Generalizing Graph Neural Networks Beyond Homophily

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Abstract

We investigate the representation power of graph neural networks in the semi-supervised node classification task under heterophily or low homophily, i.e., in networks where connected nodes may have different class labels and dissimilar features. Most existing GNNs fail to generalize to this setting, and are even outperformed by models that ignore the graph structure (e.g., multilayer perceptrons). Motivated by this limitation, we identify a set of key designs—ego- and neighbor-embedding separation, higher-order neighborhoods, and combination of intermediate representations—that boost learning from the graph structure under heterophily, and combine them into a new graph convolutional neural network, H$_2$GCN. Going beyond the traditional benchmarks with strong homophily, our empirical analysis on synthetic and real networks shows that, thanks to the identified designs, H$_2$GCN has consistently strong performance across the full spectrum of low-to-high homophily, unlike competitive prior models without them.

1 Introduction

We focus on the effectiveness of graph neural networks (GNNs) [38] in tackling the semi-supervised node classification task in challenging settings: the goal of the task is to infer the unknown labels of the nodes by using the network structure [39], given partially labeled networks with node features (or attributes). Unlike most prior work that considers networks with strong homophily, we study the representation power of GNNs in settings with different levels of homophily or class label smoothness.

Homophily is a key principle of many real-world networks, whereby linked nodes often belong to the same class or have similar features (“birds of a feather flock together”) [17]. For example, friends are likely to have similar political beliefs or age, and papers tend to cite papers from the same research area [19]. GNNs model the homophily principle by propagating features and aggregating them within various graph neighborhoods via different mechanisms (e.g., averaging, LSTM) [13][32]. However, in the real world, there are also settings where “opposites attract”, leading to networks with heterophily: linked nodes are likely from different classes or have dissimilar features. For instance, the majority of people tend to connect with people of the opposite gender in dating networks, different amino acid types are more likely to connect in protein structures, fraudsters are more likely to connect to accomplices than to other fraudsters in online purchasing networks [20].

Since GNNs assume strong homophily, most existing models fail to generalize to networks with heterophily (or low/medium level of homophily). In such cases, we find that even models that ignore
We further assume a class label vector \( y \) with strong homophily/heterophily:

\( \text{as for } f \text{ (or hidden state vector) at round } \)

The edge homophily ratio in Dfn. 1 gives an overall trend with strong heterophily (i.e., low/weak homophily) have small edge homophily ratio \( h \to 0 \).

The edge homophily ratio in Dfn. 1 gives an overall trend for all the edges in the graph. The actual level of homophily may vary within different pairs of node classes, i.e., there is different tendency of the graph structure altogether, such as multilayer perceptrons or MLPs, can outperform a number of existing GNNs. Motivated by this limitation, we make the following contributions:

- **Current Limitations**: We reveal the limitation of GNNs to learn over networks with heterophily, which is ignored in the literature due to evaluation on few benchmarks with similar properties. § 3
- **Key Design Choices for Heterophily & New Model**: We identify a set of key design choices that can boost learning from the graph structure in heterophily settings without trading off accuracy in homophily settings: (D1) ego- and neighbor-embedding separation, (D2) higher-order neighborhoods, and (D3) combination of intermediate representations. We justify the designs theoretically and empirically, combine them into a new model, \( H_2 \text{GCN} \), that effectively adapts to both heterophily and homophily settings, and compare our framework to prior GNN models. § 3
- **Extensive Empirical Evaluation**: We empirically analyze our model and competitive existing GNN models on both synthetic and real networks covering the full spectrum of low-to-high homophily (besides the typically-used benchmarks with high homophily). We show that \( H_2 \text{GCN} \) has consistently strong performance unlike existing models tailored to homophily. § 5

2 Notation and Preliminaries

We summarize our notation in Table A.1 (App. A). Let \( G = (V, \mathcal{E}) \) be an undirected, unweighted graph with nodeset \( V \) and edgset \( \mathcal{E} \). We denote a general neighborhood centered around \( v \) as \( N(v) \) (\( G \) may have self-loops), the corresponding neighborhood that does not include the ego (node \( v \)) as \( \bar{N}(v) \), and the general neighbors of node \( v \) at exactly \( i \) hops/steps away (minimum distance) as \( N_i(v) \). For example, \( N_1(v) = \{ u : (u, v) \in \mathcal{E} \} \) are the immediate neighbors of \( v \). Other examples are shown in Fig. 1. We represent the graph by its adjacency matrix \( A \in \{0, 1\}^{n \times n} \) and its node feature matrix \( X \in \mathbb{R}^{n \times P} \), where the vector \( x_v \) corresponds to the ego-feature of node \( v \), and \( \{ x_u : u \in \bar{N}(v) \} \) to its neighbor-features.

We further assume a class label vector \( y \), which for each node \( v \) contains a unique class label \( y_v \). The goal of semi-supervised node classification is to learn a mapping \( \ell : \mathcal{V} \to \mathcal{Y} \), where \( \mathcal{Y} \) is the set of labels, given a set of labeled nodes \( \mathcal{T}_V = \{ (v_1, y_1), (v_2, y_2), ... \} \) as training data.

Graph neural networks From a probabilistic perspective, most GNN models assume the following local Markov property on node features: for each node \( v \in V \), there exists a neighborhood \( N(v) \) such that \( y_v \) only depends on the ego-feature \( x_v \) and neighbor-features \( \{ x_u : u \in N(v) \} \). Most models derive the class label \( y_v \) via the following representation learning approach:

\[
r_v^{(K)} = f \left( r_v^{(k-1)}, \{ r_u^{(k-1)} : u \in N(v) \} \right), \quad r_v^{(0)} = x_v, \quad \text{and} \quad y_v = \arg \max \{ \text{softmax}(r_v^{(K)}) \mathbf{W} \},
\]

(1)

where the embedding function \( f \) is applied repeatedly in \( K \) total rounds, node \( v \)'s representation (or hidden state vector) at round \( k \), \( r_v^{(k)} \), is learned from its ego- and neighbor-representations in the previous round, and a softmax classifier with learnable weight matrix \( \mathbf{W} \) is applied to the final representation of \( v \). Most existing models differ in their definitions of neighborhoods \( N(v) \) and embedding function \( f \). A typical definition of neighborhood is \( N_1(v) \) —i.e., the 1-hop neighbors of \( v \). As for \( f \), in graph convolutional networks (GCN) [13] each node repeatedly averages its own features and those of its neighbors to update its own feature representation. Using an attention mechanism, GAT [32] models the influence of different neighbors more precisely as a weighted average of the ego- and neighbor-features. GraphSAGE [8] generalizes the aggregation beyond averaging, and models the ego-features distinctly from the neighbor-features in its subsampled neighborhood.

Homophily and heterophily In this work, we focus on heterophily in class labels. We first define the edge homophily ratio \( h \) as a measure of the graph homophily level, and use it to define graphs with strong homophily/heterophily:

**Definition 1** The edge homophily ratio \( h = \frac{|\{(u,v) : (u,v) \in \mathcal{E} \land y_u = y_v \}|}{|\mathcal{E}|} \) is the fraction of edges in a graph which connect nodes that have the same class label (i.e., intra-class edges).

**Definition 2** Graphs with strong homophily have high edge homophily ratio \( h \to 1 \), while graphs with strong heterophily (i.e., low/weak homophily) have small edge homophily ratio \( h \to 0 \).

Figure 1: Neighborhoods.
connection between each pair of classes. In App. [H] we give more details about capturing these more complex network characteristics via an empirical class compatibility matrix $H$, whose $i$, $j$-th entry is the fraction of outgoing edges to nodes in class $j$ among all outgoing edges from nodes in class $i$.

Heterophily ≠ Heterogeneity. We remark that heterophily, which we study in this work, is a distinct network concept from heterogeneity. Formally, a network is heterogeneous [30] if it has at least two types of nodes and different relationships between them (e.g., knowledge graphs), and homogeneous if it has a single type of nodes (e.g., users) and a single type of edges (e.g., friendship). The type of nodes in heterogeneous graphs does not necessarily match the class labels $y_i$, therefore both homogeneous and heterogeneous networks may have different levels of homophily.

3 Learning Over Networks with Heterophily

While many GNN models have been proposed, most of them are designed under the assumption of homophily, and are not capable of handling heterophily. As a motivating example, Table 1 shows the mean classification accuracy for several leading GNN models on our synthetic benchmark syn-cora, where we can control the homophily/heterophily level (see App. [G] for details on the data and setup). Here we consider two homophily ratios, $h = 0.1$ and $h = 0.7$, one for high heterophily and one for high homophily. We observe that for heterophily ($h = 0.1$) all existing methods fail to perform better than a Multilayer Perceptron (MLP) with 1 hidden layer, a graph-agnostic baseline that relies solely on the node features for classification (differences in accuracy of MLP for different $h$ are due to randomness). Especially, GCN [13], GAT [32] and MixHop [1] show up to 42% worse performance than MLP, highlighting that methods that work well under high homophily ($h = 0.7$) may not be appropriate for networks with low/medium homophily.

Motivated by this limitation, in the following subsections, we discuss and theoretically justify a set of key design choices that, when appropriately incorporated in a GNN framework, can improve the performance in the challenging heterophily settings. Then, we present $H_2$GCN, a model that, thanks to these designs, adapts well to both homophyly and heterophily (Table 1, last row). In Section 5, we provide comprehensive empirical analysis on both synthetic and real data with varying homophily levels, and show that $H_2$GCN performs consistently well across different levels, and improves over MLP by effectively leveraging the graph structure in challenging settings.

### 3.1 Effective Designs for Networks with Heterophily

We have identified three key designs that—when appropriately integrated—can help improve the performance of GNN models in heterophily settings: (D1) ego- and neighbor-embedding separation; (D2) higher-order neighborhoods; and (D3) combination of intermediate representations.

#### 3.1.1 (D1) Ego- and Neighbor-Embedding Separation

The first design entails encoding each ego-embedding (i.e., a node’s embedding) separately from the aggregated embeddings of its neighbors, since they are likely to be dissimilar in heterophily settings. Formally, the representation (or hidden state vector) learned for each node $v$ at round $k$ is given as:

$$r_v^{(k)} = \text{COMBINE} \left( r_v^{(k-1)}, \text{AGGR}(r_u^{(k-1)} : u \in \bar{N}(v)) \right),$$

(2)

the neighborhood $\bar{N}(v)$ does not include $v$ (no self-loops), the AGGR function aggregates representations only from the neighbors (in some way—e.g., average), and COMBINE and AGGR may be followed by a non-linear transformation. For heterophily, after aggregating the neighbors’ representations, the definition of COMBINE (akin to ‘skip connection’ between layers) is critical: a simple way of combining the ego- and the aggregated neighbor-embeddings without ‘mixing’ them is to concatenate them—rather than average all of them as in the GCN model by Kipf and Welling [13].
Below we formalize this observation for 2-hop neighborhoods, and prove

Theoretical Justification. We prove theoretically that, under some conditions, a GCN layer that

aggregation over higher-order neighborhoods that most GNN models achieve through multiple rounds

of first-order propagation based on variants of Eq. (2).

Theorem 2 Consider a graph $\mathcal{G}$ without self-loops ($\S$2) with label set $\mathcal{Y}$, where for each node $v$, its neighbors' class labels $\{y_u : u \in N(v)\}$ are conditionally independent given $y_v$, and $P(y_u = y | y_v) = P(y_u = y)$ for any $y$. 

1 These models consider self-loops, which turn each ego also into a neighbor, and thus mix the ego- and neighbor-representations. E.g., GCN and MixHop operate on the symmetric normalized adjacency matrix augmented with self-loops: $\tilde{A} = \tilde{D}^{-\frac{1}{2}}(A + I)\tilde{D}^{-\frac{1}{2}}$, where $I$ is the identity and $\tilde{D}$ the degree matrix of $A + I$. 

\[ A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 4 \\ 3 & 4 & 1 \end{pmatrix} \]

\[ \tilde{A} = \begin{pmatrix} 1 & \frac{2}{2} & \frac{3}{2} \\ \frac{2}{2} & 1 & \frac{4}{2} \\ \frac{3}{2} & \frac{4}{2} & 1 \end{pmatrix} \]
$y_v | y_e = h, \ P(y_u = y | y_e) = \frac{1-h}{|V|-1}, \ \forall y \neq y_v$. Then, the 2-hop neighborhood $N_2(v)$ for a node $v$ will always be homophily-dominant in expectation.

**Observations.** Under heterophily ($h = 0.1$), GCN-Cheby, which models different neighborhoods by combining Chebyshev polynomials to approximate a higher-order graph convolution operation [5], outperforms GCN and GAT, which aggregate over only the immediate neighbors $N_1$, by up to +31% (Table 1). MixHop, which explicitly models 1-hop and 2-hop neighborhoods (though ‘mixes’ the ego- and neighbor-embeddings[^1]), violating design D1, also outperforms these two models.

### 3.1.3 (D3) Combination of Intermediate Representations

The third design combines the intermediate representations of each node from multiple rounds at the final layer:

$$r_v^{(\text{final})} = \text{COMBINE} \left( r_v^{(1)}, r_v^{(2)}, \ldots, r_v^{(K)} \right)$$

(4)

to explicitly capture local and global information via COMBINE functions that leverage each representation separately—e.g., concatenation, LSTM-attention [34]. This design is introduced in jumping knowledge networks [34] and shown to increase the representation power of GCNs under homophily.

**Intuition.** Intuitively, each round collects information with different locality—earlier rounds are more local, while later rounds capture increasingly more global information (implicitly, via propagation). Similar to D2 (which models explicit neighborhoods), this design models the distribution of neighbor representations in low-homophily networks more accurately. It also allows the class prediction to leverage different neighborhood ranges in different networks, adapting to their structural properties.

**Theoretical Justification.** The benefit of combining intermediate representations can be theoretically explained from the spectral perspective. Assuming a GCN-style layer—where propagation can be viewed as spectral filtering—, the adjacency matrix $A$ is a low-pass filter [33], so intermediate outputs from earlier rounds contain higher-frequency components than outputs from later rounds. At the same time, the following theorem holds for graphs with heterophily, where we view class labels as graph signals (as in graph signal processing):

**Theorem 3** Consider graph signals (label vectors) $s, t \in \{0,1\}^{|V|}$ defined on an undirected graph $G$ with edge homophily ratios $h_s$ and $h_t$, respectively. If $h_s < h_t$, then signal $s$ has higher energy (Dfn. 5) in high-frequency components than $t$ in the spectrum of unnormalized graph Laplacian $L$.

In other words, in heterophily settings, the label distribution contains more information at higher than lower frequencies (see proof in App. C.3). Thus, by combining the intermediate outputs from different layers, this design captures both low- and high-frequency components in the final representation, which is critical in heterophily settings, and allows for more expressiveness in the general setting.

**Observations.** By concatenating the intermediate representations from two rounds with the embedded ego-representation (following the jumping knowledge framework [34]), GCN’s accuracy increases to 58.93% ± 3.17 for $h = 0.1$, a 20% improvement over its counterpart without design D3 (Table 1).

**Summary of designs** To sum up, D1 models (at each layer) the ego- and neighbor-representations distinctly, D2 leverages (at each layer) representations of neighbors at different distances distinctly, and D3 leverages (at the final layer) the learned ego-representations at previous layers distinctly.

### 3.2 H2-GCN: A Framework for Networks with Homophily or Heterophily

We now describe H2-GCN, which combines designs D1-D3 to adapt to heterophily. It has three stages (Alg. 1, App. D): (S1) feature embedding, (S2) neighborhood aggregation, and (S3) classification.

**The feature embedding stage (S1)** uses a graph-agnostic dense layer to generate for each node $v$ the feature embedding $r_v^{(0)} \in \mathbb{R}^p$ based on its ego-feature $x_v$: $r_v^{(0)} = \sigma(x_v, W_e)$, where $\sigma$ is an optional non-linear function, and $W_e \in \mathbb{R}^{F \times p}$ is a learnable weight matrix.

In the **neighborhood aggregation stage (S2)**, the generated embeddings are aggregated and repeatedly updated within the node’s neighborhood for $K$ rounds. Following designs D1 and D2, the neighborhood $N(v)$ of our framework involves two sub-neighborhoods without the egos: the 1-hop graph neighbors $\bar{N}_1(v)$ and the 2-hop neighbors $\bar{N}_2(v)$, as shown in Fig. 1.

$$r_v^{(k)} = \text{COMBINE} \left( \text{AGGR}\{r_u^{(k-1)} : u \in \bar{N}_1(v)\}, \text{AGGR}\{r_u^{(k-1)} : u \in \bar{N}_2(v)\} \right).$$

(5)

[^1]: Violating design D1
We set COMBINE as concatenation (as to not mix different neighborhood ranges), and AGGR as a degree-normalized average of the neighbor-embeddings in sub-neighborhood \( \tilde{N}_i(v) \):

\[
r_v^{(k)} = \left( r_{v,1}^{(k)} \right| r_{v,2}^{(k)} \right) \quad \text{and} \quad r_v^{(k)} = \text{AGGR}(r_u^{(k-1)} : u \in \tilde{N}_i(v)) = \sum_{u \in \tilde{N}_i(v)} r_u^{(k-1)} d_{u,i}^{-1/2} d_{u,i}^{-1/2},
\]

where \( d_{v,i} = |\tilde{N}_i(v)| \) is the i-hop degree of node \( v \) (i.e., number of nodes in its i-hop neighborhood). Note that unlike Eq. (2), here we do not combine the ego-embedding of node \( v \) with the neighbor-embeddings. We found that removing the typical non-linear embedding transformations per round, as in SGC [33], works better (App. D.2), and in such case including the ego-embedding only in the final representation avoids redundancies. By design D3, the final representation of each node \( v \) combines all its intermediate representations:

\[
r_v^{(\text{final})} = \text{COMBINE}(r_v^{(0)}, r_v^{(1)}, \ldots, r_v^{(K)}),
\]

where we empirically find concatenation works better than max-pooling [34] as the COMBINE function.

In the classification stage (S3), the node is classified based on its final embedding \( r_v^{(\text{final})} \):

\[
y_v = \arg \max \{ \text{softmax}(r_v^{(\text{final})} W_e) \},
\]

where \( W_e \in \mathbb{R}^{(2K+1)p \times |\mathcal{Y}|} \) is a learnable weight matrix. We visualize our framework in App. D.

**Time complexity** The feature embedding stage (S1) takes \( O(\text{nnz}(X)p) \), where \( \text{nnz}(X) \) is the number of non-0s in feature matrix \( X \in \mathbb{R}^{n \times F} \), and \( p \) is the dimension of the feature embeddings. The neighborhood aggregation stage (S2) takes \( O(|E|d_{\text{max}}) \) to derive the 2-hop neighborhoods via sparse-matrix multiplications, where \( d_{\text{max}} \) is the maximum degree of all nodes, and \( O(2K(|E| + |E_2|)p) \) for \( K \) rounds of aggregation, where \( |E_2| = \frac{1}{2} \sum_{v \in V} |\tilde{N}_2(v)| \). We give a detailed analysis in App. D.

4 Other Related Work

We discuss relevant work on GNNs here, and give other related work (e.g., classification under heterophily) in App. E. Besides the models mentioned above, there are various comprehensive reviews describing previously proposed architectures [38][39][47]. Recent work has investigated GNN’s ability to capture graph information, proposing diagnostic measurements based on feature smoothness and label smoothness [9] that may guide the learning process. To capture more graph information, other works generalize graph convolution outside of immediate neighborhoods. For example, apart from MixHop [1] (cf. § 3.1), Graph Diffusion Convolution [14] replaces the adjacency matrix with a sparsified version of a diffusion matrix (e.g., heat kernel or PageRank). Geom-GCN [21] precomputes unsupervised node embeddings and uses neighborhoods defined by geometric relationships in the resulting latent space to define graph convolution. Some of these works [1][21][9] acknowledge the challenges of learning from graphs with heterophily. Others have noted that node labels may have complex relationships that should be modeled directly. For instance, Graph Agreement Models [29] augment the classification task with an agreement task, co-training a model to predict whether pairs of nodes share the same label. Graph Markov Neural Networks [22] model the joint label distribution with a conditional random field, trained with expectation maximization using GNNs.

**Comparison of H²GCN to existing GNN models** As shown in Table 2, H²GCN differs from existing GNN models with respect to designs D1-D3, and their implementations (we give more details in App. D). Notably, H²GCN learns a graph-agnostic feature embedding in stage (S1), and skips the non-linear embeddings of aggregated representations per round that other models use (e.g., GraphSAGE, MixHop, GCN), resulting in a simpler yet powerful architecture.

| Method   | D1 | D2 | D3 |
|----------|----|----|----|
| GCN [13] | x  | x  | x  |
| GAT [12] | x  | x  | x  |
| GCN-Cheby [8] | x | x | x |
| GraphSAGE [6] | ✓ | ✓ | ✓ |
| MixHop [1] | x  | ✓  | x  |
| H²GCN (proposed) | ✓  | ✓  | ✓  |

5 Empirical Evaluation

In our analysis, we (1) compare H²GCN to existing GNN models on synthetic and real graphs with a wide range of low-to-high homophily values; and (2) evaluate the significance of designs D1-D3.

**Baseline models** We consider MLP with 1 hidden layer, and all the methods listed in Table 2. For H²GCN, we model the first- and second-order neighborhoods (\( \tilde{N}_1 \) and \( \tilde{N}_2 \)), and consider two variants: H²GCN-1 uses one embedding round (\( K = 1 \)) and H²GCN-2 uses two rounds (\( K = 2 \)). We tune all the models on the same train/validation splits (see App. E for details).
5.1 Evaluation on Synthetic Benchmarks

Synthetic datasets & setup We generate synthetic graphs with various homophily ratios $h$ (cf. table below) by adopting an approach similar to [2]. In App. G we describe the data generation process, the experimental setup, and the data statistics in detail. All methods share the same training, validation and test splits (25%, 25%, 50% per class), and we report the average accuracy and standard deviation (stdev) over three generated graphs per heterophily level and benchmark dataset.

Model comparison Figure 2 shows the mean test accuracy (and stdev) over all random splits of our synthetic benchmarks. We observe similar trends on both benchmarks: $H_2GCN$ has the best trend overall, outperforming the baseline models in most heterophily settings, while tying with other models in homophily. The performance of GCN, GAT and MixHop, which mix the ego- and neighbor-embeddings, increases with respect to the homophily level. But, while they achieve near-perfect accuracy under strong homophily ($h \to 1$), they are significantly less accurate than MLP (near-flat performance curve as it is graph-agnostic) for many heterophily settings. GraphSAGE and GCN-Cheby, which leverage some of the identified designs D1-D3 (Table 2 § 1), are more competitive in such settings. We note that all the methods—except GCN and GAT—learn more effectively under perfect heterophily ($h=0$) than weaker settings (e.g., $h \in [0.1, 0.3]$), as evidenced by the J-shaped performance curves in low-homophily ranges.

Significance of design choices Using syn-products, we show the significance of designs D1-D3 (§ 5.1) through ablation studies with variants of $H_2GCN$ (Fig. 3 Table G.4).

(D1) Ego- and Neighbor-embedding Separation. We consider $H_2GCN$-1 variants that separate the ego- and neighbor-embeddings and model: (S0) neighborhoods $\bar{N}_1$ and $\bar{N}_2$ (i.e., $H_2GCN$-1); (S1) only the 1-hop neighborhood $N_1$ in Eq. 5; and their counterparts that do not separate the two embeddings and use: (S0) neighborhoods $N_1$ and $N_2$ (including $v$); and (S1) only the 1-hop neighborhood $N_1$. In Fig. 3a, we see that the two variants that learn separate embedding functions significantly outperform the others (S0) in heterophily settings ($h < 0.7$) by up to 40%, which shows that design D1 is critical for success in heterophily. Vanilla $H_2GCN$-1 (S0) performs best for all homophily levels.

(D2) Higher-order Neighborhoods. For this design, we consider three variants of $H_2GCN$-1 without specific neighborhoods: (H0) without the 0-hop neighborhood $N_0(v) = \{i\}$, (H1) without $N_1(v)$; and (H2) without $N_2(v)$. Figure 3b shows that $H_2GCN$ consistently performs better than all the variants, indicating that combining all sub-neighborhoods works best. Among the variants, in heterophily settings, $N_0(v)$ contributes most to the performance (H0 causes significant decrease in accuracy), followed by $N_1(v)$, and $N_2(v)$. However, when $h \geq 0.7$, the importance of sub-neighborhoods is reversed. Thus, the ego-features are the most important in heterophily, and higher-order neighborhoods contribute the most in homophily. The design of $H_2GCN$ allows it to effectively combine information from different neighborhoods, adapting to all levels of homophily.

(D3) Combination of Intermediate Representations. We consider three variants (K-0.1, 2) of $H_2GCN$ that drop from the final representation of Eq. 7 the $0^{th}$, $1^{st}$ or $2^{nd}$-round intermediate representation, respectively. We also consider only the $2^{nd}$ intermediate representation as final, which is akin to what the other GNN models do. Figure 3c shows that $H_2GCN$-2, which combines all the intermediate representations, performs the best, followed by the variant K2 that skips the round-2 representation. The ego-embedding is the most important for heterophily $h \leq 0.5$ (see trend of K0).

Table 3: Statistics for Synthetic Datasets

| Benchmark Name | #Nodes $|V|$ | #Edges $|E|$ | #Classes $|Y|$ | #Features $F$ | Homophily $h$ | #Graphs |
|----------------|--------|---------|---------|----------------|--------------|---------|
| syn-cora       | 1,490  | 2,965   | 5       | cora           | [0.1,1]      | 33 (3 per h) |
| syn-products   | 10,000 | 59,640  | 10      | ogbn-products  | [0.1,1]      | 33 (3 per h) |

5.1 Evaluation on Synthetic Benchmarks
The challenging case of low-degree nodes Figure 3 plots the mean accuracy of H₂GCN variants on syn-products for different node degree ranges both in a heterophily and a homophily setting \( h \in \{0.2, 0.8\} \). We observe that under heterophily there is a significantly bigger performance gap between low- and high-degree nodes: 13% for H₂GCN-1 (10% for H₂GCN-2) vs. less than 3% under homophy. This is likely due to the importance of the distribution of class labels in each neighborhood under heterophily, which is harder to estimate accurately for low-degree nodes with few neighbors. On the other hand, in homophy, neighbors are likely to have similar classes \( y \in \mathcal{Y} \), so the neighborhood size does not have as significant impact on the accuracy.

5.2 Evaluation on Real Benchmarks

Real datasets & setup We now evaluate the performance of our model and established GNN models on a variety of real-world datasets [31, 24, 25, 18, 5, 27] with edge homophy ratio \( h \) ranging from strong heterophy to strong homophy, going beyond the traditional Cora, Pubmed and Citeseer graphs that have strong homophy (hence the good performance of existing GNNs on them). We summarize the data in Table 4 (top), and describe them in App. [H] where we also point out potential data limitations. For all benchmarks (except Cora-Full), we use the feature vectors, class labels, and 10 random splits (48%/32%/20% of nodes per class for train/validation/test) provided by [21].

Model comparison Table 4 gives the mean accuracy and stdv of H₂GCN variants and other models. We observe that the H₂GCN variants have consistently strong performance across the full spectrum of low-to-high homophy: H₂GCN-2 achieves the best average rank (2.9) across all datasets (or homophy ratios \( h \)), followed by H₂GCN-1 (3.7). Other models that use some of the designs D1-D3 (§3.1), including GraphSAGE and GCN-Cheby, also perform significantly better than GCN and GAT which lack these designs. Here, we also report the best results among the three recently-proposed GEOM-GCN variants (§4), directly from the paper [21]: other models (including ours) outperform this method significantly under heterophy. We note that MLP is a competitive baseline under strong heterophy, indicating that the existing models do not use the graph information effectively, or the latter is misleading in such cases. All models perform poorly on Squirrel and Actor likely due to their low-quality node features (small correlation with class labels). Also, Squirrel and Chameleon are dense, with many nodes sharing the same neighbors.

Table 4: Real data: mean accuracy ± stdv over different data splits. Best graph-aware model highlighted in gray. Asterisk “*” denotes results obtained from [21] and “N/A” results (for Cora Full) not reported in the paper. We note that GAT runs out of memory on Cora Full in our experiments.

| Hom. ratio \( h \) | Texas | Wisconsin | Actor | Squared | Chameleon | Corneil | Cora Full | Citeseer | Pubmed | Cora | Avg Rank |
|-------------------|-------|-----------|-------|---------|-----------|---------|-----------|---------|--------|------|----------|
| 0.11              | 92.20 | 83.41     | 92.96 | 90.72   | 91.92     | 88.62   | 90.72     | 91.92   | 88.62  | 92.20| 88.62    |
| 0.22              | 84.31 | 75.62     | 90.80 | 88.62   | 92.20     | 86.46   | 90.80     | 92.20   | 86.46  | 84.31| 86.46    |
| 0.33              | 76.47 | 68.79     | 88.62 | 86.46   | 88.62     | 84.31   | 88.62     | 86.46   | 84.31  | 76.47| 84.31    |
| 0.44              | 68.79 | 61.12     | 86.46 | 84.31   | 86.46     | 82.08   | 84.31     | 86.46   | 82.08  | 68.79| 82.08    |
| Cora Full         | 59.46 | 52.55     | 59.80 | 56.50   | 62.00     | 57.03   | 62.00     | 62.00   | 57.03  | 59.46| 57.03    |
| GAT*              | 58.38 | 49.41     | 58.38 | 50.34   | 54.32     | N/A     | 54.32     | N/A     | 54.32  | 58.38| 54.32    |
| GEOM-GCN*         | 87.57 | 64.12     | 87.57 | 60.90   | 60.90     | 77.99   | 77.99     | 77.99   | 77.99  | 87.57| 77.99    |
| MLP               | 81.08 | 54.41     | 81.08 | 55.38   | 56.50     | 80.81   | 80.81     | 80.81   | 80.81  | 81.08| 80.81    |

\[\text{[21]}\] claims that the ratios are 60%/20%/20%, which is different from the actual data splits shared on GitHub.
6 Conclusion

We have focused on characterizing the representation power of GNNs in challenging settings with heterophily or low homophily, which is understudied in the literature. We have highlighted the current limitations of GNNs, presented designs that increase representation power under heterophily and are theoretically justified with perturbation analysis and graph signal processing, and introduced a new model that adapts to both heterophily and homophily by effectively synthetizing these designs. We analyzed various challenging datasets, going beyond the often-used benchmark datasets (Cora, Pubmed, Citeseer), and leave as future work extending to a larger-scale experimental testbed.

Broader Impact

Homophily and heterophily are not intrinsically ethical or unethical—they are both phenomena existing in the nature, resulting in the popular proverbs “birds of a feather flock together” and “opposites attract”. However, existing GNN models implicitly assume homophily, thus ignoring the heterophily phenomena which may exist in some networks. As a result, if they are applied to networks that do not satisfy the assumption, the results may be biased, unfair, or erroneous.

Beyond the node classification problem that we tackle in this work, GNN models have been employed in a wide range of applications, such as recommendation systems, analysis of molecules and proteins, and more. In some of these cases, the homophily assumption may have ethical implications: For example, a GNN model that intrinsically assumes homophily may contribute to the so-called “filter bubble” phenomenon in a recommendation system (reinforcing existing beliefs/views, and downplaying the opposite ones), or make the minority groups less visible in social networks. In other cases, a reliance on homophily may hinder scientific progress: Among other domains, this is critical for the emerging research field of applying GNN models to molecular and protein structures, where the connected nodes often belong to different classes; the performance of existing GNNs may be poor in such cases (as we have shown in our analysis) and could hinder new discoveries. Moreover, if the input data contain many errors (e.g., wrong class labels, noisy network with incorrect and missing links), these may be propagated over the network, and lead to compounding errors in the classification results (this is common in most, if not all, machine learning problems).

Our work has the potential to rectify some of these potential negative consequences of existing GNN work. While our methodology does not change the amount of homophily in a network, moving beyond a reliance on homophily can be a key to improve the fairness, diversity and performance for the applications using GNN. We hope that this paper will raise more awareness and discussions regarding the homophily limitations of existing GNN models, and help researchers design models which have the power of learning in both homophily and heterophily settings.

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A  Nomenclature

We summarize the main symbols used in this work and their definitions below:

| Symbols | Definitions |
|---------|-------------|
| $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ | graph $\mathcal{G}$ with nodeset $\mathcal{V}$, edgeset $\mathcal{E}$ |
| $A$ | $n \times n$ adjacency matrix of $\mathcal{G}$ |
| $X$ | $n \times F$ node feature matrix of $\mathcal{G}$ |
| $x_v$ | $F$-dimensional feature vector for node $v$ |
| $L$ | unnormalized graph Laplacian matrix |
| $\mathcal{Y}$ | set of class labels |
| $y_v$ | class label for node $v \in \mathcal{V}$ |
| $y$ | $n$-dimensional vector of class labels (for all the nodes) |
| $T_\mathcal{V}$ | training data for semi-supervised node classification |
| $N(v)$ | general type of neighbors of node $v$ in graph $\mathcal{G}$ |
| $\bar{N}(v)$ | general type of neighbors of node $v$ in $\mathcal{G}$ without self-loops (i.e., excluding $v$) |
| $N_i(v), \bar{N}_i(v)$ | $i$-hop/step neighbors of node $v$ in $\mathcal{G}$ (at exactly distance $i$) maybe-with/without self-loops, resp. |
| $E_2$ | set of pairs of nodes $(u, v)$ with shortest distance between them being 2 |
| $d, d_{\text{max}}$ | node degree, and maximum node degree across all nodes $v \in \mathcal{V}$, resp. |
| $h$ | edge homophily ratio |
| $H$ | class compatibility matrix |
| $r_v^{(k)}$ | node representations learned in GNN model at round / layer $k$ |
| $K$ | the number of rounds in the neighborhood aggregation stage |
| $W$ | learnable weight matrix for GNN model |
| $\sigma$ | non-linear activation function |
| $\parallel$ | vector concatenation operator |
| AGGR | function that aggregates node feature representations within a neighborhood |
| COMBINE | function that combines feature representations from different neighborhoods |

B  Homophily and Heterophily: Compatibility Matrix

As we mentioned in §2, the edge homophily ratio in Definition 1 gives an overall trend for all the edges in the graph. The actual level of homophily may vary within different pairs of node classes, i.e., there is different tendency of connection between each pair of classes. For instance, in an online purchasing network [20] with three classes—fraudsters, accomplices, and honest users—, fraudsters connect with higher probability to accomplices and honest users. Moreover, within the same network, it is possible that some pairs of classes exhibit homophily, while others exhibit heterophily. In belief propagation [36], a message-passing algorithm used for inference on graphical models, the different levels of homophily or affinity between classes are captured via the class compatibility, propagation or coupling matrix, which is typically pre-defined based on domain knowledge. In this work, we define the empirical class compatibility matrix $H$ as follows:

**Definition 4** The class compatibility matrix $H$ has entries $[H]_{i,j}$ that capture the fraction of outgoing edges from a node in class $i$ to a node in class $j$:

$$[H]_{i,j} = \frac{|\{(u, v) : (u, v) \in \mathcal{E} \land y_u = i \land y_v = j\}|}{|\{(u, v) : (u, v) \in \mathcal{E} \land y_u = i\}|}$$

By definition, the class compatibility matrix is a stochastic matrix, with each row summing up to 1.
C Proofs and Discussions of Theorems

C.1 Detailed Analysis of Theorem 1

Proof 1 (for Theorem 1) We first discuss the GCN layer formulated as 
\[ f(X; A, W) = (A + I)XW. \]
Given training set \( T_V \), the goal of the training process is to optimize the weight matrix \( W \) to minimize the loss function \( L((A + I)X \mid T_V, W, [Y]_{T_V,:}) \), where \([Y]_{T_V,:}\) is the one-hot encoding of class labels provided in the training set, and \((A + I)X \mid T_V, :\) is the predicted probability distribution of class labels for each node \( v \) in the training set \( T_V \).

Without loss of generality, we reorder \( T_V \) accordingly such that the one-hot encoding of labels for nodes in training set \([Y]_{T_V,:}\) is in increasing order of the class label \( y_v \):

\[
[Y]_{T_V,:} = \begin{bmatrix}
1 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 1 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 1
\end{bmatrix}
\]  
\[
|V| \times |Y| \tag{9}
\]

Now we look into the term \((A + I)X \mid T_V, :\) which is the aggregated feature vectors within neighborhood \( N_1 \) for nodes in the training set. Since we assumed that all nodes in \( T_V \) have degree \( d \), proportion \( h \) of their neighbors belong to the same class, while proportion \( 1 - h \) \( |Y| - 1 \) of them belong to any other class uniformly, and one-hot representations of node features \( x_v = \text{onehot}(y_v) \) for each node \( v \), we obtain:

\[
(A + I)X \mid T_V, : = \begin{bmatrix}
hd + 1 & \frac{1 - h}{|Y| - 1}d & \frac{1 - h}{|Y| - 1}d & \cdots & \frac{1 - h}{|Y| - 1}d \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{1 - h}{|Y| - 1}d & hd + 1 & \frac{1 - h}{|Y| - 1}d & \cdots & \frac{1 - h}{|Y| - 1}d \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{1 - h}{|Y| - 1}d & \frac{1 - h}{|Y| - 1}d & \frac{1 - h}{|Y| - 1}d & \cdots & hd + 1 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{1 - h}{|Y| - 1}d & \frac{1 - h}{|Y| - 1}d & \frac{1 - h}{|Y| - 1}d & \cdots & hd + 1
\end{bmatrix}
\]  
\[
|V| \times |Y| \tag{10}
\]

For \([Y]_{T_V,:}\) and \((A + I)X \mid T_V, :\) that we derived in Eq. (9) and (10), we can find an optimal weight matrix \( W_\ast \) such that \((A + I)X \mid T_V, : W_\ast = [Y]_{T_V,:}\), making the loss \( L((A + I)X \mid T_V, : W_\ast, [Y]_{T_V,:}) = 0\). We can use the following way to find \( W_\ast \): First, sample one node from each class to form a smaller...
Applying the optimal weight matrix we learned on the Morrison formula, we can find its inverse as:

Now we move on to discuss the GCN layer formulated as:

Notice that we always have:

In this case we have:

Let \( W_* = (\mathbf{A} + I)^{-1} \mathbf{T}_S \), and we have \( (\mathbf{A} + I)_{\mathbf{T}_S} : W_* = \mathbf{Y}_{\mathbf{T}_S} : \). It is also easy to verify that \( (\mathbf{A} + I)_{\mathbf{T}_S} : W_* = \mathbf{Y}_{\mathbf{T}_S} : \) is the optimal weight matrix we can learn under \( \mathcal{T}_V \), since it satisfies \( \mathcal{L}((\mathbf{A} + I)_{\mathbf{T}_S} : W_* : \mathbf{Y}_{\mathbf{T}_S} : ) = 0 \).

Now consider an arbitrary training datapoint \((v, y_v) \in \mathcal{T}_V\), and a perturbation added to the neighborhood \( N(v) \) of node \( v \), such that the number of nodes with a randomly selected class label \( y_p \in \mathcal{Y} \neq y_v \) is \( \delta_1 \) less than expected in \( N(v) \). We denote the perturbed graph adjacency matrix as \( \mathbf{A}_\Delta \). Without loss of generality, we assume node \( v \) has \( y_v = 1 \), and the perturbed class is \( y_p = 2 \). In this case we have:

Applying the optimal weight matrix we learned on \( \mathcal{T}_V \) to the aggregated feature on the perturbed neighborhood \( (\mathbf{A} + I)_{\mathbf{T}_S} : \mathbf{X} : \), we obtain \( (\mathbf{A} + I)_{\mathbf{T}_S} : W_* : \mathbf{X} : \), which equals to:

Notice that we always have 1:

Solving the above inequality for \( \delta_1 \), we get the amount of perturbation needed as:

\begin{align}
\delta_1 < \frac{-h|\mathcal{Y}|-d-|\mathcal{Y}|+d+1}{|\mathcal{Y}|d} - \frac{|\mathcal{Y}|-d}{|\mathcal{Y}|d}, &\text{ when } h < \frac{|\mathcal{Y}|-d}{|\mathcal{Y}|d} \\
\delta_1 > \frac{-h|\mathcal{Y}|-d-|\mathcal{Y}|+d+1}{|\mathcal{Y}|d} - \frac{|\mathcal{Y}|-d}{|\mathcal{Y}|d}, &\text{ when } h > \frac{|\mathcal{Y}|-d}{|\mathcal{Y}|d},
\end{align}

and the least absolute amount of perturbation needed is:

\[
|\delta_1| = \begin{cases} 
\frac{|\mathcal{Y}|-d-|\mathcal{Y}|+d+1}{|\mathcal{Y}|d}, & \text{when } h < \frac{|\mathcal{Y}|-d}{|\mathcal{Y}|d} \\
\frac{|\mathcal{Y}|-d-|\mathcal{Y}|+d+1}{|\mathcal{Y}|d}, & \text{when } h > \frac{|\mathcal{Y}|-d}{|\mathcal{Y}|d}.
\end{cases}
\]

Now we move on to discuss the GCN layer formulated as \( f(\mathbf{X}; A, \mathbf{W}) = \mathbf{AXW} \) without self loops. Following similar derivations, we obtain the optimal weight matrix \( \mathbf{W}_* \) which makes \( \mathcal{L}((\mathbf{AX})_{\mathbf{T}_V} : \mathbf{W}_* : \mathbf{Y}_{\mathbf{T}_V} : ) = 0 \) as:

\[
\mathbf{W}_* = (\mathbf{AX})_{\mathbf{T}_V} : \mathbf{W}_* : \mathbf{Y}_{\mathbf{T}_V} : = \frac{1}{(1-h|\mathcal{Y}|d)\mathbf{I}} 
\begin{bmatrix}
-|\mathcal{Y}|-2+h & 1-h & \cdots & 1-h \\
1-h & -|\mathcal{Y}|-2+h & \cdots & 1-h \\
\vdots & \vdots & \ddots & \vdots \\
1-h & 1-h & \cdots & -(|\mathcal{Y}|-2+h)
\end{bmatrix}
\]
Again if for an arbitrary \((v, y_v) \in T_Y\), a perturbation is added to the neighborhood \(N(v)\) of the node \(v\), such that the number of nodes with a randomly selected class label \(y_p \in Y \neq y_v\) is \(\delta_2\) less than expected in \(N(v)\), we have:

\[
[A_\Delta X]_{v,:} = \left[ \frac{1-h}{|Y|-1} d - \delta_2 \quad \frac{1-h}{|Y|-1} d \quad \cdots \quad \frac{1-h}{|Y|-1} d \right]
\]

Then applying the optimal weight matrix that we learned on \(T_Y\) to the aggregated feature on perturbed neighborhood \([A_\Delta X]_{v,:} W\), we obtain \([A_\Delta X]_{v,:} W\) which equals to:

\[
\begin{bmatrix}
1 - \frac{(1-h)\delta_2}{(1-h)|Y|d} & \frac{(|Y| - 2 + h)\delta_2}{(1-h)|Y|d} & \cdots & \frac{(1-h)\delta_2}{(1-h)|Y|d}
\end{bmatrix}
\]

Thus, the GCN layer formulated as \(AXW\) would misclassify when the following inequality holds:

\[
1 - \frac{(1-h)\delta_2}{(1-h)|Y|d} < \frac{(|Y| - 2 + h)\delta_2}{(1-h)|Y|d}
\]

Or the amount of perturbation is:

\[
\begin{cases}
\delta_2 > \frac{(1-h)|Y|d}{1-h|Y|d}, & \text{when } 0 \leq h < \frac{1}{|Y|} \\
\delta_2 < \frac{(1-h)|Y|d}{1-h|Y|d}, & \text{when } h > \frac{1}{|Y|}
\end{cases}
\]

As a result, the least absolute amount of perturbation needed is \(|\delta_2| = \frac{(1-h)|Y|d}{1-h|Y|d}|.\)

By comparing the least absolute amount of perturbation needed for both formulations to misclassify \(|\delta_1| = \frac{-h|Y|d - |Y|d + d + 1}{|Y|-1}\) derived in Eq. (11) for the \((A + I)XW\) formulation; \(|\delta_2| = \frac{(1-h)|Y|d}{1-h|Y|d}|\) derived in Eq. (13) for the \(AXW\) formulation, we can see that \(|\delta_1| = |\delta_2|\) if and only if \(\delta_1 = -\delta_2\), which happens when \(h = \frac{1-|Y|+2d}{2|Y|d}\). When \(h < \frac{1-|Y|+2d}{2|Y|d}\) (heterophily), we have \(|\delta_1| < |\delta_2|\), which means the \((A + I)XW\) formulation is less robust to perturbation than the \(AXW\) formulation.

**Discussions** From the above proof, we can see that the least absolute amount of perturbation \(|\delta|\) needed for both GCN formulations is a function of the assumed homophily ratio \(h\), the node degree \(d\) for each node in the training set \(T_Y\), and the size of the class label set \(|Y|\). Fig. 4 shows the plots of \(|\delta_1|\) and \(|\delta_2|\) as functions of \(h\), \(|Y|\) and \(d\). From Fig. 4, we can see that the least absolute amount of perturbations \(|\delta|\) needed for both formulation first decreases as the assumed homophily level \(h\) increases, until \(\delta\) reaches 0, where the GCN layer predicts the same probability for all class labels; after that, \(\delta\) decreases further below 0, and \(|\delta|\) increases as \(h\) increases; the \((A + I)XW\) formulation is less robust to perturbation than the \(AXW\) formulation at low homophily level until \(h = \frac{1-|Y|+2d}{2|Y|d}\) as our proof shows, whereas \(|\delta_1| = |\delta_2|\). Figure 4 shows the changes of \(|\delta|\) as a function of \(|Y|\) when fixed \(h = 0.1\) and \(d = 20\). For both formulations, \(|\delta|\) first decrease rapidly as \(|Y|\) increases until \(\delta\) reaches 0, after that \(\delta\) increases slowly as \(|Y|\) increases; this reveals that both GCN formulations are more robust when \(|Y| << d\) under high homophily level, and in that case \(AXW\) formulation is more robust than the \((A + I)XW\) formulation. Figure 4 shows the changes of \(|\delta|\) as a function of \(d\) for fixed \(h = 0.1\) and \(|Y| = 5\): in this case the \(AXW\) formulation is always more robust than the \((A + I)XW\) formulation, and for the \((A + I)XW\) formulation, \(|\delta|\) follows again a “V”-shape curve as \(d\) changes.

**C.2 Detailed Analysis of Theorem 2**

**Proof 2 (for Theorem 2)** For all \(v \in V\), since its neighbors’ class labels \(\{y_u : u \in N(v)\}\) are conditionally independent given \(v\), we can define a matrix \(P_v\) for each node \(v\) as \(P_v(i,j) = P(y_u = \mathbf{1}) v, i, j \in V, u \in N(v)\). Following the assumption that for all \(v \in V\), \(P(y_u = y_v) = h\), \(\forall v \in V\), \(y \neq y_v\), we have

\[
P_v = P_v = \begin{bmatrix}
\hbar & \frac{1-h}{|Y|-1} & \frac{1-h}{|Y|-1} & \cdots & \frac{1-h}{|Y|-1} \\
\frac{1-h}{|Y|-1} & \hbar & \frac{1-h}{|Y|-1} & \cdots & \frac{1-h}{|Y|-1} \\
\vdots & \vdots & \ddots & \cdots & \vdots \\
\frac{1-h}{|Y|-1} & \frac{1-h}{|Y|-1} & \cdots & \hbar
\end{bmatrix}, \forall v \in V
\]
Now consider node \( w \in N_2(v) \), we have:

\[
P(y_w = k | y_v = i) = \sum_{j \in |\mathcal{Y}|} P(y_w = k | y_u = j) P(y_u = j | y_v = i) = \sum_{j \in |\mathcal{Y}|} [P]_{j,k} [P]_{i,j} = P^2 \quad (15)
\]

Therefore, to prove that the 2-hop neighborhood \( N_2(v) \) for any node \( v \in \mathcal{V} \) is homophily-dominant in expectation (i.e. \( P(y_w = i | y_v = i) \geq P(y_w = j | y_v = i), \forall j \in |\mathcal{Y}| \neq i, w \in N_2(v) \)), we need to show that the diagonal entries \([P^2]_{i,i}\) of \( P^2 \) are larger than the off-diagonal entries \([P^2]_{i,j}\).

Denote \( \rho = \frac{1-h}{|\mathcal{Y}|-1} \). From Eq. (14), we have

\[
[P^2]_{i,i} = h^2 + (|\mathcal{Y}| - 1)\rho^2
\]

and for \( i \neq j \)

\[
[P^2]_{i,j} = 2h\rho + (|\mathcal{Y}| - 2)\rho^2
\]

Thus,

\[
[P^2]_{i,i} - [P^2]_{i,j} = h^2 - 2h\rho + \rho^2 = (h - \rho)^2 \geq 0
\]

with equality if and only if \( h = \rho \), namely \( h = \frac{1}{|\mathcal{Y}|} \). Therefore, we proved that the 2-hop neighborhood \( N_2(v) \) for any node \( v \in \mathcal{V} \) will always be homophily-dominant in expectation. \( \blacksquare \)

C.3 Detailed Analysis of Theorem 3

Preliminaries We define unnormalized Laplacian matrix of graph \( \mathcal{G} \) as \( L = D - A \), where \( A \in \{0, 1\}^{|\mathcal{V}| \times |\mathcal{V}|} \) is the adjacency matrix and \( D \) is the diagonal matrix with \( |D|_{i,i} = \sum_{j} |A|_{i,j} \). Without loss of generality, since the eigenvalues \( \{\lambda_i\} \) of \( L \) are real and nonnegative \([28]\), we assume the following order for the eigenvalues of \( L \): \( 0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{|\mathcal{V}|-1} = \lambda_{\max} \). Furthermore, since \( L \) is real and symmetric, there exists a set of orthonormal eigenvectors \( \{v_i\} \) that form a complete basis of \( \mathbb{R}^{|\mathcal{V}|} \). This means that for any graph signal \( s \in \mathbb{R}^{|\mathcal{V}|} \), where \( s_u \) is the value of the signal on node \( u \in \mathcal{V} \), it can be decomposed to a weighted sum of \( \{v_i\} \). Mathematically, \( s \) is represented as \( s = \sum_{i=1}^{n} c_{s,i} v_i \), where \( c_{s,i} = s^T v_i \). We regard \( c_{s,i} \) as the coefficient of \( s \) at frequency component \( i \) and regard the coefficients at all frequencies components \( \{c_{s,i}\} \) as the spectrum of signal \( s \) with respect to graph \( \mathcal{G} \). In the above order of the eigenvalues, \( \lambda_i \) which are closer to 0 would correspond to lower-frequency components, and \( \lambda_i \) which are closer to \( \lambda_{\max} \) would correspond to higher-frequency components. Interested readers are referred to \([28]\) for further details regarding signal processing on graphs.

The smoothness score of a signal \( s \) on graph \( \mathcal{G} \), which measures the amount of changes of signal \( s \) along the edges of graph \( \mathcal{G} \), can be defined using \( L \) as

\[
s^T L s = \sum_{i,j} A_{ij} (s_i - s_j)^2 = \sum_{u \in \mathcal{V}} \sum_{v \in \mathcal{N}(u)} (s_u - s_v)^2. \quad (18)
\]
Then, for two eigenvectors $v_i$ and $v_j$ corresponding to eigenvalues $\lambda_i \leq \lambda_j$ of $L$, we have:

$$v_i^T L v_i = \lambda_i \leq \lambda_j = v_j^T L v_j$$

which means that $v_i$ is more smooth than $v_j$. This matches our expectations that a lower-frequency signal on $G$ should have smaller smoothness score. The smoothness score for arbitrary graph signal $s \in \mathbb{R}^{|V|}$ can be represented by its coefficients of each frequency component as:

$$s^T L s = \left( \sum_i c_{s,i} v_i \right)^T L \left( \sum_i c_{s,i} v_i \right) = \sum_{i=0}^{|V| - 1} c_{s,i}^2 \lambda_i$$

with the above preliminaries, we can define the following concept:

**Definition 5** Suppose $s = \sum_{i=0}^{|V| - 1} c_{s,i} v_i$ and $t = \sum_{i=0}^{|V| - 1} c_{t,i} v_i$ are two graph signals defined on $G$. In the spectrum of the unnormalized graph laplacian $L$, graph signal $s$ has higher energy on high-frequency components than $t$ if there exists integer $0 < M \leq |V| - 1$ such that $\sum_{i=M}^{|V| - 1} c_{s,i}^2 > \sum_{i=M}^{|V| - 1} c_{t,i}^2$.

Based on these preliminary definitions, we can now proceed with the proof of the theorem:

**Proof 3 (for Theorem 3)** We first prove that for graph signals $s, t \in \{0, 1\}^{|V|}$, edge homophily ratio $h_s < h_t$ if and only if $s^T L s > t^T L t$. Following Dfn. the edge homophily ratio for signal $s$ (similarly for $t$) can be calculated as:

$$h_s = \frac{1}{2|E|} \sum_{u \in V} \left( d_u - \sum_{v \in N(u)} (s_u - s_v)^2 \right) = \frac{1}{2|E|} \sum_{u \in V} d_u - \frac{1}{2|E|} \sum_{u \in V} \sum_{v \in N(u)} (s_u - s_v)^2$$

Plugging this in Eq. (18), we obtain:

$$h_s = \frac{1}{2|E|} \sum_{u \in V} d_u - \frac{1}{2|E|} s^T L s = 1 - \frac{1}{2|E|} s^T L s$$

where $|E|$ is the number of edges in $G$. From the above equation, we have

$$h_s < h_t \Leftrightarrow 1 - \frac{1}{2|E|} s^T L s < 1 - \frac{1}{2|E|} t^T L t \Leftrightarrow s^T L s > t^T L t$$

i.e. edge homophily ratio $h_s < h_t$ if and only if $s^T L s > t^T L t$.

Next we prove that if $s^T L s > t^T L t$, then following Dfn. signal $s$ has higher energy on high-frequency components than $t$. We prove this by contradiction: suppose integer $0 < M \leq |V| - 1$ does not exist such that $\sum_{i=M}^{|V| - 1} c_{s,i}^2 > \sum_{i=M}^{|V| - 1} c_{t,i}^2$ when $s^T L s > t^T L t$, then all of the following inequalities must hold, as the eigenvalues of $L$ satisfy $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{|V| - 1} = \lambda_{\text{max}}$:

$$0 = \lambda_0 (c_{s,0}^2 + c_{s,1}^2 + c_{s,2}^2 + \cdots + c_{s,|V| - 1}^2) = \lambda_0 (c_{t,0}^2 + c_{t,1}^2 + c_{t,2}^2 + \cdots + c_{t,|V| - 1}^2) = 0$$

$$(\lambda_1 - \lambda_0) (c_{s,0}^2 + c_{s,1}^2 + c_{s,2}^2 + \cdots + c_{s,|V| - 1}^2) \leq (\lambda_1 - \lambda_0) (c_{t,0}^2 + c_{t,1}^2 + c_{t,2}^2 + \cdots + c_{t,|V| - 1}^2)$$

$$(\lambda_2 - \lambda_1) (c_{s,0}^2 + c_{s,1}^2 + c_{s,2}^2 + \cdots + c_{s,|V| - 1}^2) \leq (\lambda_2 - \lambda_1) (c_{t,0}^2 + c_{t,1}^2 + c_{t,2}^2 + \cdots + c_{t,|V| - 1}^2)$$

Summing over $|V| - 1$ both sides of all the above inequalities, we have

$$\lambda_0 \sum_{i=0}^{|V| - 1} c_{s,i}^2 \lambda_i \leq \sum_{i=0}^{|V| - 1} c_{s,i}^2 \lambda_i \leq \sum_{i=0}^{|V| - 1} c_{s,i}^2 \lambda_i \leq \sum_{i=M}^{|V| - 1} c_{s,i}^2 \lambda_i \leq \sum_{i=M}^{|V| - 1} c_{s,i}^2 \lambda_i \leq \sum_{i=0}^{|V| - 1} c_{s,i}^2 \lambda_i \leq \sum_{i=0}^{|V| - 1} c_{s,i}^2 \lambda_i$$

i.e., $\sum_{i=0}^{|V| - 1} c_{s,i}^2 \lambda_i \leq \sum_{i=0}^{|V| - 1} c_{s,i}^2 \lambda_i$. However, from Eq. (19), we should have

$$s^T L s > t^T L t \Leftrightarrow \sum_{i=0}^{|V| - 1} c_{s,i}^2 \lambda_i > \sum_{i=0}^{|V| - 1} c_{t,i}^2 \lambda_i$$

which contradicts with the previous resulting inequality. Therefore, the assumption should not hold, and there must exist an integer $0 < M \leq |V| - 1$ such that $\sum_{i=0}^{|V| - 1} c_{s,i}^2 > \sum_{i=0}^{|V| - 1} c_{t,i}^2$ when $s^T L s > t^T L t$. \[\square\]
Extension of Theorem 3 to one-hot encoding of class label vectors

Theorem 3 discusses only the graph signal \( s, t \in \{0, 1\}^{|V|} \) with only 1 channel (i.e., with only 1 value assigned to each node). It is possible to generalize the theorem to one-hot encoding \( Y_s, Y_t \in \{0, 1\}^{|V| \times |Y|} \) as graph signal with \(|Y|\)-channels by modifying Dfn. 5 as follows:

**Definition 6** Suppose \([Y_s]_{i,j} = \sum_{t=0}^{|V|-1} c_{s,i,j} v_t\) and \([Y_t]_{i,j} = \sum_{t=0}^{|V|-1} c_{t,i,j} v_t\) are one-hot encoding of class label vector \(y_s, y_t\) defined as graph signals on \(\mathcal{G}\), where \(c_{s,i,j} = [Y_s]_{i,j}^T v_t\) is the coefficient of the \(j\)-th-channel of \(Y_s\), at frequency component \(i\). In the spectrum of the unnormalized graph laplacian \(L\), graph signal \(Y_s\) has higher energy on high-frequency components than \(Y_t\) if there exists integer \(0 < M \leq |V| - 1\) such that \(\sum_{i=M}^{\phi} \sum_{j=1}^{\phi} c_{s,i,j}^2 \geq \sum_{i=M}^{\phi} \sum_{j=1}^{\phi} c_{t,i,j}^2\).

Under this definition, we can prove Theorem 3 for one-hot encoding of class label vectors \(Y_s, Y_t\) as before, with the modification that in this case we have for signal \(Y_s\) (similarly for \(Y_t\)):

\[
h_s = \frac{1}{4|E|} \sum_{u \in V} \left( 2d_u - \sum_{v \in N(u)} \sum_{j=1}^{\phi} (|Y_s|_{u,j} - |Y_t|_{v,j})^2 \right)
\]

instead of Eq. \((20)\). The rest of the proof is similar to Proof 3.

**D Our H₂GCN model: Details**

In this section, we give the pipeline and pseudocode of H₂GCN, elaborate on its differences from existing GNN models, and present a detailed analysis of its computational complexity.

**D.1 Pseudocode & Pipeline**

In Fig. 5, we visualize H₂GCN, which we describe in § 3.2. We also give its pseudocode in Algorithm 1.

Figure 5: Pipeline of H₂GCN-2

\(r_v^{(0)} = \sigma(x_v W_c)\)

(S1)

(S2-Round 1)

(S2-Round 2)

(S3)
Algorithm 1: H₂GCN Framework for Node Classification under Homophily & Heterophily

**Input:** Graph Adjacency Matrix $A \in \{0, 1\}^{n \times n}$; Node Feature Matrix $X \in \mathbb{R}^{n \times F}$; Set of Labels $\mathcal{Y}$; Labeled Nodes $\mathcal{T}$.

**Hyper-parameters:** Dropout Rate; Non-linearity function $\sigma$; Number of Embedding Rounds $K$; Dimension of Feature Embedding $p$.

**Network Parameters:** $W_e \in \mathbb{R}^{F \times p}$, $W_c \in \mathbb{R}^{(2^K + 1)p \times |\mathcal{Y}|}$

**Output:** Class label vector $y$

```
begin
  /* All new variables defined below are initialized as all 0 */
  /* Stage S1: Feature Embedding */
  for $v \in \mathcal{V}$ do
    $r_v^{(0)} \leftarrow \sigma(x_v, W_c)$ /* Embeddings stored in matrix $R$ */
  /* Stage S2: Neighborhood Aggregation */
  /* Calculate higher-order neighborhoods $\bar{N}_1$ and $\bar{N}_2$ without self-loops and their corresponding adjacency matrices $A_1$ and $A_2$ */
  $A_0 \leftarrow I_n$ /* $I_n$ is the $n \times n$ identity matrix */
  $A_1 \leftarrow [A - I_n > 0]$ /* $I$ is a element-wise indicator function for matrix */
  $A_2 \leftarrow [A^2 - A - I_n > 0]$;
  for $i \leftarrow 1$ to 2 do
    for $v \in \mathcal{V}$ do
      $d_{v,i} \leftarrow \sum_{k} \bar{a}_{vk,i}$ /* degree of node $v$ at neighborhood $\bar{N}_i$ */
      $D_i \leftarrow \text{diag}\{d_{v,i} : v \in \mathcal{V}\}$;
      $A_i \leftarrow D_i^{-\frac{1}{2}} A D_i^{-\frac{1}{2}}$ /* symmetric degree-normalization of matrices $A_i$ */
  for $k \leftarrow 1$ to $K$ do
    $R_x^{(k)} \leftarrow A_1 R^{(k-1)}$ /* Designs D1 + D2 */
    $R_y^{(k)} \leftarrow A_2 R^{(k-1)}$;
    /* $\|$ is the vector concatenation operator */
    $R^{(k)} \leftarrow \left[ R_x^{(k)} \| R_y^{(k)} \right]$ /* Design D3 */
  /* Stage S3: Classification */
  $R^{(\text{final})} \leftarrow \text{dropout}(R^{(\text{final})})$ /* default dropout rate: 0.5 */
  for $v \in \mathcal{V}$ do
    $p_v \leftarrow \text{softmax}(r_v^{(\text{final})} W_c)$;
    $y_v \leftarrow \text{arg max}(p_v)$ /* class label */
end
```

D.2 Detailed Comparison of H₂GCN to existing GNN models

In §4, we discussed several high-level differences between H₂GCN and the various GNN models that we consider in this work, including the inclusion or not of designs D1-D3. Here we give some additional conceptual and mechanism differences.

As we have mentioned, H₂GCN differs from GCN [13] in a number of ways: (1) In each round of propagation/aggregation, GCN “mixes” the ego- and neighbor-representations by repeatedly averaging them to obtain the new node representations, while H₂GCN keeps them distinct via concatenation; (2) GCN considers only the 1-hop neighbors (including the ego / self-loops), while H₂GCN considers higher-order neighborhoods ($\bar{N}_1$ and $\bar{N}_2$); (3) GCN applies non-linear embedding transformations per round (e.g., RELU), while H₂GCN perform feature embedding for the ego in the first layer and drops all other non-linearities in the aggregation stage; and (4) GCN does not use the jumping knowledge framework (unlike H₂GCN), and makes the node classification predictions based on the last-round representations.

Unlike GAT, H₂GCN does not use any attention mechanism. Creating attention mechanisms that can generalize well to heterophily is an interesting future direction. Moreover, GCN-Cheby uses entirely
different mechanisms than the other GNN models that we consider (i.e., Chebyshev polynomials), though it has some conceptual similarities to H₂GCN in terms of the higher-order neighborhoods that it models.

GraphSAGE differs from H₂GCN in the same ways that are described in (2)-(4) above. In addition to leveraging only the 1-hop neighborhood, GraphSAGE also samples a fixed number of neighbors per round, while H₂GCN uses the full neighborhood. With respect to ego- and neighbor-representations, GraphSAGE concatenates them (as we do) but subsequently applies non-linear embedding transformations to them jointly (while we simplify all non-linear transformations). Our empirical analysis has revealed that such transformations lead to a decrease in performance in heterophily settings (see paragraph below on “Non-linear embedding transformations...”).

Finally, MixHop differs from H₂GCN in the same ways that are described in (1) and (3)-(4) above. It explicitly considers higher-order neighborhoods up to N₂, though [1] defines the 2-hop neighborhoods as that including neighbors up to 2-hop away neighbors. In our framework, we define the i-hop neighborhood as the set of neighbors with minimum distance exactly i from the ego (§ 2). Finally, the output layer of MixHop uses a tailored, column-wise attention layer, which prioritizes specific features, before the softmax layer. In contrast, before the classification layer, H₂GCN uses concatenation-based jumping knowledge in order to represent the high-frequency components that are critical in heterophily.

Non-linear embedding transformations per round in H₂GCN? GCN [13], GraphSAGE [8] and other GNN models embed the intermediate representations per round of feature propagation and aggregation. However, as we show in the ablation study in App. § G.2 (Table G.4 last row “Non-linear”), introducing non-linear transformations per round of the neighborhood aggregation stage (S2) of H₂GCN-2 (i.e., with K = 2) as follows leads to worse performance than the framework design that we introduce in Eq. (5) of § 3.2.

\[ r_u^{(k)} = \text{COMBINE}(\sigma(W r_u^{(k-1)}), \text{AGGR}(r_u^{(k-1)}: u \in N_1(v)), \text{AGGR}(r_u^{(k-1)}: u \in N_2(v))) \]  

where \( \sigma \) is RELU and W is a learnable matrix. Our design in Eq. (5) aggregates different neighborhoods in a similar way to SGC [33], which has shown that removing non-linearities does not negatively impact performance in homophily settings. We actually find that removing non-linearities even improves the performance under heterophily.

D.3 H₂GCN: Time Complexity in Detail

Preliminaries The worst case time complexity for calculating A · B when both A and B are sparse matrices is \( \mathcal{O}(\text{nnz}(A) \cdot c_B) \), where \( \text{nnz}(A) \) is the number of non-zero elements in matrix A, and \( c_B = \max(\sum_j \|b_{ij} > 0\|) \) is the maximum number of non-zero elements in any row of matrix B. The time complexity for calculating A · X, when X is a dense matrix with \( F \) columns, is \( \mathcal{O}(\text{nnz}(A) F) \).

Time complexity of H₂GCN We analyze the time complexity of H₂GCN by stage (except the classification stage).

The feature embedding stage (S1) takes \( \mathcal{O}(\text{nnz}(X) p) \) to calculate \( \sigma(XW_e) \) where \( W_e \in \mathbb{R}^{F \times p} \) is a learnable dense weight matrix, and \( X \in \mathbb{R}^{n \times F} \) is the node feature matrix.

In the neighborhood aggregation stage (S2), we perform the following computations:

- **Calculation of higher-order neighborhoods.** Given that A is sparse, we can obtain the 2-hop neighborhood by calculating \( A^2 \) in \( \mathcal{O}(|\mathcal{E}| d_{\text{max}}) \), where \( |\mathcal{E}| \) is the number of edges in \( \mathcal{G} \) (equal to the number of non-zeroes in A), and \( d_{\text{max}} \) is the maximum degree across all nodes \( v \in \mathcal{V} \) (which is equal to the maximum number of non-zeroes in any row of A).

- **Feature Aggregation.** We begin with a p-dimensional embedding for each node after feature embedding. In round \( k \), since we are using the neighborhoods \( N_1 \) and \( N_2 \), we have an embedding \( \mathbf{R}_{k-1} \in \mathbb{R}^{n \times 2^{k-1} p} \) as input. We aggregate embedding vectors within neighborhood by \( \mathbf{R}_{k} = (\mathbf{A}_1 \mathbf{R}_{k-1} | \mathbf{A}_2 \mathbf{R}_{k-1}) \), in which \( \mathbf{A}_1 \) corresponds to the adjacency matrix of neighborhood \( N_1 \). The two sparse matrix-matrix multiplications in the concatenation take \( \mathcal{O}(|\mathcal{E}| 2^{k-1} p + |\mathcal{E}_2| 2^{k-1} p) \), where \( |\mathcal{E}_2| = \frac{1}{2} \sum_{v \in \mathcal{V}} |N_2(v)| \). Over \( K \) rounds of embedding, the complexity becomes \( \mathcal{O}(2^K (|\mathcal{E}| + |\mathcal{E}_2|) p) \).
Adding all the big-O terms above, we have the overall time complexity for stages \((S1)\) and \((S2)\) of H\(_2\)GCN as:

\[
O \left( \text{nnz}(X) p + |E|d_{\text{max}} + 2^K(|E| + |E_2|)p \right),
\]

where \(K\) is usually a small number (e.g., 2). For small values of \(K\), the complexity becomes \(O \left( |E|d_{\text{max}} + \text{nnz}(X) + |E| + |E_2| \right)\).

### E Additional Related Work

In § 4, we discuss relevant work on GNNs. Here we briefly mention other approaches for node classification. Collective classification in statistical relational learning focuses on the problem of node classification by leveraging the correlations between the node labels and their attributes [26]. Since exact inference is NP-hard, approximate inference algorithms (e.g., iterative classification [11, 16], loopy belief propagation) are used to solve the problem. Belief propagation (BP) [36] is a classic message-passing algorithm for graph-based semi-supervised learning, which can be used for graphs exhibiting homophily or heterophily [15] and has fast linearized versions [7, 6]. Different from the setup where GNNs are employed, BP does not leverage node features, and assumes a pre-defined class compatibility or edge potential matrix (§ 2).

### F Experimental Setup & Hyperparameter Tuning

#### F.1 Setup

**H\(_2\)GCN Implementation** We use \(K = 1\) for H\(_2\)GCN-1 and \(K = 2\) for H\(_2\)GCN-2. For loss function, we calculate the cross entropy between the predicted and the ground-truth labels for nodes within the training set, and add \(L_2\) regularization of network parameters \(W_e\) and \(W_c\). (cf. Alg. 1)

**Baseline Implementations** For all baselines besides MLP, we used the official implementation released by the authors on GitHub.

- **GCN & GCN-Cheby** [13]: https://github.com/tkipf/gcn
- **GraphSAGE** [8]: https://github.com/williamleif/graphsage-simple
- **MixHop** [1]: https://github.com/samihaija/mixhop
- **GAT** [32]: https://github.com/PetarV-/GAT

For MLP, we used our own implementation of MLP with 1-hidden layer, which is equivalent to the case of \(K = 0\) in Algorithm 1. We use the same loss function as H\(_2\)GCN for training MLP.

**Hardware Specifications** We run all the experiments on an Amazon EC2 instance with instance size as p3.2xlarge, which features 8 CPU cores, 61 GB Memory and a Tesla V100 GPU with 16 GB GPU Memory.

#### F.2 Tuning the GNN Models

To avoid bias, we tuned the hyperparameters of each method (H\(_2\)GCN and baseline models) on each benchmark. Below we list the hyperparameters tested on each benchmark per model. As the hyperparameters defined by each baseline model differ significantly, we list the combinations of non-default command line arguments we tested, without explaining them in detail. We refer the interested reader to the corresponding original implementations for further details on the arguments, including their definitions.

**Synthetic Benchmark Tuning** For each synthetic benchmark, we report the results for different heterophily levels under the same set of hyperparameters for each method, so that we can compare how the same hyperparameters perform across the full spectrum of low-to-high homophily. We report the best performance, for the set of hyperparameters which performs the best on the validation set on the majority of the heterophily levels for each method.
For syn-cora, we test the following command-line arguments for each baseline method:

- **H$_2$GCN-1 & H$_2$GCN-2:**
  - Dimension of Feature Embedding $p$: 64
  - Non-linearity Function $\sigma$: ReLU
  - Dropout Rate: $a \in \{0, 0.5\}$
  We report the best performance, for $a = 0$.

- **GCN [13]:**
  - hidden1: $a \in \{16, 32, 64\}$
  - early_stopping: $b \in \{40, 100, 200\}$
  - epochs: 2000
  We report the best performance, for $a = 32, b = 40$.

- **GCN-Cheby [13]:**
  - Set 1:
    * hidden1: $a \in \{16, 32, 64\}$
    * dropout: 0.6
    * weight_decay: $b \in \{1e-5, 5e-4\}$
    * max_degree: 2
    * early_stopping: 40
  - Set 2:
    * hidden1: $a \in \{16, 32, 64\}$
    * dropout: 0.5
    * weight_decay: 5e-4
    * max_degree: 3
    * early_stopping: 40
  We report the best performance, for Set 1 with $a = 64, b = 5e-4$.

- **GraphSAGE [8]:**
  - hid_units: $a \in \{64, 128\}$
  - lr: $b \in \{0.1, 0.7\}$
  - epochs: 500
  We report the performance with $a = 64, b = 0.7$.

- **MixHop [1]:**
  - adj_pows: 0, 1, 2

- **GAT [32]:**
  - hid_units: $a \in \{8, 16, 32, 64\}$
  - n_heads: $b \in \{1, 4, 8\}$
  We report the performance with $a = 8, b = 8$.

- **MLP**
  - Dimension of Feature Embedding $p$: 64
  - Non-linearity Function $\sigma$: ReLU
  - Dropout Rate: 0.5

For syn-products, we test the following command-line arguments for each baseline method:

- **H$_2$GCN-1 & H$_2$GCN-2:**
  - Dimension of Feature Embedding $p$: 64
  - Non-linearity Function $\sigma$: ReLU
  - Dropout Rate: $a \in \{0, 0.5\}$
  We report the best performance, for $a = 0.5$. 

• **GCN** [13]:
  - hidden1: 64
  - early_stopping: $a \in \{40, 100, 200\}$
  - epochs: 2000
  In addition, we disabled the default feature normalization in the official implementation, as the feature vectors in this benchmark have already been normalized, and we found the default normalization method hurts the performance significantly. We report the best performance, for $a = 40$.

• **GCN-Cheby** [13]:
  - hidden1: 64
  - max_degree: 2
  - early_stopping: 40
  - epochs: 2000
  We also disabled the default feature normalization in the official implementation for this baseline.

• **GraphSAGE** [8]:
  - hid_units: $a \in \{64, 128\}$
  - lr: $b \in \{0.1, 0.7\}$
  - epochs: 500
  We report the performance with $a = 128, b = 0.1$.

• **MixHop** [1]:
  - adj_pows: 0, 1, 2

• **MLP**
  - Dimension of Feature Embedding $p$: 64
  - Non-linearity Function $\sigma$: ReLU
  - Dropout Rate: 0.5

**Real Benchmark (except Cora-Full) Tuning**
For each real benchmark in Table 4 (except Cora-Full), we perform hyperparameter tuning (see values below) and report the best performance of each method on the validation set. So, for each method, its performance on different benchmarks can be reported from different hyperparameters. We test the following command-line arguments for each baseline method:

• **H$_2$GCN-1 & H$_2$GCN-2**:
  - Dimension of Feature Embedding $p$: 64
  - Non-linearity Function $\sigma$: $a \in \{\text{ReLU, None}\}$
  - Dropout Rate: 0

• **GCN** [13]:
  - hidden1: 64
  - early_stopping: $a \in \{40, 100, 200\}$
  - epochs: 2000

• **GCN-Cheby** [13]:
  - Set 1:
    * hidden1: 64
    * dropout: 0.6
    * weight_decay: $b$
    * max_degree: 2
    * early_stopping: 40
    with $b \in \{1e-5, 5e-4\}$
  - Set 2:
    * hidden1: 64
    * dropout: 0.5
* weight_decay: 5e-4
* max_degree: 3
* early_stopping: 40

• **GraphSAGE** [8]:
  - hid_units: \( a \in \{64, 128\} \)
  - lr: \( b \in \{0.1, 0.7\} \)
  - epochs: 500

• **MixHop** [1]:
  - adj_pows: 0, 1, 2

• **MLP**
  - Dimension of Feature Embedding \( p \): 64
  - Non-linearity Function \( \sigma \): \( a \in \{\text{ReLU}, \text{None}\} \)
  - Dropout Rate: \( b \in \{0, 0.5\} \)

**Cora Full Benchmark Tuning**  
The number of class labels in Cora-Full are many more compared to the other benchmarks (Table 4), which leads to a significant increase in the size of training parameters for each model. Therefore, we need to re-tune the hyperparameters, especially the regularization weights and learning rates, in order to get reasonable performance. We test the following command-line arguments for each baseline method:

• **H\_2GCN-1 & H\_2GCN-2:**
  - Dimension of Feature Embedding \( p \): 64
  - Non-linearity Function \( \sigma \): \( a \in \{\text{ReLU}, \text{None}\} \)
  - Dropout Rate: 0
  - L2 Regularization Weight: \( b \in \{1e-5, 1e-6\} \)
  - Learning Rate: \( c \in \{0.01, 0.05\} \)

• **GCN** [13]:
  - hidden1: 64
  - early_stopping: \( a \in \{40, 100, 200\} \)
  - weight_decay: \( b \in \{1e-5, 5e-5, 1e-6\} \)
  - epochs: 2000

• **GCN-Cheby** [13]:
  - hidden1: 64
  - dropout: 0.6
  - weight_decay: \( a \in \{1e-5, 5e-4\} \)
  - max_degree: 2
  - early_stopping: 40

• **GraphSAGE** [8]:
  - hid_units: \( a \in \{64, 128\} \)
  - lr: \( b \in \{0.1, 0.7\} \)
  - epochs: 500

• **MixHop** [1]:
  - adj_pows: 0, 1, 2
  - l2reg: \( b \in \{5e-4, 5e-5\} \)

• **MLP**
  - Dimension of Feature Embedding \( p \): 64
  - Non-linearity Function \( \sigma \): \( a \in \{\text{ReLU}, \text{None}\} \)
  - Dropout Rate: \( b \in \{0, 0.5\} \)
  - L2 Regularization Weight: 1e-5
  - Learning Rate: 0.05

24
G Synthetic Datasets: Details

G.1 Data Generation Process & Setup

**Synthetic graph generation** We generate synthetic graphs with various heterophily levels by adopting an approach similar to [1, 12]. In general, the synthetic graphs are generated by a modified preferential attachment process [2]: The number of class labels $|\mathcal{Y}|$ in the synthetic graph is prescribed. Then, starting from a small initial graph, new nodes are added into the graph one by one, until the number of nodes $|\mathcal{V}|$ has reached the preset level. The probability $p_{uv}$ for a newly added node $u$ in class $i$ to connect with an existing node $v$ in class $j$ is proportional to both the class compatibility $H_{ij}$ between class $i$ and $j$, and the degree $d_v$ of the existing node $v$. As a result, the degree distribution for the generated graphs follow a power law, and the heterophily can be controlled by class compatibility matrix $\mathbf{H}$. Table G.1 shows an overview of these synthetic benchmarks, and more detailed statistics can be found in Table G.1.

**Node features & classes** Nodes are assigned randomly to each class during the graph generation. Then, in each synthetic graph, the feature vectors of nodes in each class are generated by sampling feature vectors of nodes from the corresponding class in a real benchmark (e.g., Cora [25,35] or ogbn-products [10]): We first establish a class mapping $\psi : \mathcal{Y}_s \rightarrow \mathcal{Y}_b$ between classes in the synthetic graph $\mathcal{Y}_s$ to classes in an existing benchmark $\mathcal{Y}_b$. The only requirement is that the class size in the existing benchmark is larger than that of the synthetic graph so that an injection between nodes from both classes can be established, and the feature vectors for the synthetic graph can be sampled accordingly. For syn-products, we further restrict the feature sampling to ensure that nodes in the training, validation and test splits are only mapped to nodes in the corresponding splits in the benchmark. This process respects the data splits used in ogbn-products, which are more realistic and challenging than random splits [10]. For simplicity, in our synthetic benchmarks, all the classes (5 for syn-cora and 10 for syn-products – Table G.1) are of the same size.

| Benchmark Name | syn-cora | syn-products |
|----------------|----------|--------------|
| # Nodes        | 1490     | 10000        |
| # Edges        | 2965 to 2968 | 59640 to 59648 |
| # Classes      | 5        | 10           |
| Features       | cora [25,35] | ogbn-products [10] |
| Homophily $h$  | [0, 0.1,...,1] | [0, 0.1,...,1] |
| Degree Range   | 1 to 94  | 1 to 336     |
| Average Degree | 3.98     | 11.93        |

**Experimental setup** For each heterophily ratio $h$ of each benchmark, we independently generate 3 different graphs. For syn-cora and syn-products, we randomly partition 25% of nodes into training set, 25% into validation and 50% into test set. All methods share the same training, validation and test splits, and the average and standard derivation of the performance values under the 3 generated graphs are reported as the performance under each heterophily level of each benchmark.

G.2 Detailed Results on Synthetic Benchmarks

Tables G.2 and G.3 give the results on syn-cora and syn-products shown in Figure 2 of the main paper (§ 5.1). Table G.4 provides the detailed results of the ablation studies that we designed in order to investigate the significance of our design choices, and complements Fig. 5 in § 5.1.
Table G.2: syn-cora (Fig. 2a): Mean accuracy and standard deviation per method and synthetic dataset (with different homophily ratio h). Best method highlighted in gray.

| h  | 0.00 | 0.10 | 0.20 | 0.30 | 0.40 | 0.50 |
|----|------|------|------|------|------|------|
| H-GCN-1 | 77.8 | 76.4 | 75.9 | 74.4 | 77.5 | 79.0 |
| H-GCN-2 | 78.6 | 76.9 | 74.0 | 73.6 | 76.4 | 80.0 |
| GraphSAGE | 75.9 | 72.9 | 70.6 | 71.8 | 72.0 | 76.5 |
| GCN-Cheby | 74.2 | 68.0 | 64.7 | 66.7 | 68.4 | 73.3 |
| MixHop | 40.6 | 39.6 | 34.3 | 37.4 | 45.4 | 61.3 |
| GCN | 33.6 | 31.4 | 28.2 | 25.1 | 25.6 | 66.2 |
| GAT | 30.1 | 33.1 | 35.9 | 48.8 | 55.5 | 64.7 |
| MLP | 72.7 | 74.1 | 74.5 | 73.8 | 73.3 | 74.8 |

| h  | 0.60 | 0.70 | 0.80 | 0.90 | 1.00 |
|----|------|------|------|------|------|
| H-GCN-1 | 84.7 | 81.0 | 91.8 | 91.5 | 100.0 |
| H-GCN-2 | 84.9 | 87.6 | 92.7 | 96.1 | 100.0 |
| GraphSAGE | 81.2 | 85.0 | 96.7 | 95.0 | 99.8 |
| GCN-Cheby | 78.9 | 84.9 | 90.9 | 95.9 | 100.0 |
| MixHop | 73.6 | 82.6 | 89.7 | 95.9 | 100.0 |
| GCN | 71.3 | 84.5 | 91.3 | 96.1 | 100.0 |
| GAT | 76.2 | 84.0 | 90.9 | 95.9 | 100.0 |
| MLP | 73.4 | 71.2 | 72.2 | 75.3 | 76.5 |

Table G.3: syn-products (Fig. 2b): Mean accuracy and standard deviation per method and synthetic dataset (with different homophily ratio h). GAT runs out of memory (“OOM”). Best method highlighted in gray.

| h  | 0.00 | 0.10 | 0.20 | 0.30 | 0.40 | 0.50 |
|----|------|------|------|------|------|------|
| H-GCN-1 | 82.0 | 78.3 | 79.3 | 81.1 | 82.4 | 88.1 |
| H-GCN-2 | 82.7 | 80.3 | 81.9 | 82.7 | 90.7 | 97.3 |
| GraphSAGE | 77.6 | 74.0 | 75.2 | 76.3 | 80.9 | 84.5 |
| GCN-Cheby | 83.4 | 76.9 | 77.0 | 78.4 | 85.0 | 89.6 |
| MixHop | 71.9 | 11.9 | 11.6 | 14.7 | 15.6 | 18.7 |
| GCN | 56.4 | 54.1 | 54.9 | 64.0 | 76.2 | 80.4 |
| GAT OOM | 68.3 | 68.2 | 68.5 | 66.5 | 68.7 | 68.7 |
| MLP OOM | 68.2 | 68.7 | 68.6 | 68.3 | 69.0 | 69.0 |

| h  | 0.60 | 0.70 | 0.80 | 0.90 | 1.00 |
|----|------|------|------|------|------|
| H-GCN-1 | 92.3 | 90.0 | 90.9 | 90.3 | 100.0 |
| H-GCN-2 | 94.1 | 97.6 | 99.1 | 99.0 | 100.0 |
| GraphSAGE | 89.5 | 96.1 | 98.6 | 98.7 | 100.0 |
| GCN-Cheby | 94.9 | 98.2 | 99.5 | 99.9 | 100.0 |
| MixHop | 20.4 | 21.4 | 22.9 | 25.1 | 25.1 |
| GCN OOM | 93.3 | 97.1 | 99.3 | 99.9 | 100.0 |
| GAT OOM | 68.2 | 68.7 | 68.6 | 68.3 | 69.0 |
| MLP OOM | 68.2 | 68.7 | 68.6 | 68.3 | 69.0 |

Table G.4: Ablation studies of H2GCN to show the significance of designs D1-D3 (Fig. 3a-c)): Mean accuracy and standard deviation per method on the syn-products networks.

| Design | h  | 0.00 | 0.10 | 0.20 | 0.30 | 0.40 | 0.50 |
|-------|----|------|------|------|------|------|------|
| D1-D3 | [S0 / K2] H-GCN-1 | 82.0 | 78.3 | 79.3 | 81.1 | 82.4 | 88.1 |
| D3-H2GCN-2 | 84.3 | 80.3 | 81.9 | 82.7 | 90.7 | 97.3 |

| Design | h  | 0.60 | 0.70 | 0.80 | 0.90 | 1.00 |
|-------|----|------|------|------|------|------|
| D1-D3 | [S0 / K2] H-GCN-1 | 92.3 | 90.0 | 90.9 | 90.3 | 100.0 |
| D3-H2GCN-2 | 94.1 | 97.6 | 99.1 | 99.0 | 100.0 |

| Design | h  | 0.00 | 0.10 | 0.20 | 0.30 | 0.40 | 0.50 |
|-------|----|------|------|------|------|------|------|
| D1-D3 | [S0 / K2] H-GCN-1 | 92.3 | 90.0 | 90.9 | 90.3 | 100.0 |
| D3-H2GCN-2 | 94.1 | 97.6 | 99.1 | 99.0 | 100.0 |

| Design | h  | 0.60 | 0.70 | 0.80 | 0.90 | 1.00 |
|-------|----|------|------|------|------|------|
| D1-D3 | [S0 / K2] H-GCN-1 | 92.3 | 90.0 | 90.9 | 90.3 | 100.0 |
| D3-H2GCN-2 | 94.1 | 97.6 | 99.1 | 99.0 | 100.0 |
H Real Datasets: Details

Datasets In our experiments, we use the following real-world datasets with varying levels of homophily ratios $h$. Some network statistics are given in Table 4.

- **Texas, Wisconsin and Cornell** are graphs representing links between web pages of the corresponding universities, originally collected by the CMU WebKB project. We used the preprocessed version in [21]. In these networks, nodes are web pages, which are classified into 5 categories: course, faculty, student, project, staff.

- **Squirrel and Chameleon** are subgraphs of web pages in Wikipedia discussing the corresponding topics, collected by [24]. For the classification task, we utilize the class labels generated by [21], where the nodes are categorized into 5 classes based on the amount of their average traffic.

- **Actor** is a graph representing actor co-occurrence in Wikipedia pages, processed by [21] based on the film-director-actor-writer network in [31]. We also use the class labels generated by [21].

- **Cora, Pubmed and Citeseer** are citation graphs originally introduced in [25, 18], which are among the most widely used benchmarks for semi-supervised node classification [27, 10]. Each node is assigned a class label based on the research field. These datasets use a bag of words representation as the feature vector for each node.

- **Cora Full** is an extended version of Cora, introduced in [3, 27], which contain more papers and research fields than Cora. This dataset also uses a bag of words representation as the feature vector for each node.

Data Limitations As discussed in [27, 10], Cora, Pubmed and Citeseer are widely adopted as benchmarks for semi-supervised node classification tasks; however, all these benchmark graphs display strong homophily, with edge homophily ratio $h \geq 0.7$. As a result, the wide adaptation of these benchmarks have masked the limitations of the homophily assumption in many existing GNN models. Open Graph Benchmark is a recent effort of proposing more challenging, realistic benchmarks with improved data quality comparing to the existing benchmarks [10]. However, with respect to homophily, we found that the proposed OGB datasets display homophily $h > 0.5$.

In our synthetic experiments ($\S$ G), we used ogbn-products from this effort to generate higher quality synthetic benchmarks while varying the homophily ratio $h$. In our experiments on real datasets, we go beyond the typically-used benchmarks (Cora, Pubmed, Citeseer) and consider benchmarks with strong heterophily (Table 4). That said, these datasets also have limitations, including relatively small sizes (e.g., WebKB benchmarks), artificial classes (e.g., Squirrel and Chameleon have class labels based on ranking of page traffic), or unusual network structure (e.g., Squirrel and Chameleon are dense, with many nodes sharing the same neighbors — cf. $\S$ 5.2). We hope that this paper will encourage future work on more diverse datasets with different levels of homophily, and lead to higher quality datasets for benchmarking GNN models in the heterophily settings.