GLINKX: A Unified Framework for Large-scale Homophilous and Heterophilous Graphs

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Abstract

In graph learning, there have been two main inductive biases regarding graph-inspired architectures: On the one hand, higher-order interactions and message passing work well on homophilous graphs and are leveraged by GCNs and GATs. Such architectures, however, cannot easily scale to large real-world graphs. On the other hand, shallow (or node-level) models using ego features and adjacency embeddings work well in heterophilous graphs. In this work, we propose a novel scalable shallow method – GLINKX – that can work both on homophilous and heterophilous graphs. To achieve scaling in large graphs, GLINKX leverages (i) novel monophilous label propagations (ii) ego/node features, (iii) knowledge graph embeddings as positional embeddings, (iv) node-level training, and (v) low-dimensional message passing. We show the effectiveness of GLINKX on several homophilous and heterophilous datasets.

1 Introduction

In recent years, graph learning methods have emerged with strong performance for various ML tasks. Graph ML methods leverage the topology of graphs underlying the data [4] to improve their performance. Two very important design options for proposing graph ML based architectures in the context of *node classification* are related to whether the data is *homophilous* or *heterophilous*.

For homophilous data – where neighboring nodes share similar labels [26, 3] – GCN-based methods (GCN, GAT, etc.) [19, 36, 45] have shown a lot of promise. With the GCN paradigm, *message passing* and *higher-order interactions* help node classification tasks in the homophilous setting since such inductive biases tend to bring the learned representations of linked nodes close to each other. However, GCN-based architectures suffer from *scalability issues*. Performing (higher-order) propagations during the training stage is hard to scale in large graphs because the number of nodes grows exponentially with the increase of the filter receptive field. Thus, for practical purposes, GCN-based methods require *node sampling* which substantially increases their training time. For this reason, architectures [16, 40, 35, 25, 30] that leverage propagations outside of the training loop (as a preprocessing step) have shown promising results in terms of scaling to large graphs.

In *heterophilous* datasets [29], the nodes that are connected tend to have different labels. Many works that address heterophily so far can be classified into two main categories concerning scale. On the one hand, recent successful architectures (in terms of accuracy) [17, 10, 42, 23, 8] that address heterophily resemble GCNs in terms of design and thus suffer from the same scalability issues. On the other hand, *shallow or node-level models* (see e.g. [22, 43]), i.e. models that are treating graph data as tabular data and do not involve propagations during training, have shown a lot of promise for large heterophilous graphs. In [22], it is shown that combining ego embeddings (aka. node features) and adjacency embeddings works in the heterophilous setting. However, their design is still impractical in real-world data since the method (LINKX) is *not* inductive, and embedding the

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adjacency matrix directly requires many parameters in a model. In LINKX, the adjacency embedding of a node can alternatively be thought of as a *positional embedding* (PE) of the node in the graph, and recent developments [18, 12, 22] have elevated the importance of PEs in both homophilous and heterophilous settings. However, most of these works suggest PE parametrizations that are difficult to compute in large-scale settings. For this reason, more scalable ways of computing PEs via *knowledge graph embeddings* [13, 20, 6, 38] are useful in practical settings.[1]

Goal & Contribution: In this work, we develop a scalable method for node classification that: (i) works both on homophilous and heterophilous graphs (ii) is *simpler and faster* than conventional message passing networks (by avoiding the neighbor sampling and message passing overhead), and (iii) can work in both a *transductive* and an *inductive*[2] setting. For a method to be scalable, we argue that it should: (i) run models on node-scale (thus leveraging i.i.d. minibatching), (ii) avoid doing message passing during training and do it a constant number of times before training, and (iii) transmit small messages along the edges. Our proposed method – GLINKX (see Section 1.1) – combines all the above desiderata. GLINKX has three components: (i) ego embeddings [3], (ii) PEs inspired by architectures suited for heterophilous settings, and (iii) *scalable 2nd*-hop-neighborhood propagations inspired by architectures suited for monophilous settings. Finally, we evaluate GLINKX's empirical effectiveness on several homophilous and heterophilous datasets (Section 2).

1.1 Our Method: GLINKX

Notation: We represent scalars with lower-case, vectors with bold lower-case letters, and matrices with bold upper-case letters. We consider a directed graph $G = G(V, E)$ with vertex set V with $|V| = n$ nodes, and edge set E with $|E| = m$ edges. Let $\boldsymbol{X} \in \mathbb{R}^{n \times d_X}$ represent the d_X dimensional node feature matrix and $\boldsymbol{P} \in \mathbb{R}^{n \times d_P}$ represent the d_P dimensional node positional embedding matrix. A node i has a feature vector $\boldsymbol{x}_i \in \mathbb{R}^{d_X}$ and a positional embedding $\boldsymbol{p}_i \in \mathbb{R}^{d_P}$ and belongs to a class $y_i \in \{1, \ldots, c\}$. The training set is denoted by V_{train}, validation set by V_{valid}, and test set by V_{test}.

Components: GLINKX is described in Alg. 1 (see App. A) and consists of three main components namely (i) Positional Embeddings, (ii) Ego Embeddings, and (iii) Monophilous Label propagation. We describe these in detail below.Fig. 1 shows the GLINKX stages from Alg. 1 on a toy graph.

Positional Embeddings (PEs): We use PEs to provide our model information about the position of each node and hypothesize that PEs are an important piece of information in the context of large-scale node classification. PEs have been used to help discriminate isomorphic graph (sub)-structures [18, 12, 34]. This is useful for both homophily [18, 12] and heterophily [22] because structural similarity can exist in both the settings and PEs can disambiguate the structural similarities in case it is needed for the node classification objective. In the homophilous case, adding positional information can help distinguish nodes that have the same neighborhood but distinct position [12, 27, 37], circumventing the need of doing higher-order propagations [12, 21, 7] which is prone to over-squashing [2]. In heterophily, PEs have been an shown to be an important component for node classification as in the case of LINKX – where adjacency embedding can be thought of as a PE. However, in a billion-node/edge (directed) graph, using adjacency embeddings or Laplacian eigenvectors (as methods such as [18] suggest) is a significant computational bottleneck.

In this work, we leverage *knowledge graph embeddings* (KGEs) to encode positional information about the nodes. Using KGEs has the following two benefits: Firstly, KGEs can be trained for large graphs and are extremely scalable. This is because KGEs essentially compress the adjacency matrix into a fixed sized embedding and adjacency matrix has been shown to be effective in heterophilous cases (e.g.[22]). Besides, KGEs have the benefit of being low-dimensional compared to the adjacency matrix (i.e. $d_P \sim 10^2$). Secondly, KGEs can be pre-trained efficiently on large-scale graphs [20] and can be used off-the-shelf for other downstream tasks including node classification (see e.g. [13]). So, in the 1st Stage of our methods in Alg. 1 (Fig. 1(a)) we train KGEs model on the available graph structure. In this work we fix the positional encoding once they are trained for downstream usage. One can fine-tune these along with learning [12] in the downstream task as future work.

[1] An extended related work section is located in App. D.

[2] For this paper, we operate in the *transductive setting*. See App. B.1 for the inductive setting.

[3] We use ego embeddings and node features interchangeably.

Ego Embeddings: We obtain ego embeddings from the node features. Such embeddings have been used both in homophilous and heterophilous settings (e.g. [22, 45]). Such embeddings are useful for tasks where the graph structure provides little/no information for the task.

Monophilous Label Propagations: Generally, a graph is said to to be monophilous if the label of a node is similar to that of its neighbors' neighbors. In the context of a directed graph, monophily can be thought of a structure that resembles Fig. 1(b) where similar nodes (in this case 3 green nodes connected to a yellow node) are connected to a node with a different label. In such cases, monophilous-inspired methods [3, 22] have been shown to perform well empirically. Graphs with monophily can exhibit heterophily, homophily, or both. Additionally, homophily or heterophily is not a binary construct. In Fig. 4 we report the node homophily and the edge-insensitive homophily distributions and we observe that node homophily can be multi-modal. For example, in the yelp-chi dataset – where we classify a review as spam/non-spam – we observe a case of monophily together with varying homophily. Specifically in this dataset, spam reviews are linked to with non-spam reviews and non-spam reviews usually connect to other non-spam reviews, which makes the node homophily distribution bimodal.

In this work we propose a novel label propagation mechanism that is based on *monophily*, which we call Monophilic Label Propagation (MLaP) as follows: First of all (2nd Stage in Alg. 1 and Fig. 1(b)), for a node we want to learn the distribution of *its neighbors*. To achieve this, we propagate the labels from a node's neighbors, i.e. calculate $\hat{\boldsymbol{y}}_i = \frac{\sum_{j \in V_{\text{train}}: j \to i} \boldsymbol{y}_j}{|\{j \in V_{\text{train}}: j \to i\}|}$ for all $i \in V_{\text{train}}$. We train a model that predicts the distribution of neighbors, which we denote with $\tilde{\boldsymbol{y}}_i$ using the ego features $\{\boldsymbol{x}_i\}_{i \in V_{\text{train}}}$ and the PEs $\{\boldsymbol{p}_i\}_{i \in V_{\text{train}}}$ and maximize the cross-entropy with treating $\{\hat{\boldsymbol{y}}_i\}_{i \in V_{\text{train}}}$ as ground truth labels. Although in this paper we assume to be in the *transductive setting*, this step allows us to be inductive (see App. B.1).

Then (3rd Stage in Alg. 1 and Fig. 1(c)), we propagate the predicted soft-labels $\tilde{\boldsymbol{y}}_i$ – by running the model of Stage 2 with the parameters that correspond to the epoch with the best validation accuracy – back to the original nodes, i.e. calculate $\boldsymbol{y}'_i = \frac{\sum_{j \in V: j \to i} \tilde{\boldsymbol{y}}_j}{|\{j \in V: i \to j\}|}$ for all $i \in V_{\text{train}}$ (back-propagated labels) and train a model using the ego features $\{\boldsymbol{x}_i\}_{i \in V_{\text{train}}}$, PEs $\{\boldsymbol{p}_i\}_{i \in V_{\text{train}}}$ and the (back)-propagated labels $\{\boldsymbol{y}'_i\}_{i \in V_{\text{train}}}$ by maximizing the cross-entropy with respect to a node's own labels (for final prediction).

Thus, MLaP can provide informative signals for node classification in heterophilous setting (e.g. [3]). MLaP fundamentally propagates 2nd hop label information, and hence it can provide informative signal for node classification in homophilous setting as nodes with similar labels are connected to each other. Such construction is inductive (see App. B.1). Refer App. B.4 for motivation on MLaP.

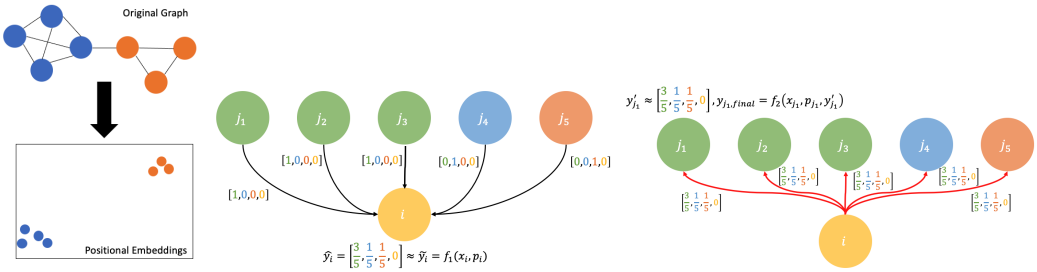
Complementary Signal & Scalability: Different components of GLINKX provide a *complementary* signal to components proposed in the GNN literature [25, 40, 30]. One can combine GLINKX with existing architectures (e.g. feature propagations [25, 30], label propagations [40]) for potential metric gains. Due to space constraints, we discuss the scalability of GLINKX at App. B.2.

2 Experiments

Comparisons: We experiment with homophilous and heterophilous datasets (see Tab. 1 and App. C.3). We train KGEs with Pytorch-Biggraph [20, 38]. For homophilous datasets we compare with vanilla GCN and GAT, FSGNN and Label Propagation (LP). For a fair comparison, we compare with one-layer GCN/GAT/FSGNN/LP since our method is one-hop. We also compare with higher-order (h.o.) GCN/GAT/FSGNN/LP with 2 and 3 layers. In the heterophilous case, we compare with LINKX[4] because it is scalable and is shown to work better than other baselines (e.g. H2GCN), as well as with FSGNN. Note that we do not compare GLINKX with other more complex methods because GLINKX is complementary towards what other methods propose (see Section 1.1) and design principles from other methods can be incorporated into GLINKX. We use a simple *ResNet* module to combine the components from stages 2 and 3 of our algorithm. We detail the hyperparameters used for each method in App. E due to space contraints.

Results: In the heterophilous datasets, GLINKX outperforms LINKX (except arxiv-year where we are within the confidence interval). Moreover, the performance gap between using KGEs and adjacency

[4]We have run our method with hyperparameter space that is a subset of the sweeps reported in [22] due to resource constraints. A bigger hyperparameter search would improve our results.



(a) 1st Stage: PEs Training (b) 2nd Stage: Learn label distribution of neighbors with ego embeddings and PEs (c) 3rd Stage: Predict your own labels with information from neighbors, ego embeddings, and PEs.

Figure 1: Example. For node i we want to learn a model that takes i's features $\boldsymbol{x}_i \in \mathbb{R}^{d_X}$, and PEs $\boldsymbol{p}_i \in \mathbb{R}^{d_P}$ and predict a value $\widetilde{\boldsymbol{y}}_i \in \mathbb{R}^c$ that matches the label distribution of it's neighbors neighbors $\hat{\boldsymbol{y}}_i$ using a shallow model. Next, we want to propagate (outside the training loop) the (predicted) distribution of a node back to its neighbors and use it together with the ego features and the PEs to make a prediction about a node's own label. We propagate $\tilde{\boldsymbol{y}}_i$ to its neighbors j_1 to j_5. For example, for j_1, we encode the propagated distribution estimate $\tilde{\boldsymbol{y}}_i$ from i to form $\boldsymbol{y}'_{j_1}$. We predict the label by using $\boldsymbol{y}'_{j_1}, \boldsymbol{x}_{j_1}, \boldsymbol{p}_{j_1}$.

	Homophilous Datasets		Heterophilous Datasets		
	PubMed	ogbn-arxiv	squirrel	yelp-chi	arxiv-year
n	19.7K	169.3K	5.2K	169.3K	45.9K
m	44.3K	1.16M	216.9K	7.73M	1.16M
Edge-insensitive homophily [22]	0.66	0.41	0.02	0.05	0.27
d_X/c	500 / 27	128 / 40	2089 / 5	32 / 2	128 / 5
GLINKX w/ KGEs	87.95 $\pm$0.30	69.27 $\pm$0.25	45.83 $\pm$2.89	87.82 $\pm$0.20	54.09 $\pm$0.61
GLINKX w/ Adjacency	88.03 $\pm$0.30	69.09 $\pm$0.13	69.15 $\pm$1.87	89.32 $\pm$0.45	53.07 $\pm$0.29
Label Propagation (1-hop)	83.02 $\pm$0.35	69.59 $\pm$0.00	32.22 $\pm$1.45	85.98 $\pm$0.28	43.71 $\pm$0.22
Label Propagation (2-hop)	83.44 $\pm$0.35	69.78 $\pm$0.00	43.41 $\pm$1.44	85.95 $\pm$0.26	46.30 $\pm$0.27
Label Prop. on $\mathbb{I}[A^2 - A - I \geq 0]$	82.14 $\pm$0.33	9.87 $\pm$0.00	24.43 $\pm$1.18	85.68 $\pm$0.32	23.08 $\pm$0.13
LINKX (from [22])	87.86 $\pm$0.77	67.32 $\pm$0.24	61.81 $\pm$1.80	85.86 $\pm$0.40	56.00 $\pm$1.34
LINKX (our runs)	87.55 $\pm$0.37	63.91 $\pm$0.18	61.46 $\pm$1.60	88.25 $\pm$0.24	53.78 $\pm$0.06
GCN w/ 1 Layer	86.43 $\pm$0.74	50.76 $\pm$0.20		N/A	
GAT w/ 1 Layer	86.41 $\pm$0.53	54.42 $\pm$0.10		N/A	
FSGNN w/ 1 Layer	88.93 $\pm$0.31	61.82 $\pm$0.84	64.06 $\pm$2.69	86.36 $\pm$0.36	42.86 $\pm$0.22
Higher-order GCN	86.29 $\pm$0.46	71.18 $\pm$0.27 (*)		N/A	
Higher-order GAT	86.64 $\pm$0.40	73.66 $\pm$0.11 (*)		N/A	
Higher-order FSGNN	89.37 $\pm$0.49	69.26 $\pm$0.36	68.04 $\pm$2.19	86.33 $\pm$0.30	44.89 $\pm$0.29

Table 1: Experimental results. (*) = results from the OGB leaderboard

embeddings shrinks as the dataset grows. In the homophilous datasets GLINKX outperforms 1-layer GCN/GAT/LP/FSGNN and LINKX. In PubMed, GLINKX outperforms h.o. GCN/GAT and in arxiv-year GLINKX is very close to the performance of GCN/GAT.

	Ablation Type	All	Remove ego embeddings	Remove propagation	Remove PEs	
Heterophilous	arxiv-year	All stages	54.09 $\pm$0.61	53.52 $\pm$0.77	50.83 $\pm$0.24	39.06 $\pm$0.35
	arxiv-year	3rd stage	54.09 $\pm$0.61	53.69 $\pm$0.65	50.83 $\pm$0.24	49.13 $\pm$1.10
Homophilous	ogbn-arxiv	All stages	69.27 $\pm$0.25	61.26 $\pm$0.33	62.70 $\pm$0.34	65.64 $\pm$0.18
	ogbn-arxiv	3rd stage	69.27 $\pm$0.25	67.60 $\pm$0.39	62.70 $\pm$0.34	69.62 $\pm$0.15

Table 2: Ablation Study. We use the hyperparameters of the best run from Tab. 1 with KGEs.

Ablation Study: We ablate each component of Alg. 1 to see the performance contribution from each of the components. We use the hyperparameters of the best model from Tab. 1. We perform two types of ablations: (i) we remove each of the components from all stages of the training, and (ii) we remove the corresponding components only from the 3rd stage of Alg. 1. With the exception of removing the PEs from the 3rd stage only on ogbn-arxiv, all components contribute in increasing performance on both datasets (where adding PEs on the 1st stage improves performance).

Future Work: We intend to run our method on bigger datasets, extend GLINKX to heterogeneous graphs and explore other stronger/more expressive methods such as attention or Wasserstein barycenters [9] for averaging the low-dimensional messages.

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Supplementary Materials

A GLINKX Algorithm

Algorithm 1 GLINKX Algorithm

Input: Graph $G(V, E)$ with train set $V_{\text{train}} \subseteq V$, node features X, labels Y
Output: Label Predictions Y_{final}
1st Stage. Pre-train knowledge graph embeddings P with Pytorch Biggraph.
2nd Stage. Propagate labels and predict neighbor distribution

1. **Forward Propagation:** Calculate $\hat{\boldsymbol{y}}_i = \frac{\sum_{j \in V_{\text{train}}: j \to i} \boldsymbol{y}_j}{|\{j \in V_{\text{train}}: j \to i\}|}$ for all $i \in V_{\text{train}}$
2. **Learn distribution of a node's neighbors:** For each epoch, calculate $\tilde{\boldsymbol{y}}_i = f_1(\boldsymbol{x}_i, \boldsymbol{p}_i; \boldsymbol{\theta}_1)$ for $i \in V_{\text{train}}$, and update the parameters s.t. $\mathcal{L}_{\text{CE},1}(\boldsymbol{\theta}_1) = \sum_{i \in V_{\text{train}}} \text{CE}(\hat{\boldsymbol{y}}_i, \tilde{\boldsymbol{y}}_i; \boldsymbol{\theta}_1)$ is maximized. Let $\boldsymbol{\theta}_1^*$ be the parameters at the end of the training that correspond to the epoch with the best validation accuracy.

3rd Stage. Propagate labels backwards and train model to predict a node's own labels

1. **Backward Propagation:** Calculate $\boldsymbol{y}'_i = \frac{\sum_{j \in V: j \to i} \tilde{\boldsymbol{y}}_j}{|\{j \in V: i \to j\}|}$ for all $i \in V_{\text{train}}$, where $\tilde{\boldsymbol{y}}_j = f_1(\boldsymbol{x}_j, \boldsymbol{p}_j; \boldsymbol{\theta}_1^*)$
2. **Learn a node's own distribution:** For each epoch, calculate $y_{\text{final},i} = f_2(\boldsymbol{x}_i, \boldsymbol{p}_i, \boldsymbol{y}'_i; \boldsymbol{\theta}_2)$, and update the parameters s.t. $\mathcal{L}_{\text{CE},2}(\boldsymbol{\theta}_2) = \sum_{i \in V_{\text{train}}} \text{CE}(y_i, y_{\text{final},i}; \boldsymbol{\theta}_2)$ is maximized.

Return Y_{final}

B Model Addendum

B.1 Inductive Setting

In the paper we focus on the transductive setting. Here we show how we can extend our framework to the inductive setting. In the inductive setting, during training we only have access to the training graph $G_{\text{train}}(V_{\text{train}}, E_{\text{train}})$. During test, the whole graph $G \subseteq G_{\text{train}}$ is revealed and we make predictions for the test set. The stages of GLINKX in the inductive setting are as follows:

1st Stage. For the KGE pretraining stage, we train KGEs on G_{train}. Then we can use existing methods in the literature such as [13, 1] to infer the KGEs of the test nodes.

2nd Stage. We train the model that predicts the distribution of the neighbors on G_{train} as in Alg. 1. Then for the test nodes, we know their ego features $\boldsymbol{x}_i$ and we can also infer their PEs (see above) from the pre-trained PEs on the training set. We use these and the pre-trained shallow model in order to predict $\tilde{\boldsymbol{y}}_i$ for the test nodes.

3rd Stage. First, we train the second shallow model by using the propagated soft-predictions only on G_{train}. Then, we infer the soft-labels $\tilde{\boldsymbol{y}}_i$ from the 2nd stage and propagate them back to the original nodes. We then use the ego features, PEs and the propagated information $\boldsymbol{y}'_i$ to make predictions on the test set.

Test set inference is illustrated by Alg. 2

B.2 Scalability

The propagations have to be done constant number (ideally once) of times by paying an $O(mc)$ cost, where the dimensionality of classes c is usually small (compared to d_X that GCNs rely on). In both stages 2 and 3 of Alg. 1 we train node-level MLPs which allow us to leverage i.i.d. (row-wise) minibatching, like tabular data, and thus our complexity is similar to other shallow methods (LINKX, FSGNN) [22, 25]; meeting our requirements. This, combined with the propagations that happen outside of the training loops, circumvent the issues of GCNs in large-scale graphs.

Cost of 1st Stage. For the first stage, we are using Pytorch-Biggraph to train PEs. Please refer to [20] for more information.

Algorithm 2 Inductive GLINKX

Input: Graph $G(V, E)$ with train set $V_{\text{train}} \subseteq V$ and test set $V_{\text{test}} \subseteq V$, node features X, labels Y
Output: Predictions for all nodes $i \in V_{\text{test}}$

Pre-training. Call Alg. 1 with input graph $G_{\text{train}}(V_{\text{train}}, E_{\text{train}})$ and compute PEs $\{\boldsymbol{p}_i\}_{i \in V_{\text{train}}}$, and pre-trained models f_1 (from 2nd stage) and f_2 (from 3rd stage)

1st Stage. Create PEs $\{\boldsymbol{p}_i\}_{i \in V_{\text{test}}}$ for the nodes of the test set (see e.g. [13, 1])

2nd Stage. Predict the distribution of neighbors for the nodes of the test set as $\tilde{\boldsymbol{y}}_i = f_1(\boldsymbol{x}_i, \boldsymbol{p}_i)$ for all $i \in V_{\text{test}}$.

3rd Stage. Propagate labels backwards and train model to predict a node's own labels Calculate $\boldsymbol{y}'_i = \frac{\sum_{j \in V: j \to i} \tilde{\boldsymbol{y}}_j}{|\{j \in V: i \to j\}|}$ for all $i \in V_{\text{test}}$. Compute $\boldsymbol{y}_{\text{final},i} = f_2(\boldsymbol{x}_i, \boldsymbol{p}_i, \boldsymbol{y}'_i)$ for all $i \in V_{\text{test}}$.

Return $\{\boldsymbol{y}_{\text{final},i}\}_{i \in V_{\text{test}}}$

Cost of 2st Stage. For the first stage we pay **once** $O(m_{\text{train}} c)$ ($m_{\text{train}} = |E_{\text{train}}|$ is the number of edges in the graph induced by the train nodes) to do the label propagation and then the MLP that takes $\boldsymbol{x}_i$ and $\boldsymbol{p}_i$ with L_X layers for the features $\boldsymbol{x}_i$ and L_P layers for the PEs $\boldsymbol{p}_i$, and L_{agg} layers for the ResNet and hidden dimension h, has forward pass complexity $O\left(n(d_X h + h^2 L_X + d_P h + h^2 L_P + h^2 L_{\text{agg}})\right)$.

Cost of 3rd Stage. For the second stage, we pay again **once** $O(m_{\text{train}} c)$ for the propagation and then, similarly, $O\Bigg(n(d_X h + h^2 L_X + d_P h + h^2 L_P + ch + h^2 L_{\text{prop}} + h^2 L_{\text{agg}})\Bigg)$ for a forward pass of the MLP, where c is the class dimensionality and L_{prop} are the layers for the MLP handling the propagated labels $\boldsymbol{y}'_i$.

Comparison with LINKX. Compared to LINKX we pay an $O(m_{\text{train}} c)$ extra cost once. Regarding embedding the adjacency matrix LINKX pays a $O(mh + nh^2 L_P)$ cost for generating the h-dimensional adjacency embeddings whereas we pay $O(nd_P h + nh^2 L_P)$ which is better for $d_P = O(m/n)$. This holds in most real-world large networks since $d_P \sim 10^2$ whereas $n \sim 1\text{B}$ and $m \sim 100\text{B}$. Also note that using KGEs as PEs has an additional benefit, since KGEs can be trained only *once* and can be used off-the-shelf for other downstream tasks.

Inference Complexity (Alg. 2). On the inductive setting, given pretrained models f_1, f_2 from stages 2 and 3, the runtime Alg. 2 without the pretraining stage is $O\left(mc + n_{\text{test}}(d_X h + h^2 L_X + d_P h + h^2 L_P + h^2 L_{\text{agg}})\right)$ to generate predictions for the test nodes, where $n_{\text{test}} = |V_{\text{test}}|$.

B.3 Stages Diagram

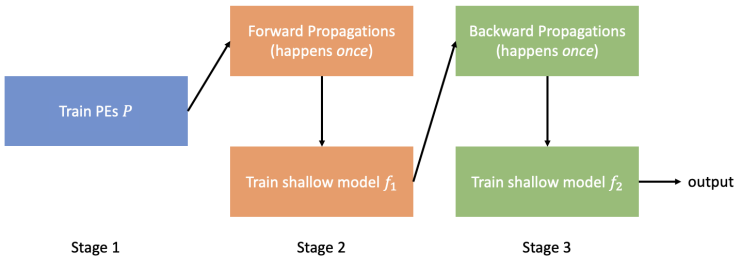
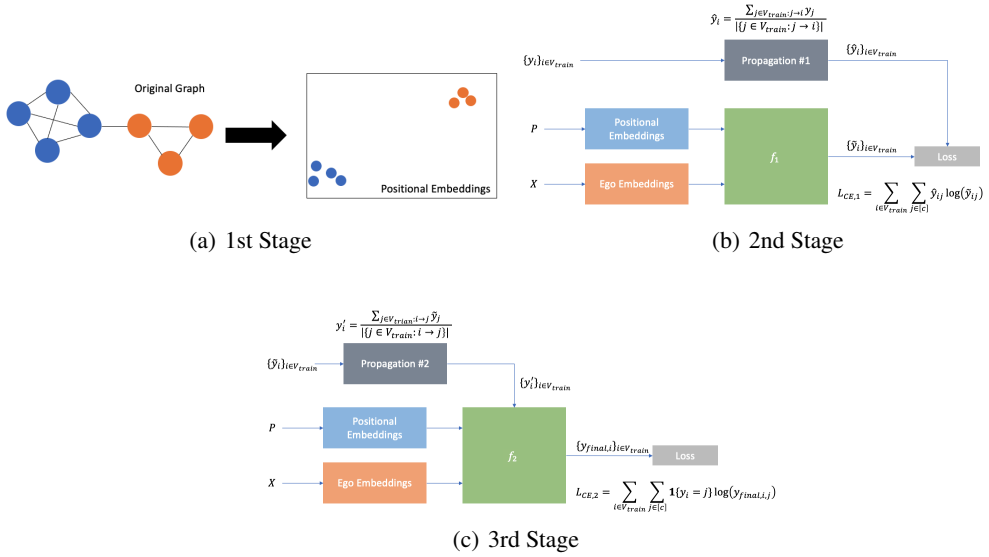


Figure 2: GLINKX stages.



(a) 1st Stage (b) 2nd Stage

(c) 3rd Stage

Figure 3: Block Diagrams of GLINKX stages.

B.4 Monophilous Label Propagation (MLaP): Motivation

In monophily, a node shares labels with its neighbors' neighbors. One way to encode monophily in Fig. 1(b) while predicting label for j_i is to get a distribution of labels of nodes connected to node i thus encoding its neighbors' distribution. The fact that there are more nodes with green color than other colors can be used by the model to make a prediction. But this information may not always be present or there may be few labelled nodes around node i. For this reason, we propose to use a model that predicts the label distribution of nodes connected to node i. And we use the node features ($\boldsymbol{x}_i$) and PE ($\boldsymbol{p}_i$) of node i to build this model, because nodes that are connected to node i share similar labels and, hence, the features of node i must be predictive of its neighbors. So, in Stage 2 for every node we train a model to predict a distribution of its neighbors. We start with the objective to provide node j_i with the neighbors' label distribution of node i. Then, we propagate this information from to j_i thus encoding monophily and train a model that uses the node features, the PEs and the propagated labels (Stage 3). This method is scalable. See App. B.2 for more details on scalability.

C Experiments Addendum

C.1 Implementation and Environment

GLINKX is implemented in Pytorch-Geometric. For the knowledge graph embeddings we use the official Pytorch-Biggraph implementation. We use the official implementation of LINKX. For hardware we used Vertex AI notebooks with 8 NVIDIA Tesla V100 with 16GB of memory and 96 CPUs.

C.2 Experimental Protocol

Error Bars. For the PubMed dataset and the heterophilous datasets provided by [28, 22, 39] we used the fixed splits provided with a fixed seed. For the OGB datasets, where there exists only one officialy released split for each dataset [15] we generate the error bars by runnning the respective experiments with 10 different seeds (0-9).

C.3 Datasets

For our experiments we use the following datasets (see Tab. 1):

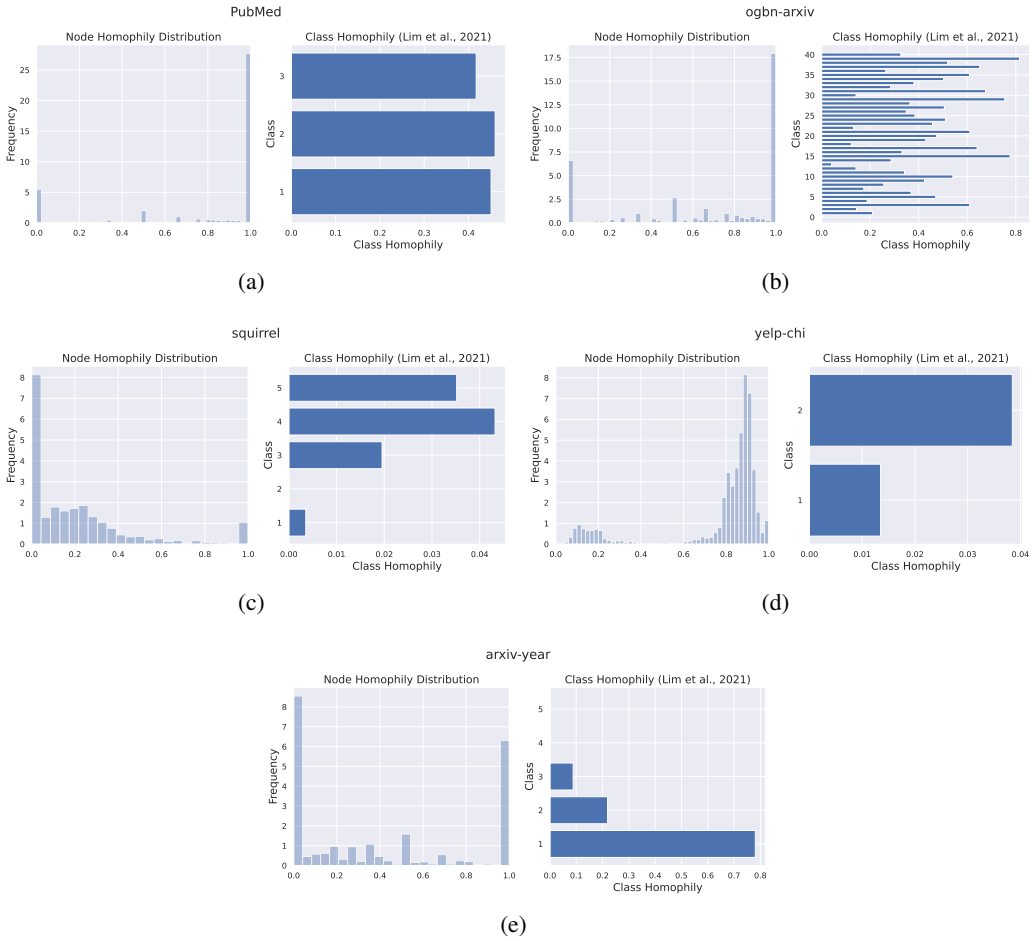


Figure 4: Node Homophily Distribution and Class (or Edge-insensitive) Homophily [22].

- *PubMed [39, 32].* The PubMed dataset consists of scientific publications from PubMed database pertaining to diabetes classified into one of three classes. Each node is described by a TF-IDF weighted word vector from a dictionary which consists of 500 unique words.

- *ogbn-arxiv [15, 5, 33].* The ogbn-arxiv dataset is a directed graph, representing the citation network between all CS papers on arxiv mined from the Microsoft Academic Graph (MAG). Nodes are papers and edges correspond to citations. The node features correspond to the average of word embeddings of the title and abstract of the papers. The task is to predict the papers' subcategories (e.g. CS.LG, CS.SI etc.).

- *squirrel [31].* The data represents page-to-page networks on squirrels mined from Wikipedia between October 2017 and November 2018. Node represent articles and edges are mutual links between the pages. The features of each node are binary and represent the existence of informative nouns that appear on the corresponding Wikipedia pages.

- *arxiv-year, yelp-chi [22].* The arXiv-year dataset is derived from the ogbn-arxiv dataset where the labels have been changed in order to convert the dataset from homophilous to heterophilous. Instead of predicting each paper's subcategories, the new task focuses on predicting the year that a paper is posted, where batches of years have been converted to labels. The yelp-chi dataset includes hotel and restaurant reviews filtered (spam) and recommended (legitimate) by Yelp. The graph structure comes from [11] and the features from [32]. The task is to predict whether a review is a spam or not.

D Further Related Work

Homophilous Methods. The backbone of graph learning is based on homophily. In a nutshell, a graph is homophilous if nodes that are connected have similar labels (and usually similar features). In such settings, propagating node embeddings and then combining these embeddings with a permutation-invariant function and perhaps an edge-wise attention mechanism yields decent results [19, 36]. Recently, a lot of attention has been given in large-scale settings where conventional GNNs – such as GCN and GAT – cannot scale. Such methods are based on multiple propagations of the features over layers and back-propagating through the weights is an infeasible task for large-scale networks.

For this reason, several methods have been proposed to tackle this computational bottleneck which are able to scale to networks with hundreds of millions of nodes. Conceptually, the most characteristic large-scale method is SIGN [30], where multiple stages of *non-trainable* filters are applied to the initial features in order to create node embeddings – which can be stored for later use – and then a shallow model (MLP) is applied on top of the final embeddings to produce the final predictions. Various follow-up methods tweak the SIGN architecture to add attention (SAGN [35]), softmax regularization, soft-selection, and hop-normalization (FSGNN [25]) and improve upon its performance. A related method is also GAMLP [40] where the authors combine label propagations and feature propagations and combine them with an attention mechanism. However, their method does not take into account heterophilous inductive biases.

Another important method for large-scale homophilous node classification is Correct-And-Smooth (C&S) [16]. C&S lifts the assumption that GNNs are essentially necessary for good performance on graph ML tasks. They propose to train a shallow classifier over the nodes and produce a set of *soft labels* from its predictions. Afterwards, the authors leverage the graph structure and the label correlations with in two steps: an error correction step that spreads residual errors in training data to correct the errors present in the test data, and a prediction correlation that smooths the predictions on the test data.

Heterophilous Methods. Recently there has been a surge in research regarding node classification in heterophilous graphs, i.e. graphs where nodes that are connected to each other may have different class labels (and maybe different features). More specifically, one of the first methods proposed is H2GCN [45] where the authors introduce a set of design principles for heterophilous model design. They propose the following design principles: ego and neighbor embedding separation, higher-order neighborhoods, and combination of intermediate representations. Accordingly they build a model – H2GCN – based on such principles and evaluate it on various real-world and synthetic datasets. Following up this work, the authors of [22] propose a significantly simpler architecture – LINKX – which combines embeddings of the ego features and embeddings of the corresponding rows of the adjacency matrix (inspired by the LINK method [41]) with a ResNet block [14]. The LINKX method is very lightweight since nodes are processed in a i.i.d. (row-wise) basis – i.e. there are no graph dependencies between the nodes – an mini-batching can be performed efficiently (contrary to propagation-based methods). LINKX is shown to outperform H2GCN on a variety of datasets. However, LINKX falls short in node classification tasks that regard homophilous datasets (such as Cora, CiteSeer, and PubMed [39]) where standard method such as GCN and GAT yield better results.

The recent framework of [23] argues that not all cases of heterophily are harmful for GNN-based architectures, and propose a set of metrics based on the construction of a similarity matrix that measures the influence of the graph and the input features on GNNs. Based on their observations, the authors design a model based on a filterbank which consists of a high-pass and a low-pass filter to address harmful heterophily achieving state-of-the-art results.

Methods for Homophily and Heterophily. Recently, there have been lots of methods which have been adapted to work both in homophily and heterophily regimes. H2GCN [45] (see above) was one of the first methods shown to work in both kinds of datasets. RAW-GNN [17] is a random-walk-based GCN that exploits both homophily and heterophily by doing random walks and aggregations in two ways: breadth-first for homophily and depth-first for heterophily. CPGNN [44] is a GCN-based architecture that uses a compatibility matrix for modeling the heterophily or homophily level in the graph, which can be learned in an end-to-end fashion, enabling it to go beyond the assumption of strong homophily. GPR-GNN [8] addresses feature over-smoothing and homophily/heterophily by combining GNNs with Generalized PageRank techniques, where each step of feature propagation is associated with a learnable weight. The amplitudes of the weights trade-off the degree of smoothing

of node features and the aggregation power of topological features. However all of the above methods suffer from the same scalability issues that GCNs have.

Regarding scalable methods for both homophily and heterophily, the FSGNN [25] method is also closely related to our work and relies on using propagations which are separate from training (similarly to SIGN) and also uses separate (higher-order) feature propagations for homophily and heterophily. On the contrary, our method, in its current form, is one-hop and relies on different components to address homophily and heterophily. Besides, their components can be added to our method, together with the ego-features, the PEs and the propagations, and thus, from another viewpoint, their work can be seen as complementary to ours. CLP [43] combines a shallow (base) predictor model with a modified Label Propagation that works both in homophily and heterophily where they use a class compatibility matrix (similarly to CPGNN) for the Label Propagation step. Our method is fundamentally different than theirs, however incorporating a compatibility matrix for the propagation stage constitutes interesting future work.

Positional Embeddings. Following up the recent success of LINKX in classifying nodes in heterophilous settings based partially on the *position* of each node (adjacency embedding) a series of methods have been suggested for incorporating positional embeddings on graph methods [18, 12]. More specifically, [12] proposes the MLPGNN-LSPE architecture which is able to simultaneously learn both structural and positional embeddings for nodes, whereas [18] proposes TokenGT, which treats all nodes and edges as independent tokens, augments them with positional embeddings – i.e. eigenvectors of the normalized Laplacian of the graph ignoring edge directions – and then feeds them to a Transformer model. They prove that their framework is at least as expressive as a 2-IGN [24] composed of equivariant linear layers which is more expressive than all message passing GNNs. However, creating positional embeddings that require the factorization of e.g. the Laplacian matrix to compute a set of orthonormal eigenvectors are infeasible for large datasets. For this reason, various methods have been proposed for embedding nodes in a graph in a scalable manner, such as TransE [6], DistMult [38][5]. The recent development of Pytorch-Biggraph [20] allows training such embeddings on billion-scale heterogeneous graphs such as the Twitter graph [13].

E Hyperparameters

For each of the methods we train for 200 epochs and report the test set accuracy on the epoch with the best validation accuracy.

E.1 KGEs

We use the following hyperparameters for the KGEs using Pytorch-Biggraph:

- dimension = 400
- 50 epochs
- negative samples = 1000
- batch size = 10000
- `dot` comparator, `softmax` loss [38]
- learning rate = 0.1

E.2 GLINKX w/ Adjacency

E.2.1 Sweeps

We perform the following sweeps:

- glinkx_init_layers_X $\in \{1, 2\}$
- glinkx_init_layers_A"$\in \{1, 2\}$
- glinkx_init_layers_agg $\in \{1, 2\}$
- glinkx_inner_dropout : $\in \{0.5\}$
- lr $\in \{0.1, 0.001\}$

[5]For more such methods see [20] and the references therein.

- optimize:r: AdamW

name	init_layers_A	init_layers_X	init_layers_agg	inner_dropout	lr
arxiv-year	1	2	1	0.5	0.001
PubMed	1	2	1	0.5	0.001
squirrel	2	1	1	0.5	0.001
yelp-chi	2	2	1	0.5	0.01

Table 3: GLINKX w/ Adjacency Hyperparameters

E.3 GLINKX w/ KGEs

E.3.1 Sweeps

We perform the following sweeps for all datasets

- glinkx_init_layers_X $\in \{1, 2\}$
- glinkx_init_layers_A $\in \{1, 2\}$
- glinkx_init_layers_agg $\in \{1, 2\}$
- glinkx_inner_dropout : $\in \{0.5\}$
- lr $\in \{0.1, 0.001\}$
- optimize:r: AdamW
- biggraph_vector_length: 400

name	biggraph_vector_length	init_layers_A	init_layers_X	init_layers_agg	inner_dropout	lr
arxiv-year	400	2	1	1	0.5	0.01
ogbn-arxiv	400	2	2	2	0.5	0.001
PubMed	400	2	2	2	0.5	0.01
squirrel	400	2	1	2	0.5	0.001
yelp-chi	400	2	2	2	0.5	0.01

Table 4: GLINKX w/ Biggraph Hyperparameters

E.4 GAT

E.4.1 Sweeps

- gat_num_layers $\in \{1\}$
- gat_hidden_channels $\in \{4, 8, 16, 32\}$
- gat_num_heads $\in \{2, 4\}$
- lr $\in \{0.01, 0.001\}$

name	gat_heads	gat_hidden_channels	gat_num_layers	lr
arxiv-year	4	8	1	0.1
ogbn-arxiv	4	4	1	0.1
PubMed	4	16	1	0.1
squirrel	4	4	1	0.1

Table 5: GAT w/ 1 layer Hyperparameters

E.5 GCN

E.5.1 Sweeps

We perform the following sweeps:

- gcn_num_layers $\in \{1\}$
- gcn_hidden_channels $\in \{4, 8, 16, 32, 64\}$
- lr $\in \{0.01, 0.001\}$

name	gcn_hidden_channels	gcn_num_layers	lr
arxiv-year	64	1	0.01
ogbn-arxiv	64	1	0.01
PubMed	64	1	0.01
squirrel	64	1	0.01
yelp-chi	64	1	0.01

Table 6: GCN w/ 1 layer Hyperparameter

E.6 FSGNN

We run the following sweeps for FSGNN

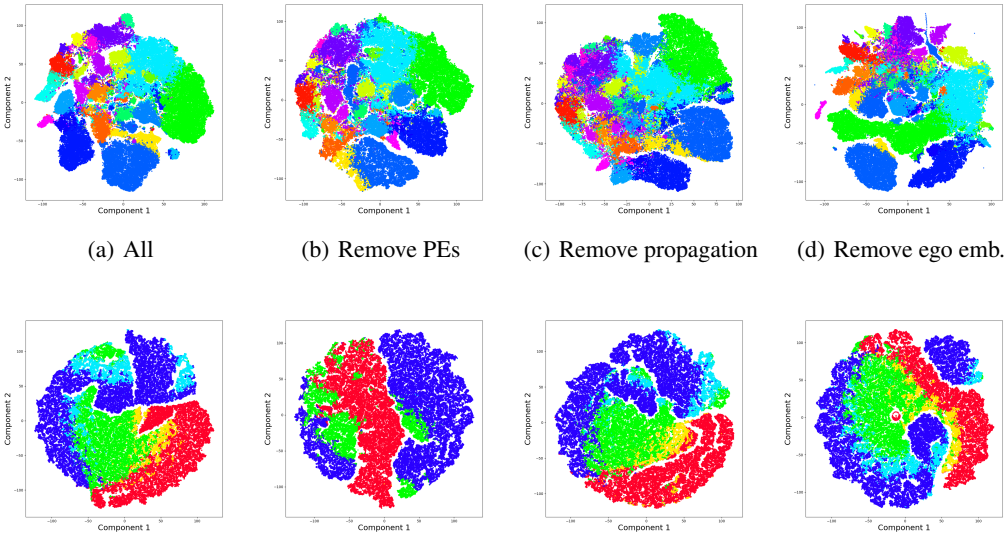
- layers = 1 for the 1-layer case and layers $\in \{2, 3\}$ for the higher-order case
- hidden channels $\in \{32, 64, 128\}$
- learning rate $\in \{0.01, 0.001\}$
- layer normalization $\in \{\text{true}, \text{false}\}$

E.7 Label Propagation

We run the following sweeps using the implementation of Label Propagation from [22]:

- $\alpha \in \{0.01, 0.1, 0.25, 0.5, 0.75, 0.99\}$
- hops $\in \{1, 2\}$

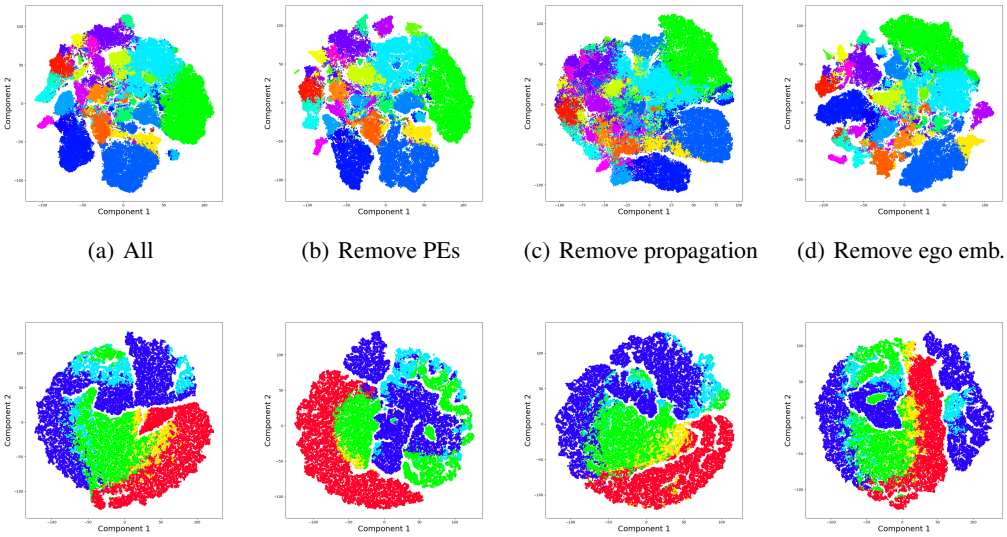
F Ablation Visualization Addendum



(a) All (b) Remove PEs (c) Remove propagation (d) Remove ego emb.

(e) All (f) Remove PEs (g) Remove propagation (h) Remove ego emb.

Figure 5: t-SNE plots of output layer embedding for ogbn-arxiv (top), arxiv-year (bottom) for ablation on both 1st and 2nd stages



(a) All (b) Remove PEs (c) Remove propagation (d) Remove ego emb.

(e) All (f) Remove PEs (g) Remove propagation (h) Remove ego emb.

Figure 6: t-SNE plots of output layer embedding for ogbn-arxiv (top), arxiv-year (bottom) for ablation on the 2nd stage