Characterizing Graph Datasets for Node Classification: Beyond Homophily–Heterophily Dichotomy

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Abstract

Homophily is a graph property describing the tendency of edges to connect similar nodes; the opposite is called heterophily. While homophily is natural for many real-world networks, there are also networks without this property. It is often believed that standard message-passing graph neural networks (GNNs) do not perform well on non-homophilous graphs, and thus such datasets need special attention. While a lot of effort has been put into developing graph representation learning methods for heterophilous graphs, there is no universally agreed upon measure of homophily. Several metrics for measuring homophily have been used in the literature, however, we show that all of them have critical drawbacks preventing comparison of homophily levels between different datasets. We formalize desirable properties for a proper homophily measure and show how existing literature on the properties of classification performance metrics can be linked to our problem. In doing so we find a measure that we call adjusted homophily that satisfies more desirable properties than existing homophily measures. Interestingly, this measure is related to two classification performance metrics — Cohen’s Kappa and Matthews correlation coefficient. We argue that adjusted homophily is a better alternative to the homophily measures commonly used in the literature. Then, we go beyond the homophily–heterophily dichotomy and propose a new property that we call label informativeness (LI) that characterizes how much information a neighbor’s label provides about a node’s label. We theoretically show that LI is comparable across datasets with different numbers of classes and class size balance. Through a series of experiments we show that LI is a better predictor of the performance of GNNs on a dataset than homophily. We show that LI explains why GNNs can sometimes perform well on heterophilous datasets — a phenomenon recently observed in the literature.

1 Introduction

Graphs are a natural way to represent data from various domains such as social networks, citation networks, molecules, protein-protein interactions, transportation networks, text, code, and many others. The field of machine learning on graph-structured data has experienced significant growth in recent years, with Graph Neural Networks (GNNs) showing particularly strong results and becoming the de facto standard for most graph representation learning tasks. Many variants of GNNs have been proposed [1–4], most of them can be unified by a general Message Passing Neural Networks (MPNNs) framework [5]. MPNNs combine node features (attributes) with graph topology to learn complex dependencies between the nodes. For this, MPNNs iteratively update the representation of

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each node by aggregating information from the previous-layer representations of the node itself and its neighbors. The node feature vector is used as the initial node representation.

In many real-world networks, edges tend to connect similar nodes. For example, users in social networks tend to connect to users with similar interests, and papers in citation networks mostly cite works from the same research area. This property is usually called homophily. However, there are also networks for which homophily does not hold. The opposite of homophily is heterophily, which describes the tendency of edges to connect dissimilar nodes. For instance, in social networks fraudsters rarely connect to other fraudsters, while in dating networks edges often connect the opposite genders.

Early works on GNNs mostly focus on homophilous graphs. However, it was later discovered that classic GNNs typically do not perform well on heterophilous graphs [6–8]. To overcome this issue, new techniques and GNN architectures have been developed for dealing with heterophilous graphs, among them are MixHop [6], Geom-GCN [7], H2GCN [8], CPGNN [9], GPR-GNN [10]. Recently, however, it has been shown that standard GNNs can perform well on certain non-homophilous graphs [11, 12]. Thus, it is not the absence of homophily that causes difficulties for GNNs.

In this paper, we aim to provide a comprehensive characterization of datasets for node classification and explore how their properties may relate to the performance of GNNs. First, we revisit the concept of homophily. There are several widely used homophily measures [6–8, 13]. However, as we theoretically show, they have some downsides and cannot be used to compare datasets with different numbers of classes and class size balance. To analyze and compare homophily measures, we formalize their desirable properties and check which measures satisfy which properties. We also show how existing literature on the properties of classification performance measures can be linked to our analysis of homophily measures. One particularly important property is called constant baseline and, informally speaking, it requires a measure to be not sensitive to the number of classes and their size balance. We conclude this investigation by recommending adjusted homophily — a measure that satisfies most of the desirable properties. Interestingly, adjusted homophily is related to both Cohen’s Kappa and Matthews correlation coefficient — two measures for evaluating classification performance. Additionally, adjusted homophily turns out to be a normalized version of a metric well known in community detection literature — modularity. We argue that adjusted homophily is a better alternative to the measures commonly used in the literature.

However, as mentioned above, it is not homophily that characterizes how difficult a dataset is for GNNs. Hence, we go beyond homophily–heterophily dichotomy and propose a new property that we call label informativeness (LI). This measure characterizes how much information a neighbor’s label provides about a node’s label. We first analyze this measure theoretically to verify that it is comparable across different datasets. Namely, we show that the constant baseline property is satisfied for this measure. Then, we empirically show that LI is a better predictor of the performance of GNNs compared to homophily. For this, we measure the correlation between different measures and GNN performance on various datasets. We show that LI explains why GNNs can sometimes perform well on heterophilous datasets — a phenomenon recently observed in the literature.

2 Homophily Measures

Assume that we are given a graph \( G = (V, E) \) with nodes \( V, |V| = n \), and edges \( E \). Throughout the paper, we assume that the graph is simple (without self-loops and multiple edges) and undirected.

Each node \( v \in V \) has a feature vector \( x_v \in \mathbb{R}^m \) and a class label \( y_v \in \{1, \ldots, C\} \). Let \( n_k \) denote the size of \( k \)-th class, i.e., \( n_k = |\{v : y_v = k\}| \). By \( N(v) \) we denote the neighbors of \( v \) in \( G \) and by \( d(v) = |N(v)| \) the degree of \( v \). Also, let \( D_k := \sum_{v : y_v = k} d(v) \). Let \( p(\cdot) \) denote the empirical distribution of class labels, i.e., \( p(k) = \frac{n_k}{n} \). Then, we also define degree-weighted distribution as

\[
\hat{p}(k) = \frac{\sum_{v : y_v = k} d(v)}{2|E|} = \frac{D_k}{2|E|}.
\]

2.1 Existing Homophily Measures

Many GNN models implicitly make a so-called homophily assumption: that similar nodes are connected. Similarity can be considered in terms of node features or node labels. Usually, label

\^[2]We further denote (unordered) edges by \( \{u, v\} \) and ordered pairs of nodes by \( (u, v) \).
homophily is analyzed, and we also focus on this aspect leaving feature homophily for further studies. There are several commonly used homophily measures in the literature. Edge homophily \[6, 8\] is the fraction of edges that connect nodes of the same class:

\[ h_{\text{edge}} = \frac{|\{u, v \in E : y_u = y_v\}|}{|E|}. \]

Node homophily \[7\] computes the fraction of neighbors that have the same class for all nodes and then averages these values across the nodes:

\[ h_{\text{node}} = \frac{1}{n} \sum_{v \in V} \frac{|\{u \in N(v) : y_u = y_v\}|}{d(v)}. \]

These two measures are intuitive; however, they have the downside of being sensitive to the number of classes and their balance, which makes them hard to interpret and incomparable across different datasets \[13\]. For example, suppose that each node in a graph is connected to one node of each class. Then, both edge homophily and node homophily for this graph will be equal to \(1\). Thus, these metrics will produce widely different values for graphs with different numbers of classes, despite these graphs being similar in exhibiting no homophily. To fix these issues, \[13\] proposed another homophily measure sometimes referred to as class homophily \[11\]. Class homophily measures excess homophily compared to a null model where edges are independent of the labels. More formally,

\[ h_{\text{class}} = \frac{1}{C-1} \sum_{k=1}^{C} \left[ \frac{\sum_{v : y_v = k} |\{u \in N(v) : y_u = y_v\}|}{\sum_{v : y_v = k} d(v)} - \frac{n_k}{n} \right]_{+}, \]

where \([x]_+ = \max\{x, 0\}\). Here the factor \(\frac{1}{C-1}\) scales the values to the interval \([0, 1]\); larger values indicate more homophilous graphs. If the graph is non-homophilous, then the value of \(h_{\text{class}}\) is expected to be close to zero.

However, there are still some issues with class homophily. First, when correcting the fraction of intra-class edges by its expected value, class homophily does not take into account the variation of node degrees. Indeed, if nodes of class \(k\) have, on average, larger degrees than \(2|E|/n\), then the probability that a random edge goes to that class can be significantly larger than \(n_k/n\). Second, only positive deviations from \(n_k/n\) contribute to class homophily, while classes with heterophilous connectivity patterns are neglected. Let us illustrate these drawbacks of class homophily with a simple example and refer to Appendix B.1 for a more formal analysis.

**Example** Let us construct non-homophilous graphs for which class homophily is significantly larger than zero. Consider the following graph on \(r^2\) nodes: first, construct a clique of size \(r\) with all nodes belonging to the red class; then, for each node in the clique, connect it to \(r - 1\) leaves, all of which belong to the blue class (example for \(r = 4\) is shown on the right). Note that all blue nodes are strictly heterophilous (i.e., only connect to nodes of the opposite class), while all red nodes are class-agnostic (i.e., have the same number of neighbors of both classes). Such graphs are clearly non-homophilous, and a meaningful homophily measure should not produce a value significantly greater than zero for them. However, class homophily for such graphs is positive and can become as large as \(\frac{1}{2}\): \(h_{\text{class}} = \frac{1}{2} - \frac{1}{r} \to \frac{1}{2}\) as \(r \to \infty\).

### 2.2 Desirable Properties for Homophily Measures

Above we have discussed some disadvantages of existing homophily measures. In this section, we formalize this discussion and propose a list of properties desirable for a good homophily measure. The properties are motivated by the recent analysis of clusterization and classification performance measures \[14, 15\], but not all of them can be easily transferred to homophily measures. For instance, we do not require symmetry since homophily compares objects of different nature (a graph and a labeling). For the same reason, the distance property cannot be defined. Finally, it is non-trivial to define monotonicity, we discuss this property in Section 2.4 and Appendix B.4.
Maximal agreement. This property states that a constant upper bound is required for perfectly homophilous graphs. Formally, we say that a homophily measure \( h \) satisfies maximal agreement if for any graph \( G \) in which \( y_u = y_v \) for all \( \{u, v\} \in E \) we have \( h(G) = c_{\text{max}} \). For all other graphs \( G \), we require \( h(G) < c_{\text{max}} \).

Minimal agreement. We say that a homophily measure \( h \) satisfies minimal agreement if \( h(G) = c_{\text{min}} \) for any graph \( G \) in which \( y_u \neq y_v \) for all \( \{u, v\} \in E \). For all other graphs \( G \), we require \( h(G) > c_{\text{min}} \). In other words, if all edges connect nodes of different classes, we expect to observe a constant minimal value.

Constant baseline. This property ensures that homophily is not biased towards particular class size distributions. Intuitively, if the graph structure is independent of labels, we would expect a low homophily value. Moreover, if we want a measure to be comparable across datasets, we expect to observe the same low value in all such cases. There are several ways to formalize the concept of independence and we choose the one based on the so-called configuration model.

**Definition 1.** Configuration model is defined as follows: take \( n \) nodes, assign each node \( v \) degree \( d(v) \) and then randomly pair edge endpoints to obtain a graph.\(^3\)

Assuming that we are given \( n \) labeled nodes and the graph is constructed according to the configuration model (independently from the labels), we expect to observe a fixed (small) homophily independently of the number of classes and class size balance. We formalize this property as follows.

**Definition 2.** A homophily measure \( h \) has asymptotic constant baseline if for \( G \) generated according to the configuration model and for any \( \varepsilon > 0 \) with probability \( 1 - o(1) \) we have \( |h(G) - c_{\text{base}}| < \varepsilon \) for some constant \( c_{\text{base}} \) as \( n \to \infty \).

We refer to Appendix B.2 for other possible ways to formalize the constant baseline requirement.

Let us stress that maximal agreement and asymptotic constant baseline are two essential properties that make the values of a homophily measure comparable across different datasets: the maximal agreement guarantees that perfectly homophilous graphs have the same value, while constant baseline corresponds to uninformative cases with neither strong homophily nor strong heterophily.

Empty class tolerance. Since homophily measures are used to compare different graph datasets, they have to be comparable across datasets with different numbers of classes. Thus, we say that a measure is tolerant to empty classes if it is defined and it does not change when we introduce an additional dummy label that is not present in the data. For instance, both edge homophily and node homophily are empty class tolerant, while class homophily is not. Empty class tolerance is a new property that was not discussed in [14, 15] since classification and clustering evaluation measures are usually not used to compare datasets, see Appendix B.4 for more details.

### 2.3 Adjusted Homophily

In this section, we propose a new homophily measure that satisfies both maximal agreement and constant baseline.

Let us start with edge homophily and first enforce the constant baseline property. For this, we subtract the expected value of the measure from \( h_{\text{edge}} \). If we assume the configuration model, then the probability that a given edge endpoint will be connected to a node with a class \( k \) is equal to \( \sum_{y_v = k} d(v) / 2|E| \). Thus, the adjusted value becomes:

\[
\frac{\left| \{u, v\} \in E : y_u = y_v \right|}{|E|} - \sum_{k=1}^C \left( \frac{\sum_{v : y_v = k} d(v)}{4|E|^2} \right)^2 = h_{\text{edge}} - \sum_{k=1}^C \frac{D_k^2}{4|E|^2}.
\] (1)

Now, to enforce maximal agreement, we normalize the measure as follows:

\[
h_{\text{adj}} = h_{\text{edge}} - \sum_{k=1}^C D_k^2 / (2|E|)^2 = h_{\text{edge}} - \sum_{k=1}^C \frac{\bar{D}(k)}{1 - \sum_{k=1}^C \bar{D}(k)^2}.
\] (2)

\(^3\)See Appendix A for additional discussions about the model.
The following proposition holds.

**Proposition 1.** Adjusted homophily satisfies maximal agreement and constant baseline and is empty class tolerant.

The proof of this proposition can be found in Appendix B.3. Note that minimal agreement is not satisfied since the value \( \frac{-\sum_{k=1}^{C} D_k^2 / |E|^2}{1 - \sum_{k=1}^{C} D_k^2 / |E|^2} \) can be different for different datasets. Thus, perfectly heterophilous datasets may get different values.

### 2.4 Connecting Edge-wise Homophily with Classification Evaluation Measures

In this section, we discover an interesting connection between some homophily measures and recent literature on characterizing classification evaluation measures. In particular, we show that edge-wise homophily measures can be matched with classification evaluation measures. We refer to [14] for a list of classification measures and their properties.

Since we consider undirected graphs, each edge \( \{u, v\} \in E \) gives two ordered pairs of nodes \((u, v)\) and \((v, u)\). Let us consider all such pairs and for each pair \((u, v)\) let us say that \(y_u\) is a true label (for some object) and \(y_v\) is a predicted label. Any classification evaluation measure (such as accuracy, balanced accuracy, etc.) reflects how well the predicted labels agree with the true labels. Similarly, edge-wise homophily measures evaluate how often nodes connected by an edge have the same label. Thus, we can define a confusion matrix \(C\) as follows: each matrix element \(c_{ij}\) denotes the number of edges \((u, v)\) such that \(y_u = i\) and \(y_v = j\). Since the graph is undirected, the matrix \(C\) is symmetric (which is not necessary the case for classification evaluation measures).

**Monotonicity.** Using the confusion matrix, we can define an additional monotonicity property for edge-wise homophily measures.

**Definition 3.** We say that a homophily measure is *monotone* if it is empty class tolerant and it increases when we increment a diagonal element by 2 (except for perfectly homophilous graphs) and decreases when we increase \(c_{ij}\) and \(c_{ji}\) by one for \(i \neq j\) (except for perfectly heterophilous graphs). These two cases correspond to adding an edge between two nodes of the same class or two nodes of different classes, respectively.

Our definition of monotonicity allows for comparing graphs with different numbers of edges and classes. The latter holds due to the empty class tolerance property. Using the analogy between homophily and classification evaluation measures, we can derive the following correspondence:

- **Accuracy** corresponds to *edge homophily* \(h_{edge}\). Edge homophily satisfies maximal and minimal agreement and is empty class tolerant and monotone. However, it does not satisfy asymptotic constant baseline, which is a critical drawback. It is known that accuracy can produce misleading results in settings with imbalanced classes, and edge homophily suffers from the same problem.

- **Balanced accuracy** corresponds to the following expression:

\[
\hat{h}_{bal} = \frac{1}{C} \sum_{k=1}^{C} \frac{|(u, v) : y_u = y_v = k|}{D_k}.
\]

We call this measure *balanced homophily*. Note that symmetric balanced accuracy introduced in [14] gives the same balanced homophily due to the symmetry of \(C\). Balanced homophily satisfies maximal and minimal agreement properties. However, it is not empty class tolerant and thus is not monotone. The asymptotic constant baseline is also not satisfied. Indeed, for the configuration model the value \(c_{base}\) depends on the number of classes and is equal to \(1/C\). Similarly to our derivations in Section 2.3, the value \(h_{bal}\) can be adjusted to have both maximal agreement and constant baseline using the following transformation:

\[
h_{adj} := \frac{C}{C - 1} \left( h_{bal} - \frac{1}{C}\right).
\]

The obtained measure satisfies maximal agreement and constant baseline, but does not satisfy minimal agreement since the value \(-1/c_{C-1}\) depends on the number of classes. Similarly to \(h_{bal}\), monotonicity and empty class tolerance are not satisfied.
Interestingly, both Cohen’s Kappa and Matthews correlation coefficient give the same expression that is adjusted homophily defined in (2). As stated in Proposition 2, adjusted homophily satisfies maximal agreement, asymptotic constant baseline, and empty class tolerance, while the minimal agreement property is not satisfied. Monotonicity is partially satisfied as stated in the theorem below.

**Theorem 1.** Adjusted homophily is monotone (see Definition (3)) if \( h_{adj} > \frac{\sum_i \tilde{p}(i)^2}{\left(\sum_i \tilde{p}(i)^2 + 1\right)} \) and we note that the bound \( \frac{\sum_i \tilde{p}(i)^2}{\left(\sum_i \tilde{p}(i)^2 + 1\right)} \) is always smaller than 0.5. When \( h_{adj} \) is small, counterexamples to monotonicity can be constructed.

We prove this theorem in Appendix B.4.

For our experiments in Section 4, we choose adjusted homophily as it is the best measure in terms of the satisfied properties. We recommend to use adjusted homophily as a measure of homophily in further works since it allows for comparing homophily levels of different datasets with varying number of classes and class balance.

Finally, we note that homophily measures can be directly related to community detection evaluation measures including the well-established characteristic in graph community detection literature called modularity [16]. While modularity measures how well a partition fits a given graph, homophily measures how well graph edges agree with the partition (class labels). It turns out that adjusted homophily measure is a normalized version of modularity. We give a detailed discussion of this in Appendix B.5.

### 2.5 Homophily of Real Graph Datasets

Finalizing the discussion of homophily, let us analyze how different homophily measures behave on real graph datasets. For this analysis, we chose 25 transductive node classification datasets of different sizes and properties. Statistics of these datasets and values of different homophily measures are provided in Table 1, see Appendix D.

Recall that both edge and node homophily are sensitive to the number of classes and class size balance. As we can see from Table 1, they may indicate high homophily levels for some heterophilous datasets (e.g., deezer-europe). In contrast, \( h_{adj} \) corrects for the expected number of edges between classes and shows that most of the considered binary classification datasets are actually heterophilous.

### 3 Label Informativeness

Let us note that non-homophilous graphs can have widely different structures. For instance, among strictly heterophilous graphs in which nodes never connect to nodes of the same class, there can be those where edges are drawn between particular pairs of classes (e.g., Graph 1 in the figure below) and those where edges do not depend on node labels besides not connecting nodes with the same label (e.g., Graph 2). While adjusted homophily will correctly capture the absence of homophily in these graphs, it is not designed to identify which type they belong to. However, distinguishing such graphs is practically important. While it is often believed that standard graph neural networks do not perform well on non-homophilous graphs [7–10, 13], recently it has been shown that they can achieve strong performance on certain non-homophilous graphs [11, 12]. This section proposes a simple measure allowing to distinguish these cases.

![Figure 1: Graph 1](image1.png)

**Figure 1:** Graph 1

![Figure 2: Graph 2](image2.png)

We define a particular characteristic measuring the informativeness of a neighbor’s label for a node’s label. For example, for Graph 1 above, the neighbor’s label uniquely defines the node’s label. Thus, the node classification task is simple on this dataset, and we want our informativeness to be maximal.
for such graphs. Let us formalize this idea. Assume that we sample an edge \((\xi, \eta) \in E\) (from some distribution). The class labels of nodes \(\xi\) and \(\eta\) are then random variables \(y_\xi\) and \(y_\eta\). We want to measure the amount of knowledge the label \(y_\eta\) gives for predicting \(y_\xi\). The entropy \(H(y_\xi)\) measures the ‘hardness’ of predicting the label of \(\xi\) without knowing \(y_\eta\). Given \(y_\eta\), this value is reduced to the conditional entropy \(H(y_\xi | y_\eta)\). In other words, \(y_\eta\) reveals \(I(y_\xi, y_\eta) = H(y_\xi) - H(y_\xi | y_\eta)\) information about the label. To make the obtained quantity comparable across the datasets, we say that label informativeness is

\[
LI := I(y_\xi, y_\eta) / H(y_\xi).
\]

We have \(LI \in [0, 1]\). If the label \(y_\eta\) allows for unique reconstruction of \(y_\xi\), then \(LI = 1\). If \(y_\xi\) and \(y_\eta\) are independent, \(LI = 0\).

Depending on the distribution used for sampling \((\xi, \eta)\), one can obtain several variants of the measure. For instance, if the edges are sampled uniformly at random, we get an edge-wise variant:

\[
LI_{\text{edge}} = \frac{\sum_{c_1, c_2} p(c_1, c_2) \log \frac{p(c_1, c_2)}{\hat{p}(c_1)\hat{p}(c_2)}}{\sum_e \hat{p}(e) \log \hat{p}(e)} = 2 - \frac{\sum_{c_1, c_2} p(c_1, c_2) \log p(c_1, c_2)}{\sum_e \hat{p}(c) \log \hat{p}(c)},
\]

where \(p(c_1, c_2) = \sum_{(u,v) \in E} \mathbb{1}_{y_u = c_1, y_v = c_2} / |E|\). For brevity, we further denote \(LI_{\text{edge}}\) by \(LI\). For alternative ways to define label informativeness we refer to Appendix C.

Recall that \(LI\) equals 1 if and only if the neighbor’s class uniquely reveals the node’s class. This property can be considered as an analog of maximum agreement. To show that \(LI\) is comparable across different datasets, it remains to prove the constant baseline. The following proposition holds, see Appendix C for the proof.

**Proposition 2.** Assume that \(|E| \to \infty\) as \(n \to \infty\) and that the entropy of \(\hat{p}(\cdot)\) is bounded from below by some constant. Let \(\hat{p}_{\min} = \min_e \hat{p}(k)\) and assume that \(\hat{p}_{\min} \gg C/\sqrt{|E|}\) as \(n \to \infty\). Then, for the random configuration model we have \(LI = o(1)\) with high probability.

### 4 Correlation of Graph Dataset Characteristics with GNN Performance

In this section, we analyze the effect of dataset characteristics on the performance of GNNs. In particular, we show that \(LI\) is a better predictor of GNN performance than homophily.

#### 4.1 Synthetic Data

**Random graph model.** To perform our analysis in a simple controlled setting, we generate synthetic graphs. Our generator is based on the *stochastic block model* (SBM) [17]. In this model, the nodes are divided into \(C\) clusters, and for each pair of nodes \(i, j\), we draw an edge between them with probability \(p_{c(i), c(j)}\) independently of all other edges. Here \(c(i)\) is a cluster assignment for a vertex \(i\), which in our case corresponds to the node label \(y_i\).

We assume that the number of classes is \(C = 4\) and each class is of equal size \(l = n/4\). It remains to define the probabilities, which we do as follows:

\[
p_{i, j} = \begin{cases} 
  p_0 K, & \text{if } i = j, \\
  p_1 K, & \text{if } i + j = 5, \\
  p_2 K, & \text{otherwise},
\end{cases}
\]

where \(p_0 + p_1 + 2p_2 = 1\) and \(K\) is a positive constant. Note that the expected degree of any node is (up to a negligible term corresponding to self-loops) \(p_0 K l + p_1 K l + 2p_2 K l = K l\).

This model allows us to explore various combinations of dataset characteristics. Indeed, \(p_0\) directly controls the homophily level, while the relation between \(p_1\) and \(p_2\) allows us to additionally vary \(LI\). To understand this, note that the condition \(i + j = 5\) gives two pairs of classes: \((1, 4)\) and \((2, 3)\). Thus, if \(p_2 = 0\) and \(p_1 > 0\), knowing the label of any neighbor from another class, we can uniquely restore the node’s label. In contrast, for given \(p_0\), the case \(p_1 = p_2\) gives the smallest amount of additional information.
To further illustrate which characteristics can be obtained with this model, let us compute their asymptotic values.

**Proposition 3.** As $n \to \infty$, the dataset characteristics of the proposed model converge to the following values (with high probability):

$$h_{adj} = 4 \frac{p_0}{3} - \frac{1}{3},$$

$$LI = 1 - \frac{H(p_0, p_1, p_2, p_2)}{\log 4},$$

where $H(x) = -\sum x_i \log(x_i)$.

In particular, we see that $h_{adj}$ can be any value between $-1/3$ and $1$ and LI can be between $0$ and $1$. If $LI = 0$, then we always have $h_{adj} = 0$; if $h_{adj} = 1$, then $LI = 1$. However, if $LI = 1$, then either $h_{adj} = -1/3$ or $h_{adj} = 1$.

**Results.** Recently, it has been shown that standard GNNs can sometimes perform well on non-homophilous datasets [11, 12]. We hypothesize that GNNs can learn more complex relationships between nodes than just homophily, and they will perform well as long as the node’s neighbors provide some information about this node. Thus, we expect LI to better predict performance of GNNs than homophily.

To test this hypothesis, we generate graphs according to the procedure described above with the expected node degree $10$ and various combinations of $p_0, p_1, p_2$. Given class labels, the features are taken from the four largest classes in the cora [18–21] dataset. We use the obtained graphs to train two popular GNN models: GCN [1] and GraphSAGE [2]. In total, we run more than 20000 experiments on synthetic datasets for each of the two models. A detailed description of data generation, training setup and hyperparameters used is provided in Appendix E.

Figure 3 shows the results for GraphSAGE. It can be seen that the performance is much better correlated with LI than with homophily. Indeed, the Spearman correlation coefficient between accuracy and LI is equal to 0.93, while between accuracy and adjusted homophily it is equal to 0.05. In particular, when LI is high, GraphSAGE achieves good performance even on strongly heterophilous graphs with negative homophily. The results for GCN follow the same patterns as for GraphSAGE; we provide them in Appendix E.

4.2 Semi-Synthetic Data from [12]

In [12] the authors argue that standard GNNs can perform well on certain heterophilous graphs. They construct semi-synthetic graphs by adding inter-class edges following different patterns to several real-world graphs, thus obtaining several sets of graphs with varying levels of homophily. The authors of [12] run experiments on these graphs and note that a standard GNN with mean aggregation achieves strong performance on some of the heterophilous graphs.
We train GraphSAGE on the same modifications of the cora graph used in [12] and find that the model achieves strong performance when the graphs have high label informativeness. The model performance is shown in Figure 4. The Spearman correlation coefficient between accuracy and LI is equal to 0.78, while between accuracy and adjusted homophily it is equal to -0.24. This confirms that label informativeness is a better predictor of GNN performance than homophily. Training setup and hyperparameters used in these experiments are the same as in Section 4.1 and are described in Appendix E, where we additionally provide results of training GraphSAGE on the modifications of the citeseer [22] graph used in [12].

4.3 Synthetic Data from [11]

In [11] it has also been shown that GNNs can achieve strong performance on certain heterophilous graphs. Again, this phenomenon can be explained by the high label informativeness of the heterophilous graphs used for these experiments.

The authors of [11] investigate how different levels of homophily affect GNN performance. Surprisingly, they find that the curve showing the dependence of GNN performance on edge homophily (as well as on node homophily) is U-shaped: GNNs show strong results not only when edge homophily is high, but also when edge homophily is very low. Our label informativeness explains this behavior. We use the same data generating process as in [11] and find that the curve of label informativeness depending on edge homophily is also U-shaped (see Figure 5). Thus, on datasets from [11], GNNs perform well exactly when label informativeness is high regardless of edge homophily. The U-shape of the label informativeness curve is not surprising: indeed, when edge homophily is very low, knowing that a node has a neighbor of a certain class provides us with information that this node probably does not belong to this class.

5 Conclusion

In this paper, we propose several new measures for characterizing graph node classification datasets. First, we revisit the concept of homophily and show that existing measures have certain drawbacks preventing the comparison of homophily levels between different datasets. We formalize desirable properties for a good homophily measure and show how existing literature on the properties of classification performance metrics can be linked to our problem. Based on our analysis, we propose a new measure called adjusted homophily and argue that it is a better measure of homophily than the ones commonly used in the literature. We believe that having a reliable measure of homophily is important for the future development of heterophily-suited GNNs: we need a characteristic that reliably differentiates homophilous and heterophilous graphs.

Then, we go beyond the homophily–heterophily dichotomy and propose a new property called label informativeness (LI) that characterizes how much information a neighbor’s label provides about a node’s label. Similarly to adjusted homophily, this measure has a constant baseline property and thus can be used to compare datasets with different numbers of classes and class size balance. Through a series of experiments, we show that LI is a better predictor of the performance of GNNs on a graph dataset than homophily.

We do not claim, however, that LI is a universal predictor of the performance of a GNN on a given dataset. We designed this measure to be both informative and simple to compute and interpret. For instance, LI considers all edges individually and do not consider the node’s neighborhood as a whole. As a result, LI can be insensitive to some complex dependencies. However, we clearly see that despite its simplicity, LI correlates with GNN performance much better than homophily.

Let us also note that our analysis is limited to graph-label interactions. In future work, it would be important to also analyze node features. Indeed, node features may have non-trivial relations with both graph and labels. It can be the case that graph is heterophilous in terms of labels but homophilous...
in terms of node features or vise- versa. These interactions may allow one to understand the properties and performance of GNNs even better.

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A  Random Configuration Model

Numerous random graph models have been proposed to reflect and predict important quantitative and topological aspects of real-world networks [23]. The simplest model is the Erdős–Rényi random graph, i.e., we assume that $G$ is sampled uniformly at random from the set of all graphs with $n$ nodes and $|E|$ edges. However, this model is known to be not a good descriptor of real-world networks since its Poisson degree distribution significantly differs from heavy-tailed degree distributions observed in real-world networks. A standard solution is to consider a random graph with a given degree sequence [24]: a graph is sampled uniformly from the set of all graphs with a given degree sequence.

A configuration model which we assume throughout the paper is defined as follows. To generate a graph, we form a set $A$ containing $d(v)$ distinct copies of each node $v$ and then choose a random matching of the elements of $A$. In this case, self-loops and multiple edges may appear. Under some conditions, the obtained graph is simple (i.e., does not contain loops and multiple edges) with probability $1 - o(1)$ [24].

Let us also note that there is another model that is similar to the one discussed above but can be easier to analyze. To obtain a graph with given expected degree sequence [25] we take the degree sequence from the observed graph and say that the number of edges between $i$ and $j$ follows a Poisson distribution with the mean $\frac{d(i)d(j)}{2|E|}$ if $i \neq j$ and the expected number of loops for a vertex $i$ is $\frac{d(i)^2}{4|E|}$. This model does not preserve the exact degree sequence, but has it in expectation. Note that usually $d(i)d(j) \ll 2|E|$, so multiple edges rarely appear. Asymptotically, this model is similar to the configuration model but a graph with given expected degree sequence is easier to analyze theoretically. In our analysis, we assume the configuration model, so we have to carefully track the error terms.

B  Analysis of Homophily

B.1  Class Homophily

Recall that class-homophily is defined as [13]:

$$h_{\text{class}} = \frac{1}{C-1} \sum_{k=1}^{C} \left[ \frac{\sum_{v: y_v = k} |\{u \in N(v) : y_u = y_v\}|}{\sum_{v: y_v = k} d(v)} - \frac{n_k}{n} \right]_+.$$  

Here the first term inside the brackets is the fraction of edges that go from a particular class $k$ to itself. The second term $n_k/n = p(k)$ is the null expected fraction. We note that $p(k)$ is the expected fraction if we assume the Erdős–Rényi model. Indeed, for this model, all edges have equal probability, and thus the expected fraction of neighbors of class $k$ is proportional to the size of this class. However, as mentioned above, the Erdős–Rényi null model has certain disadvantages since it does not take into account node degrees. This may lead to incorrect estimates of null probabilities for degree-imbalanced classes, as shown in the example below.

**Proposition 4.** Assume that we have two classes of size $n/2$. Further assume that the degrees of nodes in the first class are equal to $d$, while nodes in the second class have degrees $\ell d$ for some $\ell > 1$.

Then, if edges are added independently of the classes (configuration model), the expected value of $h_{\text{class}}$ is

$$Eh_{\text{class}} = \frac{l}{l+1} - \frac{1}{2}.$$  

Thus, for randomly connected nodes we get $Eh_{\text{class}} \to 1/2$ as $l \to \infty$.

**Proof.** We need to compute the expected number of intra-class edges for each class. For the first class, we multiply the number of nodes by the degree of each node and by the probability of a particular edge to go to the same class: $\frac{n}{2} \cdot d \cdot \frac{|E|}{n|E|} = \frac{nd}{2}$. Normalizing by the sum of the degrees, we get $\frac{1}{\ell+1}$. Similarly, for the second class, the normalized number of the intra-class edges is $\frac{l}{\ell+1}$. Hence,

$$Eh_{\text{class}} = \left[ \frac{1}{\ell+1} - \frac{1}{2} \right]_+ + \left[ \frac{l}{l+1} - \frac{1}{2} \right]_+ = \frac{l}{l+1} - \frac{1}{2},$$

$\square$
In the example above, we see that the undesirable behavior of \( h_{\text{class}} \) is caused by the \( \lfloor \cdot \rfloor \) operation. Interestingly, if we remove this operation, then \( h_{\text{class}} \) becomes equal to \( h_{\text{adj}}^{\text{bal}} \) introduced in Section 2.4, equation (3):

\[
\frac{1}{C - 1} \sum_{k=1}^{C} \left( \frac{\sum_{v,y_k = k} \{ \{ u \in N(v) : y_u = y_v \} \}}{\sum_{v,y_k = k} d(v)} \frac{n_k}{n} \right) = C h_{\text{bal}} - 1 \frac{1}{C - 1} .
\]

**Proposition 5.** For the configuration model with an arbitrary number of classes \( C \), we have \( E h_{\text{bal}} = 0 \).

**Proof.** Let us denote the sizes of the classes by \( n_1, \ldots, n_C \). Recall that we use the notation \( D_k = \sum_{v,y_k = k} d(v) \). It is easy to see that

\[
E h_{\text{bal}} = \sum_{i=1}^{C} \left( \frac{D_i}{\sum_j D_j} - \frac{n_i}{\sum_j n_j} \right) = 1 - 1 = 0 .
\]

\( \square \)

**B.2 Constant Baseline**

There are several possible ways to formalize the constant baseline property. In the literature [14, 15], this property is often formalized as follows: assuming some randomized model, the expected value of a measure should be equal to some constant. For homophily measures, this corresponds to the following definition.

**Definition 4.** A homophily measure \( h \) has constant baseline if for \( G \) generated according to the configuration model we have \( E h(G) = c_{\text{base}} \) for some constant \( c_{\text{base}} \).

This property is very strict as minor variations in the definition of the model (e.g., different alternatives of the configuration model discussed in Appendix A) may lead to negligibly small error terms preventing us from getting exactly the same constant \( c_{\text{base}} \). Thus, in the main text, we use the alternative Definition 2. This definition is weaker in the sense that we allow asymptotically negligible deviations from the constant \( c_{\text{base}} \). On the other hand, our definition is somewhat stronger since we also require the concentration of the value around its expectation. In that sense, our definition is stronger than the asymptotic constant baseline defined in [14].

**B.3 Proof of Proposition 1**

The fact that adjusted homophily is empty class tolerant directly follows from its definition: an empty class does not contribute to neither the numerator nor the denominator of \( h_{\text{adj}} \).

Maximal agreement is also straightforward: we have \( h_{\text{edge}} = \sum_{k=1}^{C} D_k/(2|E|)^2 \leq 1 - \sum_{k=1}^{C} D_k/(2|E|)^2 \) with equality if and only if all edges are homophilous.

Now, let us formulate and prove the constant baseline property.

**Proposition 6.** Let \( G \) be a graph generated according to the configuration model. Assume that the degree-weighted distribution of classes is not very unbalanced, i.e., that \( 1 - \sum_k \bar{p}(k)^2 \gg 1/\sqrt{E} \). Then, \( |h_{\text{adj}}| \leq \phi \) with probability \( 1 - o(1) \) for some \( \phi = \phi(|E|) \to 0 \text{ as } |E| \to \infty \).

Let us first analyze the numerator of \( h_{\text{adj}} \) which we denote by \( h_{\text{mod}} \) (since it corresponds to the network’s modularity — see Appendix B.5).

Let \( \xi \) denote the number of intra-class edges in a graph constructed according to the configuration model. We may write:

\[
\xi = \frac{1}{2} \sum_{k=1}^{C} \sum_{i=1}^{n_k} \sum_{i,k} 1_{i,k} ,
\]

where \( 1_{i,k} \) indicates that an endpoint \( i \) of some node with class \( k \) is connected to another endpoint of class \( k \). Note that the probability of this event is \( D_k^{-1} \). Thus, we have

\[
E h_{\text{mod}} = \xi |E| - \sum_{k=1}^{C} \frac{D_k^2}{4|E|^2} = \frac{1}{2} \sum_{k=1}^{C} \frac{D_k(D_k - 1)}{2(2|E| - 1)} - \sum_{k=1}^{C} \frac{D_k^2}{4|E|^2} = O \left( \frac{1}{|E|} \right) .
\]

(4)
Now, let us estimate the variance of the number of intra-class edges. We may write:

\[
\text{Var}(2\xi) = \mathbb{E}(2\xi)^2 - (\mathbb{E}(2\xi))^2 = \mathbb{E}\left(\sum_{k=1}^{C} \sum_{i=1}^{D_k} 1_{i,k}\right)^2 - (\mathbb{E}2\xi)^2
\]

\[
= \mathbb{E}(2\xi) + \sum_{k=1}^{C} 2 \cdot \frac{D_k}{2|E| - 1} \cdot \left(\frac{1}{2|E| - 1} + \frac{D_k - 2}{2|E| - 3} \cdot \frac{D_k - 3}{2|E| - 3}\right) + \sum_{k=1}^{C} \sum_{l=k+1}^{C} 2D_kD_l \cdot \frac{D_k - 1}{2|E| - 1} \cdot \frac{D_l - 1}{2|E| - 3} - (\mathbb{E}2\xi)^2
\]

\[
= \mathbb{E}(2\xi) + \sum_{k=1}^{C} \frac{D_k^2 + O(D_k^3)}{4|E|^2} + \sum_{k=1}^{C} \sum_{l=k+1}^{C} \frac{2D_k^2D_l^2 + O(D_k^2D_l + D_kD_l^2)}{4|E|^2} - \left(\sum_{k=1}^{C} \frac{D_k^2 + O(D_k)}{2|E|}\right)^2
\]

\[
= \mathbb{E}(2\xi) + O\left(\frac{|E|}{|E|^2}\right) = \mathbb{E}(2\xi) + O\left(\frac{1}{|E|}\right) = O\left(\frac{1}{|E|}\right).
\]

Let \(\varphi = \varphi(|E|)\) be any function such that \(\varphi \to \infty\) as \(|E| \to \infty\). Using the Chebyshev’s inequality and (4), we get:

\[
P\left(|h_{mod}| \geq \frac{\varphi}{\sqrt{|E|}}\right) = P\left(|h_{mod} - \mathbb{E}h_{mod}| > \frac{\varphi}{\sqrt{|E|}} + O\left(\frac{1}{|E|}\right)\right)
\]

\[
= O\left(\frac{\text{Var}(\xi)|E|}{|E|^2\varphi^2}\right) = O\left(\frac{1}{\varphi^2}\right) = o(1).
\]

Recall that \(h_{adj} = \frac{h_{mod}}{1 - \sum_{k=1}^{C} \bar{p}(k)^2}\). Since we have \(1 - \sum_{k=1}^{C} \bar{p}(k)^2 \gg \frac{1}{\sqrt{|E|}}\) and \(|h_{mod}| \leq \frac{\varphi}{\sqrt{|E|}}\) with probability \(1 - o(1)\), we can choose such slowly growing \(\varphi\) that \(h_{adj} \leq \frac{\varphi}{\sqrt{|E|}\left(1 - \sum_{k=1}^{C} \bar{p}(k)^2\right)} = o(1)\) with probability \(1 - o(1)\).

### B.4 Monotonicity Property

#### B.4.1 Definition

In this section, we discuss why it is difficult to define monotonicity for general homophily measures and how we define it for edge-wise measures.

First, let us revisit how monotonicity is defined for measures used in other areas. In general, the monotonicity property is defined as follows: if an object \(B'\) is definitely more similar to an object \(A\) than \(B\), then the similarity between \(B'\) and \(A\) should be larger than between \(B\) and \(A\). The only problem is to define what it means to be “definitely more similar”. In [15] the monotonicity property was introduced for cluster similarity measures. Such measures evaluate how close are two partitions of the same set of items. To formally define the concept of more similar partitions, the authors of [15] use the concept of perfect splits and perfect merges — such transformations of a partition \(B\) that make it more similar to \(A\). Later, monotonicity was defined for classification evaluation measures that compare the predicted labels for a set of items with the reference ones. Here it is easier to formalize what it means that a labeling \(B'\) is definitely more similar to the reference labeling than \(B\). Indeed, if we consider a labeling \(B\) and change one incorrect label to the correct one, then we become closer to the reference labeling.

Now, let us return to homophily measures. Such measures evaluate the agreement between a graph and a labeling of its nodes. To define monotonicity, we need such transformations that make a graph and a labeling definitely more similar. Since the problem is not symmetric, we can either rewire edges or relabel nodes. Regarding relabeling of nodes, we may say that taking a perfectly heterophilous node (that is not connected to any node of its class) and relabeling it in such a way that it becomes
perfectly homophilous (which is only possible when all its neighbors belong to one class) should make the graph and labeling more similar to each other. Regarding the edges, we may say that taking an edge that connects two nodes of different classes and rewiring it in such a way that it connects two nodes of the same class should increase the measure. However, note that rewiring edges may also affect the graph structure in a non-trivial way (degree distribution, diameter, etc.). Since the definition of monotonicity is non-trivial for homophily measures, we do not focus on this property in the paper. Instead, we define and analyze monotonicity for edge-wise measures only, where the definition is straightforward.

Recall that in Section 2.4 we reformulated the edge-wise measures as functions over confusion matrices, where each matrix element $c_{ij}$ denotes the number of edges $(u,v)$ such that $y_u = i$ and $y_v = j$. Since the graph is undirected, the confusion matrix $C$ has to be symmetric.

If we follow the definition of monotonicity in [14, 15], we could define it for homophily measures as follows. We say that a homophily measure is monotone if it increases when we decrement $c_{i,j}$ and $c_{j,i}$ by one and increment either $c_{i,j}$ or $c_{j,i}$ by two for $i \neq j$. This condition corresponds to taking an edge with $y_u \neq y_v$, and changing $y_u$ to $y_v$ or vice versa. However, an important property that has to be taken into account when discussing monotonicity for homophily measures is the fact that such measures are used to compare different graph datasets, in contrast to classification evaluation measures that compare the agreement between predicted labelings for a fixed given reference labeling. This means that for classification measures, monotonicity and constant baseline are critical for a fixed number of classes and a fixed number of elements, while homophily measures have to be comparable across datasets with different sizes and numbers of classes. For instance, balanced accuracy has a constant baseline with the expected value of $\frac{1}{2}$ which is sufficient for classification evaluation but is a drawback for measuring homophily. Because of this, we do not consider the standard definition of monotonicity as it is restricted to a fixed number of classes only. Instead, we introduce tolerance to empty classes and, based on that, we introduce a stronger version of monotonicity. In fact, our definition of monotonicity (Definition 3) is similar to strong monotonicity in [14, 15], but also requires empty class tolerance since comparing measures across different numbers of classes is crucial.

### B.4.2 Monotonicity of Adjusted Homophily

In this section, we analyze monotonicity of adjusted homophily and prove Theorem 1.

Recall that we say that a homophily measure is monotone if it is empty class tolerant and it increases when we increment a diagonal element by 2 (except for perfectly homophilous graphs) and decreases when we increase $c_{i,j}$ and $c_{j,i}$ by one for $i \neq j$ (except for perfectly heterophilous graphs).

Empty class tolerance is clearly satisfied for adjusted homophily, so let us now analyze what happens when we increment a diagonal element or decrement two (symmetric) off-diagonal elements.

Let us denote $N := 2|E|, a_i := \sum_j c_{ij}$. Then, we have $\bar{p}(i) = \frac{a_i}{N}$. Thus, we have to prove that the measure is monotone when $h_{adj} > \frac{N \sum_i c_{ii} - \sum_i a_i^2}{N^2 - \sum_i a_i^2}$.

Using the notation with a confusion matrix, adjusted homophily can be written as follows:

$$h_{adj} = \frac{N \sum_i c_{ii} - \sum_i a_i^2}{N^2 - \sum_i a_i^2}.$$  

To check whether the measure increases when we increment diagonal elements, let us compute the derivative w.r.t. $c_{kk}$ for some $k$:

$$\frac{\partial h_{adj}}{\partial c_{kk}} = \frac{\left(\sum_i c_{ii} + N - 2a_k\right) \left( N^2 - \sum_i a_i^2 \right) - \left(2N - 2a_k\right) \left(N \sum_i c_{ii} - \sum_i a_i^2\right)}{(N^2 - \sum_i a_i^2)^2}.$$  

Let us simplify the numerator:

$$\left(\sum_i c_{ii} + N - 2a_k\right) \left( N^2 - \sum_i a_i^2 \right) - \left(2N - 2a_k\right) \left(N \sum_i c_{ii} - \sum_i a_i^2\right)$$

$$= N^3 - 2N^2 a_k - \sum_i c_{ii} \sum_i a_i^2 - N^2 \sum_i c_{ii} + 2a_k N \sum_i c_{ii} + N \sum_i a_i^2.$$  

15
For monotonicity, we need the derivative to be positive, i.e.,
\[ N^3 + 2a_k N \sum_i c_{ii} + N \sum_i a_i^2 > 2N^2 a_k + \sum_i c_{ii} \sum_i a_i^2 + N^2 \sum_i c_{ii}. \]
Let us denote by \( \bar{D} \) the sum of all off-diagonal elements, i.e., \( \bar{D} := N - \sum_i c_{ii} \). Then, we can rewrite the above condition as follows:
\[ N^2 \bar{D} + \bar{D} \sum_i a_i^2 > 2Na_k \bar{D}, \]
\[ N^2 + \sum_i a_i^2 > 2Na_k. \]
The latter equality holds since
\[ N^2 + \sum_i a_i^2 > N^2 + a_k^2 \geq 2Na_k. \]
Thus, \( h_{\text{adj}} \) increases when we increment a diagonal element.

To see whether the measure decreases when we increment the off-diagonal elements, let us compute the derivative of the measure w.r.t. \( c_{k,l} \) (which is equal to \( c_{l,k} \)) for \( k \neq l \):
\[ \frac{\partial h_{\text{adj}}}{\partial c_{k,l}} = \frac{(2 \sum_i c_{ii} - 2a_k - 2a_l) \left( N - \sum_i a_i^2 \right) - (4N - 2a_k - 2a_l) \left( N \sum_i c_{ii} - \sum_i a_i^2 \right)}{(N^2 - \sum_i a_i^2)^2}. \]
The numerator is:
\[ -2(a_k + a_l)N^2 - 2 \sum_i c_{ii} \sum_i a_i^2 - 2N^2 \sum_i c_{ii} + 2(a_k + a_l)N \sum_i c_{ii} + 4N \sum_i a_i^2. \]
For monotonicity, we need the following inequality:
\[ (a_k + a_l)N^2 + \sum_i c_{ii} \sum_i a_i^2 + N^2 \sum_i c_{ii} > (a_k + a_l)N \sum_i c_{ii} + 2N \sum_i a_i^2. \quad (5) \]
This inequality is not always satisfied. Indeed, both \( a_k + a_l \) and \( \sum_i c_{ii} \) can be small. Let us note, however, that the inequality is satisfied if \( h_{\text{adj}} \) is large enough. Indeed, the sufficient condition for (5) is
\[ \sum_i c_{ii} \left( \sum_i a_i^2 + N^2 \right) > 2N \sum_i a_i^2. \]
This is equivalent to the following inequality for \( h_{\text{adj}} \):
\[ h_{\text{adj}} = \frac{N \sum_i c_{ii} - \sum_i a_i^2}{N^2 - \sum_i a_i^2} > \frac{N \sum_i \frac{2N \sum_i a_i^2}{\sum_i a_i^2 + N^2} - \sum_i a_i^2}{N^2 - \sum_i a_i^2} \]
\[ = \frac{N^2 \sum_i a_i^2 - \left( \sum_i a_i^2 \right)^2}{\left( N^2 - \sum_i a_i^2 \right) \left( \sum_i a_i^2 + N^2 \right)} = \frac{\sum_i a_i^2}{\left( \sum_i a_i^2 + N^2 \right)}. \]
Thus, \( h_{\text{adj}} \) is monotone if its values are at least \( \frac{\sum_i a_i^2}{\left( \sum_i a_i^2 + N^2 \right)} \). Note that we have \( \frac{\sum_i a_i^2}{\left( \sum_i a_i^2 + N^2 \right)} < 0.5 \), so when \( h_{\text{adj}} > 0.5 \) it is always monotone.

However, the non-monotone behavior may occur when the numerator of \( h_{\text{adj}} \) is small. This undesirable behavior is somewhat expected: due to the normalization, \( h_{\text{adj}} \) satisfies constant baseline and maximal agreement, but violates minimal agreement. Since minimal agreement does not hold, one can also expect monotonicity to be violated for small values of \( h_{\text{adj}} \).
Characterizing Graph Datasets for Node Classification: Beyond Homophily–Heterophily Dichotomy

For instance, we can construct the following counter-example to monotonicity. Assume that we have four classes (0, 1, 2, 3) and non-zero entries of the confusion matrix are \( c_{23} = c_{32} = M, c_{33} = 2 \). Then, the adjusted homophily is:

\[
h_{adj} = \frac{2(2M + 2) - M^2 - (M + 2)^2}{(2M + 2)^2 - M^2 - (M + 2)^2} = \frac{-2M^2}{2M^2 + 4M} = \frac{-M}{M + 2}.
\]

Now, we increment the entries \( c_{01} \) and \( c_{10} \) by 1. The new adjusted homophily is:

\[
h'_{adj} = \frac{2(2M + 4) - M^2 - (M + 2)^2 - 2}{(2M + 4)^2 - M^2 - (M + 2)^2 - 2} = \frac{-2M^2 + 2}{2M^2 + 12M + 10} = \frac{1 - M}{M + 5}.
\]

We disprove modularity if we have \( h'_{adj} > h_{adj} \), i.e.,

\[
\frac{1 - M}{M + 5} > \frac{-M}{M + 2},
\]

\[
2 - M - M^2 > -M^2 - 5M,
\]

\[
2 > -4M,
\]

which holds for all \( M \geq 1 \).

B.5 Modularity

**Background.** Modularity is arguably the most well-known measure of goodness of a partition for a graph. It was first introduced in [16] and is widely used in community detection literature: modularity is directly optimized by some algorithms, used as a stopping criterion in iterative methods, or used as a metric to compare different algorithms when no ground truth partition is available. The basic idea is to consider the fraction of intra-community edges among all edges of \( G \) and penalize it for avoiding trivial partitions like those consisting of only one community of size \( n \). In its general form and using notation adopted in this paper, modularity is

\[
h_{mod} = \frac{1}{|E|} \left( \frac{|\{u, v\} \in E : y_u = y_v|}{|E|} - \gamma \mathbb{E} \xi \right),
\]

where \( \xi \) is a random number of intra-class edges in a graph constructed according to some underlying random graph model; \( \gamma \) is the resolution parameter which allows for varying the number of communities obtained after maximizing modularity. The standard choice is \( \gamma = 1 \), which also guarantees that the expected value of modularity is 0 if a graph is generated independently of class labels according to the underlying model.

Usually, modularity assumes the configuration model. In this case, we have \( \mathbb{E} \xi = \frac{\sum_k D_k (D_k - 1)}{2(2|E| - 1)} \approx \frac{1}{4|E|} \sum_k D_k^2 \), giving the following expression:

\[
h_{mod} = \frac{|\{u, v\} \in E : y_u = y_v|}{|E|} - \sum_{k=1}^C \frac{D_k^2}{4|E|^2}.
\]

We refer to [26, 27] for more details regarding modularity and its usage in community detection literature.

**Relation to homophily.** While modularity measures how well a partition fits a given graph, homophily measures how well graph edges agree with the partition (class labels). Thus, they essentially measure the same thing, and modularity can be used as a homophily measure. Indeed, it is easy to see that modularity coincides with the expression (1). In other words, the numerator of adjusted homophily is equal to modularity. Hence, adjusted homophily can be viewed as a normalized version of modularity. Note that for modularity the normalization is not crucial as modularity is usually used to compare several partitions of the same graph. In contrast, homophily is usually used to compare different graphs, and that is why it is essential to use normalization.
C Analysis of LI

C.1 Proof of Proposition 2

In this section, we prove Proposition 2. Let us give a formal statement of this proposition.

**Proposition 1.** Assume that $|E| \to \infty$ as $n \to \infty$. Assume that the entropy of $\bar{p}(\cdot)$ is bounded from below by some constant. Let $p_{\min} = \min_k \bar{p}(k)$. Assume that $p_{\min} \gg C/\sqrt{|E|}$ as $n \to \infty$. Let $\varepsilon = \varepsilon(n)$ be any function such that $\varepsilon \gg \frac{C}{p_{\min} \sqrt{|E|}}$ and $\varepsilon = o(1)$ as $n \to \infty$. Then, with probability $1 - o(1)$, we have $|LI| \leq K \varepsilon = o(1)$ for some constant $K > 0$.

**Proof.** Recall that

$$LI = - \sum_{c_1, c_2} p(c_1, c_2) \log \frac{p(c_1, c_2)}{\bar{p}(c_1) \bar{p}(c_2)}.$$

Thus, for each pair $k, l$, we need to estimated $p(k, l)$. Let us denote:

$$E(k, l) := \sum_{u=1}^{n} \sum_{v=1}^{n} \mathbb{1}_{\{u, v\} \in E, y_u = k, y_v = l},$$

so we have $p(k, l) = \frac{E(k, l)}{|E|}$.

As before, we use the notation $D_k = \sum_{v:y_v=k} d(v)$. First, consider the case $k \neq l$. Let us compute the expectation of $E(k, l)$:

$$EE(k, l) = \frac{D_k D_l}{2|E| - 1} \quad \text{for } k \neq l, \text{ and } EE(k, k) = \frac{D_k (D_k - 1)}{2|E| - 1}.$$

Now, we estimate the variance. Below, $1_{i,j}$ indicates that two endpoints are connected.

$$\text{Var} E(k, l) = E \left( \sum_{i=1}^{D_k} \sum_{j=1}^{D_l} 1_{i,j} \right)^2 - (EE(k, l))^2$$

$$= EE(k, l) + \frac{D_k D_l (D_k - 1)(D_l - 1)}{(2|E| - 1)(2|E| - 3)} - (EE(k, l))^2$$

$$= EE(k, l) + O \left( \frac{D_k D_l (D_k + D_l)}{|E|^2} \right) = O \left( \frac{D_k D_l}{|E|} \right).$$

Similarly,

$$\text{Var} E(k, k) = E \left( \sum_{i=1}^{D_k} \sum_{j=1}^{D_k} 1_{i,j} \right)^2 - (EE(k, k))^2 = EE(k, k) + O \left( \frac{D_k^3}{|E|^2} \right) = O \left( \frac{D_k^3}{|E|} \right).$$

From Chebyshev’s inequality, we get:

$$P \left( |E(k, l) - EE(k, l)| > \varepsilon EE(k, l) \right) = O \left( \frac{|E|}{D_k D_l \varepsilon^2} \right) = O \left( \frac{1}{p_{\min} \varepsilon^2} \right) = o \left( \frac{1}{C^2} \right).$$

Thus, with probability $1 - o(1)$, $P \left( |E(k, l) - EE(k, l)| < \varepsilon EE(k, l) \right)$ for all pairs of classes. In this case,

$$LI = - \frac{\sum_{k,l} p(k, l) \log (1 + O(\varepsilon))}{\sum_{l} \bar{p}(k) \log \bar{p}(k)} = O(\varepsilon).$$

\[\Box\]
C.2 Alternative Definition

Recall that in Section 3 we define the label informativeness in the following general form:

\[ LI := I(y_{\xi}, y_{\eta}) / H(y_{\xi}) \]

Then, to define \( LI_{edge} \), we say that \( \xi \) and \( \eta \) are two endpoints of an edge sampled uniformly at random. Another possible variant is when we first sample a random node and then sample its random neighbor. The probability of an edge becomes \( p(c_1, c_2) = \sum_{u=1}^{n} \sum_{v=1}^{n} \mathbb{1}(\{u, v\} \in E, y_u = c_1, y_v = c_2) / \sum_{u=1}^{n} d(u) \). In this case, \( H(y_\eta) \) is the entropy of the distribution \( p(c) \), \( H(y_\eta) \) is the entropy of \( p(c) \). Thus, we obtain:

\[ LI_{node} = - \sum_{c_1, c_2} p(c_1, c_2) \log \frac{p(c_1, c_2)}{p(c_1)p(c_2)} \]

In this paper, we mostly focus on \( LI_{edge} \) and refer to it as LI for brevity. First, this measure is conceptually similar to adjusted homophily discussed above: they both give equal weights to all edges. Second, in our analysis of real datasets we do not notice any substantial difference between \( LI_{edge} \) and \( LI_{node} \), see Table 1.

D Analysis of Real Datasets

D.1 Datasets

Cora, citeseer, and pubmed [18–22] are three classic paper citation network benchmarks. For cora and citeseer labels correspond to paper topics, while for pubmed labels specify the type of diabetes addressed in the paper. Coauthor-CS and coauthor-physics [28] are co-authorship networks. Nodes represent authors, and two nodes are connected by an edge if the authors co-authored a paper. Node labels correspond to fields of study. Amazon-computers and amazon-photo [28] are co-purchasing networks. Nodes represent products, and an edge means that two products are frequently bought together. Labels correspond to product categories. Lastfm-asia is a social network of music streaming site LastFM users who live in Asia. Edges represent follower relationships, and labels correspond to user’s nationality. In the facebook [29] graph nodes correspond to official Facebook pages, and links indicate mutual likes. Labels represent site categories. In the github [29] graph, nodes represent GitHub users and edges represent follower relationships. A binary label indicates that a user is either a web or a machine learning developer. Ogbn-arxiv and ogbn-products [30] are two datasets from the recently proposed Open Graph Benchmark. Ogbn-arxiv is a citation network graph with labels corresponding to subject areas. ogbn-products is a co-purchasing network with labels corresponding to product categories. Squirrel, chameleon, and actor [7, 29, 31] are popular datasets for node classification in heterophilous graphs. In squirrel and chameleon nodes represent Wikipedia pages, and edges indicate links between pages. The labels correspond to a page’s popularity. In the actor graph, nodes correspond to actors and edges represent co-occurrence on the same Wikipedia page. The labels are based on words from an actor’s Wikipedia page. Flickr [32] is a graph of images with labels corresponding to image types. Deezer-europe [29] is a user network of the music streaming service Deezer with labels representing a user’s gender. Twitch-de and twitch-pt [29] are social network graphs of gamers from the streaming service Twitch. The labels indicate if a streamer uses explicit language. Genius, twitch-gamers, arxiv-year, snap-patents, and wiki [13] are recently proposed large-scale heterophilous datasets. For the wiki dataset we remove all isolated nodes. We additionally construct one more binary classification graph — twitter-hate. This graph is based on data from Hateful Users on Twitter dataset on Kaggle.\(^4\) The labels indicate if a user posts hateful messages or not. We remove all the unlabeled nodes from the graph and use the largest connected component of the resulting graph.

D.2 Dataset Characteristics

Dataset characteristics are shown in Table 1. It can be seen that the typically used homophily measures — \( h_{edge} \) and \( h_{node} \) — often overestimate homophily levels, since they do not take into account the number of classes and class size balance. This is particularly noticeable for datasets with two classes. If fact, according to these measures all binary classification datasets in our table

\(^4\)https://www.kaggle.com/datasets/manoelribeiro/hateful-users-on-twitter
Table 1: Dataset characteristics, more homophilous datasets are above the line

| Dataset            | n      | |E| | C | h_{edge} | h_{node} | h_{class} | h_{adj} | LI_{edge} | LI_{node} |
|--------------------|--------|-----|-----|-----|----------|----------|----------|----------|----------|----------|
| cora               | 2708   | 5278| 7   | 0.81| 0.83     | 0.77     | 0.77     | 0.59     | 0.61     |
| citeseer           | 3327   | 4552| 6   | 0.74| 0.71     | 0.63     | 0.67     | 0.45     | 0.43     |
| pubmed             | 19717  | 44324| 3   | 0.80| 0.79     | 0.66     | 0.69     | 0.41     | 0.40     |
| coauthor-cs       | 18333  | 81894| 15  | 0.81| 0.83     | 0.75     | 0.78     | 0.65     | 0.68     |
| coauthor-physics   | 34493  | 247962| 5   | 0.93| 0.92     | 0.85     | 0.87     | 0.72     | 0.76     |
| amazon-computers   | 13752  | 245861| 10  | 0.78| 0.79     | 0.70     | 0.68     | 0.53     | 0.60     |
| amazon-photo       | 7650   | 119081| 8   | 0.83| 0.84     | 0.77     | 0.79     | 0.67     | 0.70     |
| lastfm-asia        | 7624   | 27806| 18  | 0.87| 0.83     | 0.77     | 0.86     | 0.74     | 0.68     |
| facebook           | 22470  | 170823| 4   | 0.89| 0.88     | 0.82     | 0.82     | 0.62     | 0.74     |
| github             | 37700  | 289003| 2   | 0.85| 0.80     | 0.38     | 0.38     | 0.13     | 0.15     |
| twitter-hate       | 2700   | 11934| 2   | 0.78| 0.67     | 0.50     | 0.55     | 0.23     | 0.51     |
| ogbn-arxiv         | 169343 | 1157799| 40  | 0.65| 0.64     | 0.42     | 0.59     | 0.45     | 0.53     |
| ogbn-products      | 2449029| 61859012| 47  | 0.81| 0.82     | 0.46     | 0.79     | 0.68     | 0.70     |
| squirrel           | 5201   | 198353| 5   | 0.22| 0.22     | 0.03     | 0.01     | 0.00     | 0.00     |
| chameleon          | 2277   | 31371| 5   | 0.23| 0.25     | 0.04     | 0.03     | 0.05     | 0.06     |
| actor              | 7600   | 26659| 5   | 0.22| 0.22     | 0.01     | 0.00     | 0.00     | 0.00     |
| flickr             | 89250  | 449878| 7   | 0.32| 0.32     | 0.07     | 0.09     | 0.01     | 0.01     |
| deezer-europe      | 28281  | 92752| 2   | 0.53| 0.53     | 0.03     | 0.03     | 0.00     | 0.00     |
| twitch-de          | 9498   | 153138| 2   | 0.63| 0.60     | 0.14     | 0.14     | 0.02     | 0.03     |
| twitch-pt          | 1912   | 31299| 2   | 0.57| 0.59     | 0.12     | 0.11     | 0.01     | 0.02     |
| genius             | 421961 | 922868| 2   | 0.59| 0.51     | 0.02     | -0.05    | 0.00     | 0.17     |
| twitch-gamers      | 168114 | 6797557| 2   | 0.55| 0.56     | 0.09     | 0.09     | 0.01     | 0.02     |
| arxiv-year         | 169343 | 1157799| 5   | 0.22| 0.29     | 0.07     | 0.01     | 0.04     | 0.12     |
| snap-patents       | 2923922| 13972547| 5   | 0.22| 0.21     | 0.04     | -0.00    | 0.02     | 0.00     |
| wiki               | 1770981| 242605360| 5   | 0.38| 0.28     | 0.17     | 0.15     | 0.06     | 0.04     |

are homophilous. In contrast, h_{adj} corrects for the expected number of edges between classes and shows that most of the considered binary classification datasets (github and twitter-hate being the exceptions) are actually heterophilous.

As for label informativeness, it can be seen that on real heterophilous datasets it is typically very low. This is in contrast to synthetic datasets used for experiments in [11, 12], which, as we have shown, sometimes exhibit a combination of low homophily and high label informativeness. High label informativeness of these datasets leads to strong GNN performance on them despite low homophily levels.

E Experimental Setup and Additional Results

For our experiments on synthetic data, we select 208 different combinations of homophily and LI. For each combination, we generate 10 random graphs with the corresponding homophily and LI values using the model described in Section 4.1. Each graph has 1000 nodes (250 nodes for each class) and the expected node degree of 10. Node features are taken from the four largest classes in the cora dataset (each of these four classes is mapped to one class in the synthetic data, and node features are sampled randomly from the corresponding class). For each synthetic graph we create 10 random 50%/25%/25% train/validation/test splits. Thus, for each model, we make 10 runs per graph or 100 runs per homophily/LI combination, totaling 20800 runs.

We use GCN [1] and GraphSAGE [2] as representative GNN architectures for our experiments. For GraphSAGE we use the version with the mean aggregation function and we do not use the node sampling technique used in the original paper. We augment both models with skip connections [33], layer normalization [34], and GELU activation functions [35]. For both models, we use two message-passing layers and a hidden dimension of 512. We use Adam [36] optimizer with learning rate of $3 \times 10^{-5}$ and train for 1000 steps, selecting the best step based on the validation set performance. We use dropout probability of 0.2 during training. Our models are implemented using PyTorch [37] and DGL [38].
In Figure 3 of the main text, we show the results for GraphSAGE, while the results for GCN are presented in Figure 6. As can be seen, GCN performance generally follows the same patterns as GraphSAGE performance, and LI is a better predictor of GCN performance than homophily. In particular, when LI is high, GCN achieves high accuracy even if homophily is negative. The Spearman correlation coefficient between GCN accuracy and LI is equal to 0.76, while between GCN accuracy and adjusted homophily it is equal to 0.19.

We use the same experimental setting described above for training GraphSAGE on modifications of the cora and citeseer graphs from [12]. The results for cora are provided in Figure 4 of the main text. The results for citeseer are shown in Figure 7. For citeseer the Spearman correlation coefficient between accuracy and LI is equal to 0.51, while between accuracy and adjusted homophily it is equal to -0.54. This once again confirms that homophily is not an appropriate measure for indicating simplicity of a dataset for GNNs, and LI is much more suitable for this purpose.