprint*
379 *arXiv:2102.06462*, 2021.
- 380 [34] J. Zhu, R. A. Rossi, A. Rao, T. Mai, N. Lipka, N. K. Ahmed, and D. Koutra. Graph neural
381 networks with heterophily. *arXiv preprint arXiv:2009.13566*, 2020.
- 382 [35] J. Zhu, Y. Yan, L. Zhao, M. Heimann, L. Akoglu, and D. Koutra. Beyond homophily in graph
383 neural networks: Current limitations and effective designs. *Advances in Neural Information*
384 *Processing Systems*, 33, 2020.

385 **Checklist**

- 386 1. For all authors...
- 387 (a) Do the main claims made in the abstract and introduction accurately reflect the paper's
388 contributions and scope? [Yes]
- 389 (b) Did you describe the limitations of your work? [Yes] In the Appendix **C**, we discussion
390 cases that high-pass filter cannot tackle.
- 391 (c) Did you discuss any potential negative societal impacts of your work? [No] It is in
392 Section 8, we have not come up with significant social negative impact.
- 393 (d) Have you read the ethics review guidelines and ensured that your paper conforms to
394 them? [Yes]
- 395 2. If you are including theoretical results...
- 396 (a) Did you state the full set of assumptions of all theoretical results? [Yes] In Section
397 3&4, we mainly define a new homophily metric and it is followed by two theorems.
- 398 (b) Did you include complete proofs of all theoretical results? [Yes] In Appendix **B&C&**
399 **E**, we justify the new metric and two theorems.
- 400 3. If you ran experiments...
- 401 (a) Did you include the code, data, and instructions needed to reproduce the main experi-
402 mental results (either in the supplemental material or as a URL)? [Yes] The settings are
403 provided in details and the source code is submitted in the supplemental material.
- 404 (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they
405 were chosen)? [Yes] In Section 6, we specify model details.
- 406 (c) Did you report error bars (e.g., with respect to the random seed after running experi-
407 ments multiple times)? [Yes] We include average test accuracy of times of running
408 with standard deviation.
- 409 (d) Did you include the total amount of compute and the type of resources used (e.g., type
410 of GPUs, internal cluster, or cloud provider)? [Yes] We include hardware details in
411 Appendix, which is not computationally expensive.
- 412 4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
- 413 (a) If your work uses existing assets, did you cite the creators? [Yes] In Section 6, we
414 specify the datasets with their data split sources in footnotes.
- 415 (b) Did you mention the license of the assets? [No]
- 416 (c) Did you include any new assets either in the supplemental material or as a URL? [No]
- 417 (d) Did you discuss whether and how consent was obtained from people whose data you're
418 using/curating? [No]
- 419 (e) Did you discuss whether the data you are using/curating contains personally identifiable
420 information or offensive content? [No] None included.
- 421 5. If you used crowdsourcing or conducted research with human subjects...
- 422 (a) Did you include the full text of instructions given to participants and screenshots, if
423 applicable? [No] None included.
- 424 (b) Did you describe any potential participant risks, with links to Institutional Review
425 Board (IRB) approvals, if applicable? [No] None included.
- 426 (c) Did you include the estimated hourly wage paid to participants and the total amount
427 spent on participant compensation? [No] None included.