

BA-GNN: On Learning Bias-Aware Graph Neural Network

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Abstract—Graph Neural Networks (GNNs) show promising results for semi-supervised learning tasks on graphs, which become favorable comparing with other approaches. However, similar to other machine learning models, GNNs might suffer from the bias issue because of the distribution shift between training and testing node distributions. More importantly, the test node distribution in the graph is generally unknown during model training in practice. In this paper, we focus on how to address the bias issue on graphs and learn a graph neural network model that is robust to arbitrary unknown distribution shifts. To address this problem, we propose a novel *Bias-Aware Graph Neural Network* (BA-GNN) framework by learning node representations that are invariant across different distributions for invariant prediction. Specifically, our BA-GNN framework contains two interactive parts, one for bias identification and the other for invariant prediction. To learn invariant feature and aggregated representation, our BA-GNN learns multiple biased graph partitions and selects feature, neighbor, and propagation steps for nodes under multiple biased graph partitions. Extensive experiments show that our proposed BA-GNN framework can significantly improve different GNNs backbones such as GCN, GAT, APPNP and GraphSAGE on different datasets.

Index Terms—Graph Neural Network; Distribution Shift

I. INTRODUCTION

Recently, Graph Neural Networks have achieved state-of-the-art performance across various tasks on graphs, such as semi-supervised node classification [1]–[4], link prediction [5], [6] and graph classification [7], [8]. Typically, GNNs exploit message propagation strategy to learn expressive node representations by propagating and aggregating the messages between neighboring nodes. Various message propagation layers have been proposed, including graph convolutional layers (GCN) [1], graph attention layers (GAT) [2] and many others [4], [5], [9]–[12]. GNNs [1], [2], [9] have achieved great success in many real world applications across different domains, such as recommender system [13], molecule design [14], financial fraud detection [15], and traffic prediction [16].

Despite the great performance of GNNs, the majority of existing methods assume that the training and testing data are independent and identically distributed (i.e., i.i.d assumption), while for many real-world graphs and applications,

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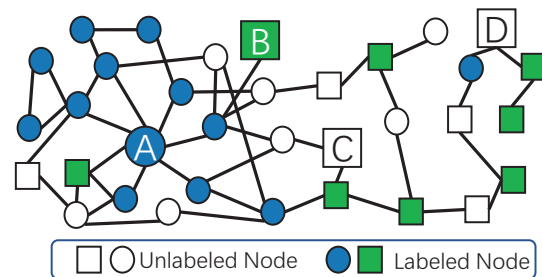


Fig. 1: Schematic diagram of the bias in node classification problem. The shape denotes the label of each node. The shape *circle* is labeled as “machine learning”, and the shape *rectangle* is labeled as “computer architecture”. The node with high-degree is more likely to be labeled and used as training nodes, however, in the testing, the node with low-degree need to be classified, leading to the distribution (of degrees and label) shifts between training and testing.

the distributions between training and testing data could be different. For instance, in the citation network, the papers with high citations (i.e., high-degree nodes) will be more likely to be labeled and used as training nodes. However, in the testing, we generally have many low-degree nodes that need to be classified. In addition, machine learning (ML)-related papers are more likely to be labeled as training nodes compared to Computer Architecture-related papers. However, a GNN model trained in this citation network may see a vastly different distribution of labels: we have many computer architecture-related papers that need to be classified. Both degree and label shifts between training and testing distributions can significantly degrade model performance as we show later. Figure 1 shows the illustration of degree and label distribution shifts in graph. As shown in the Figure 1, A is the high-degree node with higher influence, which can dominate the training/learning of GNNs. However, the degree of test nodes C and D differ from nodes in training, and most of unlabeled nodes are at the fringes of the graph. The difference of degree distribution can hurt the message-passing mechanism

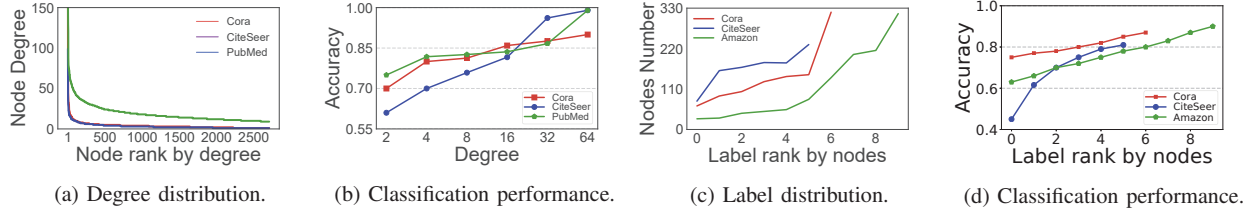


Fig. 2: Empirical investigation of bias in graphs. (a) shows the degree distribution of the Cora, CiteSeer and PubMed datasets. The node degrees are characterized by a long-tailed distribution, where the performance of nodes with different degree varies considerably. (c) shows the label distributions, and the performance of nodes with different labels is shown in (d).

of GNNs. Obviously, GNNs which train on high-degree nodes results in unsatisfying or even poor prediction performance on low-degree nodes. Moreover, as shown in Figure 1 the label of most labeled nodes in training graph is *circle*, which may warp GNNs biased towards *circle* nodes. However, the label of test nodes C and D is *rectangle* rather than *circle*. Such label-related distribution shift may also degrade the prediction performance on test environments.

Empirical investigation of bias in graph. To further verify and study the distribution shift caused by the bias, we conduct empirical investigation of two common distribution shifts: label-related distribution shift and degree-related distribution shift. Figure 2 (a) shows the degree distribution of the Cora, CiteSeer and PubMed datasets. The node degrees are characterized by a long-tailed distribution, where a significant fraction of the nodes belong to the tail with very low degrees. Generally, the node degrees varies considerably across the graph and are not uniformly distributed, which leads to degree-related distribution shift between training and testing. In addition, Figure 2 (b) shows that the performance of nodes with different degree vary considerably across the graph. The label distributions of datasets are shown in Figure 2 (c), which are not uniformly distributed. GNNs rely on message-passing mechanism, and aggregate the information from neighbors to learn representations. Thus, the nodes where their label has fewer nodes receive less information during the aggregation, which leads to poor performance as shown in Figure 2 (d).

More importantly, the test distribution is always unknown during GNNs optimizing on training graph data, where the unknown distribution shift might be caused by node labels, node degrees, or both. Generally, the unknown distribution shift between training and testing would render traditional GNNs over-optimized on the labeled training samples and render their predictions error prone on test samples, resulting in variant predictions. Therefore, learning GNNs that are resilient to distribution shifts and able to make invariant predictions on graphs will be important for real-world applications.

In this paper, we focus on the bias issue on graph and study a novel problem of learning de-biased graph neural networks for unknown testing distributions. To address this problem, we are still facing the following challenges: 1) *How to address bias problem in graph tasks.* Previous methods [17]–[36] are for bias problem with independent and identically distributed

(i.i.d) data. [26], [37] propose bias aware learning method via heterogeneous risk minimization. However, graph-structured data are not i.i.d, and the properties of graph-structured data are not explicitly utilized in these methods. Some works [38]–[44] focus on graph-level task or one specific bias in node-level task, which could not address agnostic bias where biases may be label-related bias, degree-related bias or both in node-level task. 2) *How to overcome bias problem in unknown test environment.* The testing distribution is always unknown during GNNs optimizing on training graph data, previous works [38]–[44] ignore the bias in unknown test environments.

In an attempt to address these challenges, in this work, we propose a novel *Bias-Aware Graph Neural Network* (BA-GNN) framework that aims to learn invariant graph representations for robust prediction across unknown testing distributions. Our BA-GNN framework contains two interactive parts, the frontend \mathcal{M}_B for bias identification and the backend \mathcal{M}_I for invariant prediction. To learn invariant feature and aggregated representation, \mathcal{M}_B learns multiple biased graph partitions, and \mathcal{M}_I selects feature, neighbor and propagation step for nodes under multiple biased graph partitions.

We compare our BA-GNN framework with a bunch of generic SOTA GNNs and methods that are specifically designed for mitigating selection biases on various public graph benchmarks. We concern both traditional task-specific evaluation metrics and protocols that are especially designed for invariant learning. Extensive experimental results demonstrate the capability of our framework on learning GNNs that makes invariant predictions on graphs with unknown testing distribution. In summary, the contributions of this paper are:

- We study the problem of learning GCNs with bias for invariant prediction across unknown test environments, which is less explored in the literature.
- We propose a novel framework *Bias-Aware Graph Neural Network* (BA-GNN) for GNNs, which learns invariant aggregated presentation for each node, and make invariant prediction on various unknown test environments.
- Extensive experiments show that our proposed BA-GNN framework can significantly improve different GNNs backbones such as GCN, GAT, APPNP and GraphSAGE on different datasets and settings.

The remainder of this paper is organized as follows. We

review about the related work in Section 2. We present problem formulation for the node classification problem with bias on unknown test environments in Section 3. It is followed by the elaboration of the proposed BA-GNN approach in Section 4. In Section 5, we theoretically analyze our BA-GNN. In Section 6, we present extensive experimental studies on various graph datasets. Finally, the conclusion of this paper and discussion of future works are presented in Section 7.

II. RELATED WORKS

A. Graph Neural Networks

GNNs have achieved great success for modeling graph structured data. Generally, GNNs can be categorized into two categories, i.e., spectral-based and spatial-based. Spectral-based GNNs define graph convolution based on spectral graph theory [3], [12], [45]. GCN [1] further simplifies graph convolutions by stacking layers of first-order Chebyshev polynomial filters together with some approximations. Spatial-based methods directly define updating rules in the spatial space. For instance, GAT [2] introduces the self-attention strategy into aggregation to assign different importance scores of neighborhoods. With the similar intuition, GraphSAGE [5] extends prior works in the inductive setting. There is a lot of spatial-based methods [2], [43], [46]–[48] are proposed to capture different neighborhood information.

The spectral based GNNs usually require to compute the Laplacian eigenvectors or the approximated eigenvalues as suggested by spectral theory, and these methods are inefficient on large scale graph. Different from the spectral based ones, the spatial-based GNNs [49]–[51] attempt to directly capture the spatial topological information and use the mini-batch training schema. For example, DCNN [49] combines graph convolutional operator with the diffusion process, and Veličković et al. propose the graph attention network [50] with the self-attention mechanism on the neighbors of nodes and assign different weights during the aggregation process.

B. Bias in Machine Learning

Recently, many methods are proposed to address bias caused by distribution shift for general machine learning problems [17]–[20]. There are mainly three branches of methods for the selection bias caused by distribution shift, namely domain adaptation [17]–[21], distributionally robust optimization (DRO) [52] and invariant learning [22]–[25], [32]–[36], [53].

Domain adaptation aims to reduce bias by learning domain-invariant representations, which is learned by minimizing a certain discrepancy between distributions of source and target features extracted by a shared representation learner [17]–[20]. [18] put forward the domain adversarial neural network (DANN). A domain discriminator is trained to distinguish source features from target features and a feature extractor to confuse the discriminator. Since then, a series of works have appeared and achieved significantly better performance. [19] proposed an architecture that employed asymmetric encodings for target and source data. [54] presented a principled framework that conducted the adversarial adaptation models using

conditional information. [20], [55] unified pixel-level and feature-level adversarial learning for domain adaptation. [17] presented a multi-modal domain adaptation framework that conducted the adversarial adaptation for multi-modal tasks.

Distributionally robust optimization methods aim to minimize the worst-case risk, where uncertainty set of the observed training distribution and potential testing distribution [52], [56]–[58]. However, the uncertainty set should be pretty large to better capture the testing distribution, which is not realistic in many real-world settings [52], [56].

Invariant learning methods presuppose the presence of causally invariant correlations between some predictors and the target value to overcome the selection bias caused by distribution shift problems without any prior information. [24] choose features that have a consistent predictive association with the target across environments. [25] improves [22] by reducing its numerous environment restrictions. [25] provides a two-stage method, in which a pre-provided biased model is used to infer the environment division, followed by invariant learning on the inferred environments.

As summary, these methods mentioned above are generally adopted from general machine learning tasks, where the data is independent and identically distributed (i.i.d). However, graph-structured data is non i.i.d, and the properties of graph-structured data are not explicitly utilized in these methods.

Recent works explore GNN's extrapolation ability to address bias caused by distribution shift. [38] proposes to learn a static adjacency matrix for a given graph and expects that the learned adjacency matrix captures general relational patterns that are free from selection biases. [39] suggests that encoding appropriate non-linearity in architecture and features can help extrapolation. [40] show how subgraph densities can be used to build size-invariant graph representations. [41] propose a Self-Supervised Learning (SSL) task aimed at learning representations of local structures to overcome the size-generalization problem. However, they concentrate on *graph-level tasks* (e.g., graph classification), where each input instance is a graph (usually with less than 100 nodes) and one dataset contains massive graphs for training and testing.

Recent works study the degree bias in node-level task. GNM [42] confronts a related problem named non-ignorable nonresponse, which indicates that the unlabeled nodes are missing not at random (MNAR). DEMO-Net [43] explicitly capture the graph topology integrated with node attributes. SL-DSGCN [44] mitigate the degree-related biases of GCNs from model and data aspects. However, these works only focus on degree bias, and ignore other bias. Moreover, these methods could not address bias in unknown environments.

Imbalanced graph classification [59], [60] focuses to the quantity or topology imbalance problems on graph [61]–[63], where both quantity or topology imbalance problems cause label-related bias. Different from them, our BA-GNN studies the agnostic bias rather than specific bias in testing environments and biases can be label-related or degree-related.

III. PRELIMINARIES

Invariant Risk Minimization. [22] propose invariant risk minimization (IRM), augmenting empirical risk minimization to learn a data representation free of spurious correlations. They assume there exists some partition of the training data \mathcal{X} into environments $e \in \mathcal{E}$, and that the model's predictions take the form $Y^e = \mathbf{w}^\top \phi(X^e)$. IRM aims to learn a representation ϕ for which the optimal linear classifier, \mathbf{w} , is invariant across e , where optimality is defined as minimizing the empirical risk R^e . We can then expect this representation and classifier to have low risk in new environment e .

$$\begin{aligned} \min_{\substack{\phi: \mathcal{X} \rightarrow \mathbb{R}^d \\ \mathbf{w} \in \mathbb{R}^d}} \sum_{e \in \mathcal{E}} R^e(\mathbf{w}^\top \phi(X^e)) \\ \text{s.t. } \mathbf{w} \in \arg \min_{\mathbf{w} \in \mathbb{R}^d} R^e(\bar{\mathbf{w}}^\top \phi(X^e)) \quad \forall e \in \mathcal{E}. \end{aligned} \quad (1)$$

Previous invariant learning methods [18]–[20], [22]–[26], [52], [56] are for bias problem with independent and identically distributed (i.i.d) data, however, graph-structured data is non i.i.d, and the properties of graph-structured data are not explicitly utilized in these methods. In this paper, we aim to learn invariant graph representations across unknown testing environments.

Problem Formulation. An input graph $G = (\mathbf{A}, \mathbf{X}, Y)$ contains two-folds information: an adjacency matrix \mathbf{A} and node features \mathbf{X} . $\mathbf{A} \in \{0, 1\}^{N \times N}$ is the adjacency matrix of G . The (i, j) -th element $\mathbf{A}_{ij} = 1$ if there exists an edge between node v_i and v_j , otherwise $\mathbf{A}_{ij} = 0$. Furthermore, $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N] \in \mathbb{R}^{N \times d}$ denotes the features of nodes, where \mathbf{x}_n is the d -dimensional feature vector of node v_n . Following the common semi-supervised node classification setting [1], [2], only a small portion of nodes are associated with observed labels $Y^o = \{y_1, y_2, \dots, y_o\}$, where y_n denotes the label of node v_n . Following [22], we define a graph environment as the joint distribution P_{XAY} on $X * A * Y$ and use \mathcal{E} denote the set of all environments. For each environment $e \in \mathcal{E}$, we have a graph dataset $G^e = (X^e, A^e, Y^e)$, where $X^e \in \mathcal{X}$ are node features, $A^e \in \mathcal{A}$ is the adjacency matrix, and $Y^e \in \mathcal{Y}$ is the response variable (e.g., node labels in the node classification problem). The joint distribution P_{XAY}^e of X^e, A^e and Y^e can vary across environments, i.e., $P_{XAY}^e \neq P_{XAY}^{e'}$ for $e, e' \in \mathcal{E}$, and $e \neq e'$. In this paper, we aim to learn node representations based on which we can make invariant predictions across environments with various unknown biases.

Node classification problem with bias on unknown test environments. Given a training graph $\mathcal{G}_{\text{train}} = \{A_{\text{train}}, X_{\text{train}}, Y_{\text{train}}\}$, the task is to learn a GNN $g_\theta(\cdot)$ with parameter θ to precisely predict the label of nodes on different unknown test environments $\{\mathcal{G}_{\text{test}}^1, \mathcal{G}_{\text{test}}^2, \dots, \mathcal{G}_{\text{test}}^e\}$, where $\mathcal{G}_{\text{test}}^e = \{A_{\text{test}}^e, X_{\text{test}}^e, Y_{\text{test}}^e\}$.

IV. METHODS

A. Graph Neural Networks

It has been observed that a broad class of graph neural network (GNN) architectures followed the 1-dimensional

Weisfeiler-Lehman (WL) graph isomorphism test [64]. From the perspective of WL isomorphism test, they mainly consist of the following crucial steps at each iteration of feature aggregation:

- Feature initialization (label initialization): The node features are initialized by original attribute vectors.
- Neighborhood detection (multiset-label determination): It decides the local neighborhood in which node gathers the information from neighbors. More specifically, a seed followed by its neighbors generates a subtree pattern.
- Neighbors sorting (multiset-label sorting): The neighbors are sorted in the ascending or descending order of degree values. The subtrees with permutation order of neighbors are recognized as the same one.
- Feature aggregation (label compression): The node feature is updated by compressing the feature vectors of the aggregated neighbors including itself.
- Graph-level pooling (graph representation): It summarizes all the node features to form a global graph representation.

We would like to point out that graph neural networks would learn the node or graph representation using continuous node attributes, whereas WL algorithms update the node attributes by directly compressing the augmented discrete attributes.

Taking 1-hop neighborhood $N(v) = \{u | (v, u) \in E\}$ into consideration at each iteration, the following node-level graph neural network variants have the same feature initialization and neighborhood detection on learning node representation. And when element-wise average or max operations are used for feature aggregation, graph neural networks would be invariant to the order of neighbors.

Graph Convolutional Network (GCN) [1]:

$$h_v^k = \sigma \left(\sum_{u \in \{v\} \cup N(v)} \hat{a}_{vu} W^k h_u^{k-1} \right) \quad (2)$$

where $\hat{A} = (\hat{a}_{vu}) \in \mathbb{R}^{n \times n}$ is the re-normalization of the adjacency matrix A with added self-loops, and W^k is the trainable matrix at k^{th} layer. It is essentially a weighted feature aggregation from node neighborhood.

B. Bias-Aware Graph Neural Network

Despite the great performance of GNNs, some distribution-specific patterns might warp the GNN biased towards a globally sub-optimal solution since mostly yield distribution shift from the training graph distribution and the testing data distribution in real-world applications.

However, it is impossible to figure out the *node classification problem with bias on unknown environments* without any prior knowledge or structural assumptions, since one cannot characterize the unseen latent environments in provided environments.

In graph data, due to the neighborhood aggregation process, each neighbor node contributing to the final aggregated representation can be viewed as a property of the root node. Thus, we should consider all invariant properties of the target node, such as *feature*, *edge* and *propagation step*. In invariant

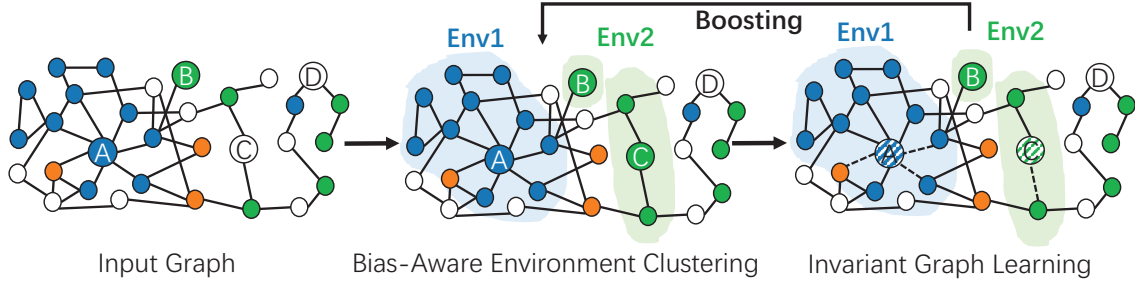


Fig. 3: The framework of BA-GNN. BA-GNN aims to learn invariant graph representations. It contains two parts: *Bias-Aware Environment Clustering* for bias identification and *Invariant Graph Learning* for learning invariant aggregated representation.

graph learning, we have assumption based on a commonly used assumption in invariant learning literature [22]–[26]:

Assumption 4.1: There exists random variable $\Phi^*(X, A)$ such that the following properties hold:

a. Invariance property: for all $e, e' \in \text{supp}(\mathcal{E})$, we have $P^e(Y|\Phi^*(X, A)) = P^{e'}(Y|\Phi^*(X, A))$ holds.

b. Sufficiency property: $Y = f(\Phi^*) + \epsilon$, $\epsilon \perp X$.

However, as shown in the Figure 1, there are degree and label biases between training and testing. The environments need to be subtly uncovered, as indicated by Theorem 4.1, not all environments are helpful to tighten the invariance set.

Theorem 4.1: For environments \mathcal{E} and corresponding invariance set $\mathcal{I}_{\mathcal{E}}$, if the maximal invariant model Φ in newly-added environment e_{new} with distribution $P^{new}(X, A, Y)$ has $P^{new}(Y|\Phi) = P^e(Y|\Phi)$, the invariance set constrained by $\mathcal{E} \cup e_{new}$ is equal to $\mathcal{I}_{\mathcal{E}}$.

Besides Assumption 4.1, we make another assumption on the existence of bias in training data as:

Assumption 4.2: Bias – Aware Assumption.

For random variable pair (X, A, Φ^*) and Φ^* satisfying Assumption 4.1, using functional representation lemma [65], there exists random variable Ψ^* such that $X = X(\Phi^*, \Psi^*)$, then we assume $P^e(Y|\Psi^*)$ can arbitrary change across environments $e \in \text{supp}(\mathcal{E})$.

With notions mentioned above, in this work, we propose a novel *Bias-Aware Graph Neural Network* (BA-GNN) framework that aims to learn a de-biased graph representation. Our BA-GNN framework contains two interactive parts, the frontend \mathcal{M}_B for bias identification and the backend \mathcal{M}_I for invariant graph learning. BA-GNN leverages the mutual promotion between the two steps via joint optimization. The general framework is shown in Figure 3.

Given the graph data, it starts with the bias identification module \mathcal{M}_B leveraging the learned variant representation $\Psi(X)$ and variant adjacency matrix $\Psi(A)$ to generate bias environments \mathcal{E}_{learn} . Then the learned environments are used by invariant graph learning module \mathcal{M}_I to learn the $\Phi(X, A)$ as well as the invariant graph learning model $\text{GNN}(\Phi(X, A))$. After that, we derive the variant $\Psi(X, A)$ to further boost the module \mathcal{M}_B , which is supported by Theorem 4.1. The boosting operation is that more variant representation can be attained in bias-aware environment clustering module when

more invariant representation is learned in invariant graph learning module. In addition, the more variant information is learned, the more invariant information could be used. Specifically, the invariant predictor of feature $\Phi(X)$ is generated as $\Phi(X) = M_x \odot X$, and the variant part $\Psi(X) = (1 - M_x) \odot X$ correspondingly, where $M \in \{0, 1\}^d$ is the binary invariant feature selection mask. The invariant predictor of adjacency $\Phi(A)$ is similar to $\Phi(X)$, where $\Phi(A) = M_a \odot A$, and the variant part $\Psi(A) = (1 - M_a) \odot A$.

Despite the surface similarity between Theorem 4.1 and generative adversarial network, our method is significantly different from that of the generative adversarial network method in the following terms: 1) Motivations of two methods are different. Discriminator and generator models in GANs contest with each other, where generator “fool” the discriminator network by producing novel candidates that the discriminator thinks are not synthesized. However, our clustering module and invariant learning module promote each other, where they have different objective function. 2) Goal of two methods are different. GAN is generative model for unsupervised learning. Our BA-GNN aims to learn invariant graph representation across environments with different agnostic bias. 3) Core insights are different. Minimax GAN loss refer to the minimization of the generator loss and the maximization of the discriminator’s loss. For our BA-GNN, environment clustering module assign nodes to environments with minimization loss, and invariant graph learning module learn invariant representation cross environments with minimization loss. 4) Optimization steps are different. Discriminator and generator models in GANs are simultaneous optimization. However, our clustering module and invariant learning module are asynchronous optimization.

For instance, the feature information is more important for final aggregated representation of node B compared with node A, the reason is that node B is low-degree nodes, low-degree nodes only have few neighbors, which receive very limited information from neighborhoods. Thus, the aggregated representation should have more information of feature for the node B. Moreover, the edges that bring the noise to the representation should be masked, as shown in Figure 4 (b), the dash line are edges that are masked. In addition, the

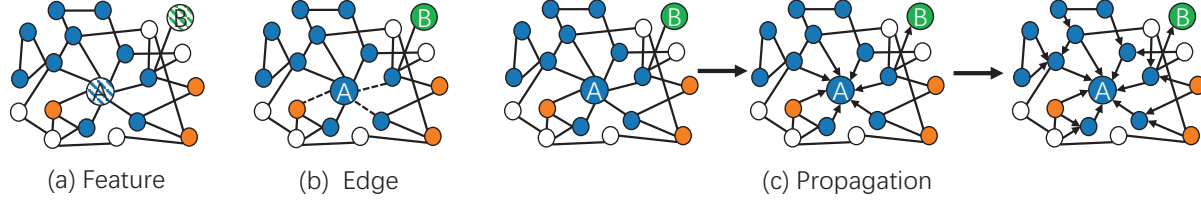


Fig. 4: Illustrations of our Invariant Graph Learning. (a) Learn most informative feature which is invariant across environments. (b) Mask edges that bring variant and noise information to final aggregated representation. (c) Learn optimal propagation step for nodes across different environments.

propagation step influences the features of nodes locally along the edges of the graph. In Figure 4 (c), we can obviously observe that the optimal propagation step for the node A is 2, however, the optimal step for the node B is 1 since more steps will bring the noise to the representation of it. Thus, the parameter of GCNs in higher layers should be masked for the node B, and should not be masked for the node A.

C. Bias-Aware Environment Clustering

The bias-aware environment clustering module \mathcal{M}_B takes a single graph as input, and outputs a multi-environment graph partition for invariant graph learning. Thus, the nodes should be clustered by the relation between variant information and target label. And the variant information $\Psi(X, A)$ is initialized as $\Psi(X, A) = (X, A)$ at the beginning of optimization.

To learn cluster centre $P(Y|\Psi(X, A))$, we assume the j -th cluster centre $P_{\theta_j}(Y|\Psi(X, A))$ parameterized by GCN f_{θ_j} as:

$$h_j(\Psi, Y) = P_{\theta_j}(Y | \Psi) = \|Y - f_{\theta_j}(\Psi(X_j, A))\|_2^2, \quad (3)$$

where Ψ means the learned variant part $\Psi(X, A)$. For the given $N = \sum_{e \in \mathcal{E}_{tr}} n_e$ nodes $(X, A) = \{\psi_i(x_i, a_{i,:}), y_i\}_{i=1}^N$, the empirical distribution is modeled as $\hat{P}_N = \frac{1}{N} \sum_{i=1}^N \delta_i(\Psi(X, A), Y)$, where $\delta_i = 1$ if $\Psi(X, A) = \psi_i(x_i, a_{i,:})$ and $Y = y_i$ and 0, otherwise.

To fit the empirical distribution \hat{P}_N , we have $\mathcal{Q} = \{Q|Q = \sum_{j \in [K]} q_j h_j(\Psi(X, A), Y), \mathbf{q} \in \Delta_K\}$ to fit the empirical distribution best, where Δ_K means K -dimension simplex. Therefore, the objective function of our bias clustering is:

$$\min_{Q \in \mathcal{Q}} D_{KL}(\hat{P}_N \| Q) \quad (4)$$

We further have:

$$\min_{\Theta, \mathbf{q}} \left\{ \mathcal{L}_c = -\frac{1}{N} \sum_{i=1}^N \log \left[\sum_{j=1}^K q_j h_j(\psi_i(x_i, a_{i,:}), y_i) \right] \right\} \quad (5)$$

For environments \mathcal{E}_{tr} , each node is assigned to environment $e_j \in \mathcal{E}_{tr}$ by:

$$P(e_j|\Psi(X, A), Y) = q_j h_j(\Psi(X, A), Y) / \left(\sum_{i=1}^K q_i h_i(\Psi(X, A), Y) \right) \quad (6)$$

D. Invariant Graph Learning

The invariant learning module takes multiple graph partition $G = \{G^e\}_{e \in \text{supp}(\mathcal{E}_{tr})}$ as input, and learn invariant predictor GNN_{θ} , the invariant feature mask M_x , invariant adjacency M_a and the propagation mask M_p . We combine feature selection, neighborhood selection and propagation selection with invariant learning under bias environments, which can learned invariant aggregated features with invariant correlations of the label across \mathcal{E}_{tr} . Specifically, the former module can select most informative features, neighbors and propagation step.

Given one graph partition G^e , the neighborhood aggregation in most GNNs with our invariant mask (M_x, M_a, M_p) is:

$$h'_i = M_{p,i} \sigma \left(\sum_{j \in \mathcal{N}_i} M_{a,ij} W(M_{x,j} \odot h_j) \right) \quad (7)$$

where h_i denotes the updated representation of the target node i , W denotes the weight matrix of the linear transformation, σ denotes the nonlinear activation function, \mathcal{N}_i denotes the indices set of node i 's neighbors, and $M_{x,j}, M_{a,ij}$ are invariant feature and neighbor selection mask, respectively. $M_{p,i}$ is the propagation mask, where $M_{p,i} = 0$ means exiting the propagation process, and $M_{p,i} = 1$ means proceeding the propagation process.

To learn invariant graph representation, we use the variance penalty regularizer similar to [23], where the regularizer is used in feature, neighbor and propagation step selection scenarios. The objective function of \mathcal{M}_I with $(M_x, M_a, M_p) \in \{0, 1\}^d$ is:

$$\mathcal{L}^e(M \odot (X, A), Y; \theta) = \mathbb{E}_{P^e} [\ell(GNN(X^e, A^e, M_x, M_a, M_p; \theta), Y^e)] \quad (8)$$

$$\mathcal{L}_p(M \odot (X, A), Y; \theta) = \mathbb{E}_{\mathcal{E}_{tr}} [\mathcal{L}^e] + \lambda \text{trace}(\text{Var}_{\mathcal{E}_{tr}}(\nabla_{\theta} \mathcal{L}^e)) \quad (9)$$

To learn invariant information, the hard mask suffers from high variance. Following [66], we use soft mask with continuous value in $[0, 1]$, and approximate mask to clipped Gaussian random variable parameterized by $\mu = [\mu_1, \dots, \mu_d]^T$ as $m_i = \max\{0, \min\{1, \mu_i + \epsilon\}\}$ where ϵ is drawn from $\mathcal{N}(0, \sigma^2)$. The objective function can be reformulated as:

$$\mathcal{L}^e(\theta, \mu) = \mathbb{E}_{P^e} \mathbb{E}_M [\ell(GNN(X^e, A^e, M_x, M_a, M_p; \theta), Y^e) + \alpha(\|M_a\|_0 + \|M_x\|_0 + \|M_p\|_0)] \quad (10)$$

Thus, we have $\|M_x\|_0 = \sum_{i \in [d]} \text{CDF}(\mu_{i,x}/\sigma)$, where CDF is the standard Gaussian CDF. Similarly, we have $\|M_a\|_0 =$

Algorithm 1 Bias-Aware Graph Neural Network (BA-GNN)

- 1: **Require:** Graph data $G = (A, X)$ and label Y .
 - 2: **while** Not converged or maximum epochs not reached **do**
 - 3: Obtain multi-environment graph partition $G^j = (A^j, X^j)$ via bias-aware environment clustering module \mathcal{M}_B .
 - 4: **for all** $e = 1$ to $|\mathcal{E}_{tr}|$ **do**
 - 5: Computing loss as in Equation 12.
 - 6: **end for**
 - 7: Optimize θ, μ to minimize \mathcal{L}_p as in Equation 11.
 - 8: **end while**
-

$\sum_{i \in [A]} \text{CDF}(\mu_{i,a}/\sigma)$ and $\|M_p\|_0 = \sum_{i \in [P]} \text{CDF}(\mu_{i,p}/\sigma)$, where P is the maximal propagation step given by layer number of GNNs. $\mu = \{\mu_x, \mu_a, \mu_p\}$. We formulate our objective as risk minimization problem:

$$\min_{\theta, \mu} \mathcal{L}_p(\theta; \mu) = \mathbb{E}_{\mathcal{E}_{tr}} [\mathcal{L}^e(\theta, \mu_x, \mu_a, \mu_p)] + \lambda \text{trace}(\text{Var}_{\mathcal{E}_{tr}}(\nabla_{\theta} \mathcal{L}^e)) \quad (11)$$

where

$$\mathcal{L}^e(\theta, \mu) = \mathbb{E}_{P^e} \mathbb{E}_M [\ell(\text{GNN}(X^e, A^e, M_x, M_a, M_p; \theta), Y^e)] \quad (12)$$

$$+ \alpha \sum_{i \in [P]} \text{CDF}(\mu_p/\sigma) + \alpha \sum_{i \in [A]} \text{CDF}(\mu_a/\sigma) + \alpha \sum_{i \in [d]} \text{CDF}(\mu_i/\sigma) \quad \left. \vphantom{\sum_{i \in [P]} \text{CDF}(\mu_p/\sigma)} \right]$$

The whole algorithm of our proposed BA-GNN framework is detailed in Algorithm 1.

V. MORE ANALYSIS

In this section, we analyze our proposed Bias-Aware Graph Neural Network (BA-GNN) method.

Proof of Theorem 4.1 We can simply prove that we have $S \in \mathcal{I}_{new}, \forall S \in \mathcal{I}_{\hat{\epsilon}}$, where the invariance set is $\text{supp}(\hat{\mathcal{E}} \cup \{e_{new}\})$, because the newly added environment cannot exclude any variables from the old invariance set.

We prove that the invariant graph learning module can learn the maximal invariant predictor $\Phi(X, A)$ with respect to the corresponding invariance set $\mathcal{I}_{\mathcal{E}_{tr}}$ given training environments \mathcal{E}_{tr} .

Theorem 5.1: Given \mathcal{E}_{tr} , the learned $\Phi(X, A) = M \odot (X, A)$ is the maximal invariant predictor of $\mathcal{I}_{\mathcal{E}_{tr}}$, where $M = \{M_x, M_a, M_p\}$.

Justification of the Promote Mechanism. The mechanism for \mathcal{M}_B and \mathcal{M}_I to mutually promote each other is the core of our BA-GNN framework. In Assumption 4.1, we assume that the invariance and sufficiency properties of the invariant information and the relationship between variance part and target value can arbitrarily change.

As shown in Figure 3, with bias-aware environment clustering module, the nodes with higher degree will be assigned to the environment where degree of nodes is higher and the nodes with lower degree will be assigned to the environment where degree of nodes is lower. With such different environments, invariant graph learning could learn more invariant representation. The bias-aware environment clustering module and

invariant graph learning module are in the loop and promote each other, where the boosting operation is that more variant representation can be attained in bias-aware environment clustering module when more invariant representation is learned in invariant graph learning module.

Complexity Analysis. The training and inference time complexity of a GCN with L layers can be bounded by $O(LmF)$, where m is the number of edges and F is the feature dimension. Our BA-GNN learns invariant representation which is in the feature transformation stage. Feature transformation can be performed with significantly less cost due to better parallelism of dense-dense matrix multiplication. Consequently, the complexity of our BA-GCN is $O(LmF)$ and has the same level complexity as the GCN backbone.

VI. EXPERIMENTS

In this section, we conduct experiments on graph benchmarks to evaluate the effectiveness of the proposed frameworks with comparison to state-of-the-art GNNs. Specifically, we aim to answer the following questions:

- **(RQ 1)** How effective is the proposed BA-GNN framework for the node classification task on different graphs and different backbones?
- **(RQ 2)** Could the proposed BA-GNN alleviate bias issue?
- **(RQ 3)** Could the proposed framework learn to identify different biases?
- **(RQ 4)** How efficiency is the proposed BA-GNN framework with comparison to state-of-the-art GNNs?

A. Datasets

We conduct experiments on 11 datasets based on citation, co-authorship, co-purchase graphs and heterophily graphs for semi-supervised node classification tasks; those are Cora [67], CiteSeer [67], PubMed [67], Coauthor CS [68], Coauthor Physics [68], Amazon Computers [68], and Amazon Photo [68], Actor [46], Cornell [46], Texas [46], and Wisconsin [46]. We follow the widely used training/validation/testing split in [10], [46], [68] The statistics of datasets are summarized in the Table I.

Citation datasets. Cora, CiteSeer and PubMed [67] are representative citation network datasets where nodes and edges denote documents and their citation relationships, respectively. Node features are formed by bay-of-words representations for documents. Each node has a label indicating what field the corresponding document belongs to.

Co-authorship datasets. Coauthor CS and Coauthor Physics [68] are co-authorship graphs datasets. Nodes denote authors, which are connected by an edge if they co-authored a paper. Node features represent paper keywords for each author's papers. Each node has a label denoting the most active fields of study for the corresponding author.

Co-purchase datasets. Amazon Computers and Amazon Photo [68] are segments of the Amazon co-purchase graph [69] where nodes are goods and edges denote that two goods are frequently bought together. Node features are

TABLE I: Statistics of datasets. The edge density is computed by $\frac{2m}{n^2}$. The standard fixed training/validation/testing split is widely used in [1]–[3], [46].

Dataset	#Classes	#Nodes	#Edges	Edge Density	#Features	#Training Nodes	#Validation Nodes	#Test Nodes
Cora	7	2708	5278	0.0014	1433	20 per class	500	1000
CiteSeer	6	3327	4552	0.0008	3703	20 per class	500	1000
PubMed	3	19717	44324	0.0002	500	20 per class	500	1000
Coauthor CS	15	18333	81894	0.0005	6805	20 per class	30 per class	Rest nodes
Coauthor Physics	5	34493	247962	0.0004	8415	20 per class	30 per class	Rest nodes
Amazon Computers	10	13381	245778	0.0027	767	20 per class	30 per class	Rest nodes
Amazon Photo	8	7487	119043	0.0042	745	20 per class	30 per class	Rest nodes
Actor	5	7600	26659	0.0009	932	48% of nodes per class	32% of nodes per class	Rest nodes
Texas	5	183	309	0.0185	1703	48% of nodes per class	32% of nodes per class	Rest nodes
Cornell	5	183	295	0.0176	1703	48% of nodes per class	32% of nodes per class	Rest nodes
Wisconsin	5	251	499	0.0158	1703	48% of nodes per class	32% of nodes per class	Rest nodes

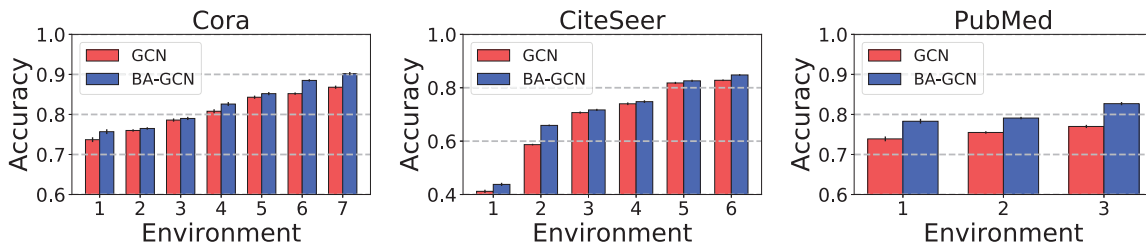


Fig. 5: Results of **GCN backbone** under **label-related distribution shift** for the task of semi-supervised node classification. Comparing with GCN method, our BA-GCN method (by applying our BA-GNN framework on GCN backbone) improves the accuracy of node classification across different label biased environments.

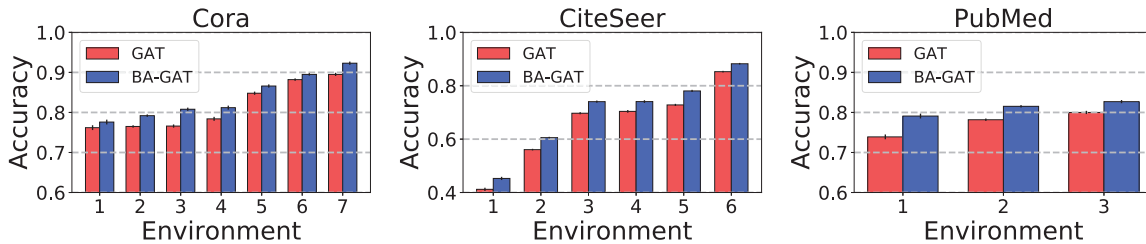


Fig. 6: Results of **GAT backbone** under **label-related distribution shift** for the task of semi-supervised node classification. Comparing with GAT method, our BA-GAT method (by applying our BA-GNN framework on GAT backbone) improves the accuracy of node classification across different label biased environments.

derived from bag-of-words representations for product reviews and class labels are given by the product category.

Heterophily graph datasets. Recent studies [10], [46], [70] show that the performance of GNNs can significantly drop on heterophily graphs, we also include heterophily benchmark in our experiments, including Actor, Cornell, Texas, and Wisconsin [10], [46].

B. Baselines

Note that the proposed framework BA-GNN is generic and can be utilized to improve arbitrary GNN backbones. To evaluate the effectiveness of BA-GNN framework, we consider three popular GNN architectures, including GCN [1], GAT [2] and APPNP [9]. We implemented our proposed BA-GNN and some necessary baselines using Pytorch [71] and Pytorch

Geometric [72], a library for deep learning on irregularly structured data built upon Pytorch.

Moreover, we further consider the methods that are designed for reducing the degree bias, including GNM [42], DEMO-Net [43], SL-DSGCN [44]. We compare our BA-GNN with studies on imbalance graph such as DR-GCN [59], ImGAGN [63]. We aim to provide a rigorous and fair comparison between different models on each dataset by using the same dataset splits and training procedure. We tune hyperparameters for all models individually and some baselines even achieve better results than their original reports.

C. RQ1. Overall performance in Graph Benchmark

To show the effectiveness of our proposed BA-GNN, we follow the widely used semi-supervised setting in [1]–[3],

TABLE II: Classification accuracy (%) results of semi-supervised node classification experiments. We follow the widely used semi-supervised setting in [1]–[3], and apply the standard fixed training/validation/testing split as shown in Table I.

Method	Cora	CiteSeer	PubMed	Coauthor-CS	Coauthor-Physics	Amazon-Computers	Amazon-Photo
GCN	81.3±0.8	71.1±0.7	78.8±0.6	91.08±0.6	93.03±0.8	81.17±1.8	90.25±1.6
GCN+Ours	82.1±0.5	72.4±0.6	79.8±0.4	92.73±0.6	94.94±0.1	84.94±2.4	91.39±1.1
GAT	83.0±0.7	72.5±0.7	79.0 ±0.4	90.28±0.7	91.92±0.9	80.38±1.5	90.41±1.8
GAT+Ours	83.5±0.7	73.4±0.5	80.3 ±0.3	91.34±0.5	92.39±0.8	81.29±2.2	91.53±1.4
APPNP	83.8±0.3	71.6±0.5	79.7±0.3	92.45±0.4	93.41±0.9	81.79±2.0	91.22±1.3
APPNP+Ours	84.2±0.3	72.0±0.5	79.9±0.3	92.94±0.5	94.36±1.1	82.64±1.9	91.81±1.3
GraphSAGE	80.7±0.8	70.7±0.6	78.9±0.7	91.38±2.8	93.03±0.8	82.46±1.8	91.31±1.3
GraphSAGE+Ours	81.6±0.7	71.4±0.8	79.2±0.5	91.50±1.4	93.87±0.8	83.15±1.7	91.90±1.2

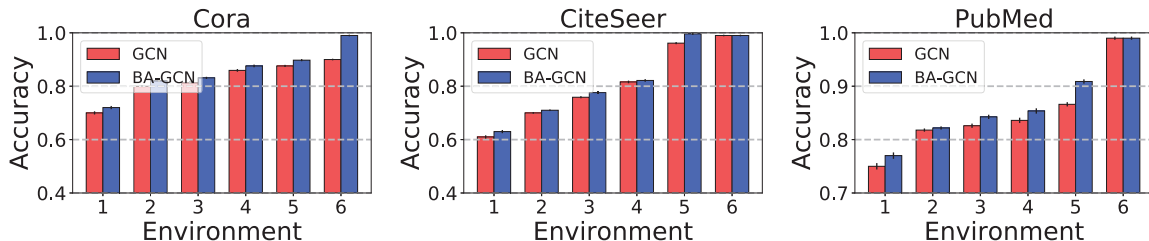


Fig. 7: Results of **GCN backbone** under **degree-related distribution shift** for the task of semi-supervised node classification. Comparing with GCN method, our BA-GCN method (by applying our BA-GNN framework on GCN backbone) improves the accuracy of node classification across different degree biased environments.

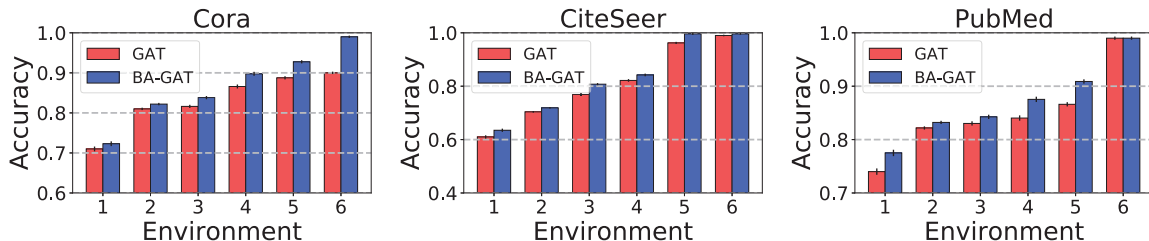


Fig. 8: Results of **GAT backbone** under **degree-related distribution shift** for the task of semi-supervised node classification. Comparing with GAT method, our BA-GAT method (by applying our BA-GNN framework on GAT backbone) improves the accuracy of node classification across different degree biased environments.

TABLE III: Classification accuracy (%) results of semi-supervised node classification experiments on heterophily graphs [46].

Method	Actor	Cornell	Texas	Wisconsin
GCN	26.86	52.71	52.16	45.88
GCN+Ours	28.31	54.93	57.48	49.97
GAT	28.45	54.32	58.38	49.41
GAT+Ours	31.59	57.08	59.26	51.19
APPNP	28.65	58.43	60.68	54.24
APPNP+Ours	29.58	59.03	61.73	55.39
GraphSAGE	30.23	60.95	64.43	56.18
GraphSAGE+Ours	31.73	61.87	66.48	58.27

and apply the standard fixed training/validation/testing split as shown in Table I. We conduct node classification on 7 graph datasets as introduced in Table I with different backbones such as GCN, GAT and APPNP. For each graph dataset, we report

the mean accuracy with standard deviation on the test nodes in Table II and III with 10 runs experiments. As shown in Table II and III, we have the following findings:

- Our BA-GNN improves the performance of all GNN backbones consistently and significantly in all settings.
- GNN backbones have worse performance due to ignoring of biases.
- The reason why our BA-GNNs outperform is that our method alleviates different biases, thus our method outperform in different bias environments, and the overall classification accuracy increases.
- We can observe that our BA-GNN outperform all backbones on four heterophily graphs, which indicates our framework can still work well on the heterophily graphs.
- In summary, our BA-GNN achieves superior performance on all these seven datasets, which significantly demonstrates the effectiveness of our proposed framework and

our motivation.

D. RQ2. Performance in unknown bias environments.

To further validate the effectiveness of our framework, besides the widely used semi-supervised setting in [1]–[3], we evaluate our framework in different biased unknown test environments. Specifically, for degree biased test environments, we group the testing nodes of each graph according to their degrees. Similarly, for label biased test environments, we group the testing nodes of each graph according to their labels. The distribution shifts between training and testing environments are various in this setting, where we evaluate methods in different environments rather than average accuracy of all testing nodes in a single environment. The training/validation/testing split in this experiment is the standard fixed split as shown in Table I, which is widely used in [1]–[3].

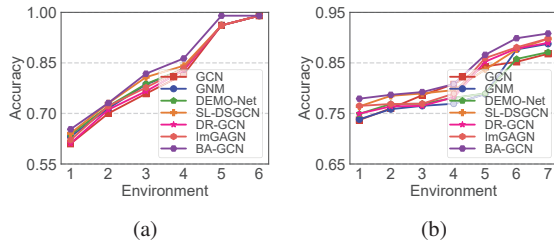


Fig. 9: Semi-supervised node classification accuracy compared with other GNN baselines for addressing the bias issue. We test all methods on (a) unknown degree bias environments on Cora (b) unknown label bias environments on Cora.

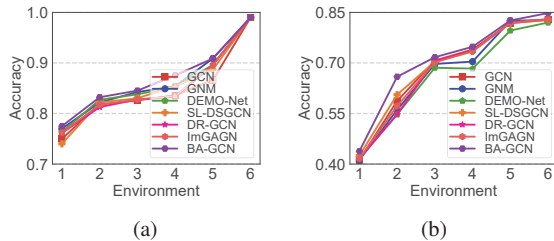


Fig. 10: Semi-supervised node classification accuracy compared with other GNN baselines for addressing the bias issue. We test all methods on (a) unknown degree bias environments on PubMed (b) unknown label bias environments on CiteSeer.

Compare with base backbone. The testing results in unknown environments are shown in Figure 5 - 8. Specifically, each figure in Figure 5 - 8 plot the evaluation results across different testing environments. From the results, we have the following observations and conclusions: Our BA-GNN outperforms all backbones such as GCN, GAT, APPNP in all bias cases. GNN backbones have worse performance due to ignoring of biases. Results illustrate the effectiveness of our BA-GNN. The reason why BA-GNN outperform in all cases is that our method could alleviate different unknown

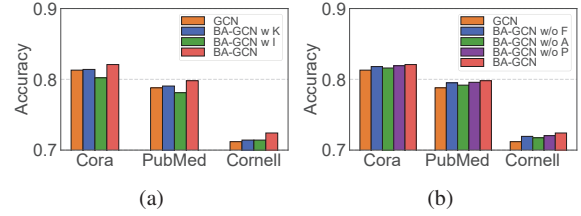


Fig. 11: Ablation study of (a) the bias-aware environment clustering and the invariant graph learning; and (b) invariant feature mask, invariant adjacency, and propagation selection.

biases with invariant representation. In summary, our BA-GNN outperforms the baselines with different backbones and different graphs, which suggests that our framework is agnostic to backbones and graphs.

Compare with previous methods designed for reducing biases. To further show the effectiveness of our framework, we compare our BA-GNN with the following baselines designed for reducing biases: GNM [42], DEMO-Net [43], SL-DSGCN [44]. Figure 9 shows the performance of different methods designed for reducing biases in unknown test environments. Specifically, Figure 9 (a) plots the evaluation results across different unknown testing environments with degree bias, and Figure 9 (b) plots the evaluation results across different unknown testing environments with label bias. From these figures, we have the following observations and findings:

- Our BA-GNN outperforms all methods in all bias cases, including methods are designed for reducing degree bias.
- Although the degree-related method DEMO-Net and SL-DSGCN can also alleviate the degree bias, they still do not outperform APPNP on label bias environments.
- Results illustrate the effectiveness of our BA-GNN. The reason why BA-GNN outperform in all cases is that our method could alleviate different biases, GNM, DEMO-Net and SL-DSGCN only focus on degree bias.
- Compared with methods focused on imbalance graph such as DR-GCN, ImGAGN, BA-GNN outperform in both degree-related and label-related bias environments.
- Our BA-GCN is the only method that performs better than all baselines across all the environments. These findings show that our BA-GCN framework can effectively adapt to different graph and alleviate different bias.
- In summary, our BA-GNN could alleviate different biases such as degree bias and label bias. Thus our method outperforms the methods designed for reducing biases.

E. RQ.3 Effectiveness of Bias-Aware Environment Clustering

Effectiveness of proposed two modules. The bias-aware environment clustering module and the invariant graph learning module in BA-GNN are not individual, they are in the loop, and promote each other. To further illustrate the effectiveness of two modules in BA-GNNs, we design experiments to compare our BA-GCN with BA-GCNwK, BA-GCNwI.

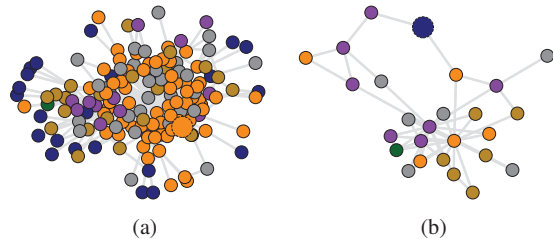


Fig. 12: Illustration of the inferred environments for the degree bias by our BA-GNN. The node assigned to environment is the bigger node in each sub-graph. (a) Node in Environment 6, where most of the nodes are high-degree. (b) Node in Environment 1, where most of the nodes are low-degree.

BA-GCNwK replace bias-aware environment clustering module with K-means method in BA-GCN, where the input of K-means is the node feature, and output is environment label of nodes. BA-GCNwI replace invariant graph learning module with IRM in BA-GCN, where the environment label is given by our proposed bias-aware environment clustering module.

As shown in Figure 11 (a), a couple of observations are worth being highlighted as: BA-GCNwI has a significant drop, the reason is that BA-GCNwI focuses on the node feature and ignore the structure information of graph. BA-GCNwK outperform GCN, which validate the effectiveness of our proposed invariant learning module, BA-GCN outperform BA-GCNwK, which demonstrate the effectiveness of promote mechanism between our proposed two modules: the better invariant representation is learned, the better variant representation can be obtained for bias identification.

Effectiveness of proposed three selection strategy. To further validate the effectiveness of the proposed three selection strategy of BA-GNN, we design experiments to show the effectiveness of invariant feature mask strategy, invariant adjacency selection strategy, and optimal propagation selection strategy. We evaluate BA-GCN with: **BA-GCNw/oF** is BA-GCN without invariant feature mask strategy. **BA-GCNw/oA** is BA-GCN without invariant adjacency selection strategy. **BA-GCNw/oP** is BA-GCN without optimal propagation selection strategy. Figure 11 (b) shows the result. The best performance is obtained by BA-GCN for all cases, indicating that each of components does contribute to the effectiveness and robustness of the whole model.

Case study. To evaluate if our BA-GNN can learn good bias identification, we study the bias identification for individual nodes. Figures 12 and 13 show the case studies of bias identification on both label bias and degree bias. In Figures 12 and 13, we plot the 3-hop neighborhood of each test node and use different colors to indicate different labels. The node with higher degree is assigned to the environment where degree of nodes is higher, as shown in Figure 12 (a), and the node with lower degree is assigned to the environment where degree of nodes is lower, as shown in Figure 12 (b). Similarly, As shown in Figure 13, we find that the node with more same class

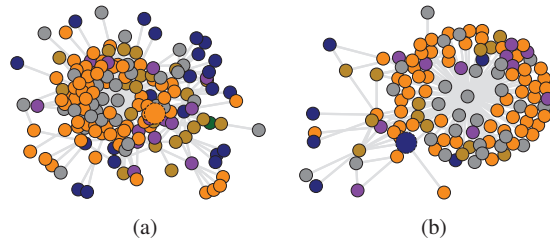


Fig. 13: Illustration of the inferred environments for the label bias by our BA-GNN. The node assigned to environment is the bigger node in each sub-graph. (a) Node in Environment 6, where node's label has more nodes. (b) Node in Environment 1, where node's label has fewer nodes.

neighbors tends to be assigned to environment where label has more nodes. In contrast, the node with fewer same class nodes will probably be assigned to environment where label has fewer nodes. Additionally, we can find that our framework successfully identifies the bias.

More details of Experiment Setup. The hyper-parameters for model architectures are set as default values in different cases. Other hyperparameters are searched with grid search on validation dataset. The searching space are as follows: learning rate for GNN backbone $\alpha \in \{0.0001, 0.0002, 0.001, 0.005, 0.01\}$, weight decay $\in \{0, 2e-2, 5e-3, 5e-4, 5e-5\}$, and dropout rate $\in \{0.5, 0.8\}$.

VII. CONCLUSION

In this paper, we argue that GNNs might suffer from the bias issue because of the distribution shift between training and testing node distributions. More importantly, the test node distribution in the graph is generally unknown during model training in real-world applications. To address this problem, we propose a novel *Bias-Aware Graph Neural Network* (BA-GNN) framework that aims to learn node representations that are invariant across different distributions for invariant prediction. Our BA-GNN framework contains two interactive parts, one for bias identification and the other for invariant prediction. To learn invariant feature and aggregated representation, our BA-GNN learns multiple biased graph partitions and selects feature, neighbor, and propagation steps for nodes under multiple biased graph partitions. With extensive empirical experiments on different graphs and different GNN backbones, we demonstrate the effectiveness of our proposed framework, which leads to the state-of-the-art performance on several benchmark datasets.

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