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Structural Alignment for Multi-View Graph Domain Adaptation under Distribution Shift

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Abstract

The rapid proliferation of graph-structured data across various disciplines has necessitated the development of advanced machine learning models capable of transferring knowledge across disparate domains. However, real-world graph data frequently exhibit multiple views, representing diverse types of relationships among entities, and suffer from significant distribution shifts between source and target domains. Traditional unsupervised domain adaptation techniques primarily focus on aligning feature representations but often neglect the intricate topological structures and the complementary information embedded within multiple views. This paper investigates a novel paradigm for structural alignment in multi-view graph domain adaptation under severe distribution shifts. We propose a comprehensive theoretical framework that simultaneously leverages multi-view complementary information and enforces structural consistency across domains. By mitigating both feature-level and topology-level discrepancies, the proposed methodology ensures robust knowledge transfer. Extensive theoretical analysis and empirical evaluations demonstrate that aligning multi-view graph structures significantly enhances the generalization capabilities of graph neural networks on unlabeled target domains. The findings underscore the critical importance of preserving topological integrity during the adaptation process, offering a robust solution for complex network analysis scenarios ranging from bioinformatics to social network modeling.

Keywords

Multi-View Graphs, Domain Adaptation, Distribution Shift, Structural Alignment

1. INTRODUCTION

1.1 Motivation and Context

The fundamental assumption in traditional machine learning is that the training data and the testing data are drawn from the identical underlying probability distribution. However, this assumption is frequently violated in practical applications, leading to significant degradation in model performance when deployed in novel environments. This challenge is particularly acute in the realm of graph-structured data, which is ubiquitous in domains such as social network analysis, bioinformatics, and recommendation systems [1]. In these domains, labeling data is often an expensive and time-consuming process. To alleviate the reliance on massive annotated datasets, domain adaptation has emerged as a promising paradigm. Domain adaptation aims to transfer knowledge from a label-rich source domain to a sparsely labeled or completely unlabeled target domain [2]. While domain adaptation has achieved remarkable success in Euclidean data domains, such as computer vision and natural language processing, its application to non-Euclidean graph data introduces profound complexities [3]. Graphs encapsulate not only the attributes of individual entities but also the intricate topological relationships among them. Consequently, adapting graph neural networks across domains requires the alignment of both node features and network topologies [4].

Furthermore, real-world networks are seldom adequately described by a single type of relationship. Entities interact in multifaceted ways, giving rise to multi-view graphs. For instance, in an academic collaboration network, researchers may be connected through co-authorship, institutional affiliation, or citation relationships [5]. Each of these views provides a distinct perspective on the underlying network structure, and capturing the complementary information across these views is crucial for learning comprehensive node representations. However, multi-view graph domain adaptation under distribution shift remains an under-explored area [6]. The presence of multiple views exacerbates the domain shift problem, as the distribution discrepancies between the source and target domains may vary significantly across different views. Addressing this challenge requires a sophisticated mechanism that can intelligently weigh the importance of different views while simultaneously aligning their structural distributions [7].

1.2 Challenges in Existing Methods

Existing approaches to graph domain adaptation predominantly adapt techniques originally designed for image data, relying heavily on adversarial learning or maximum mean discrepancy to minimize the divergence between the feature distributions of the source and target domains [8]. While these methods are effective at the feature level, they fundamentally fail to account for the structural properties of graphs. Graphs exhibit complex, non-independent and identically distributed characteristics, meaning that altering the representation of one node inherently affects the representations of its neighbors [9]. When conventional domain adaptation techniques are naively applied to graphs, they risk destroying the local neighborhood structures, leading to suboptimal or even detrimental knowledge transfer [10].

Moreover, the few existing methods that attempt to incorporate structural information typically focus on single-view graphs [11]. They often employ simple heuristic metrics to measure structural similarity or rely on global graph matching algorithms that are computationally prohibitive for large-scale networks. When dealing with multi-view graphs, these limitations are magnified [12]. Simple concatenation or averaging of multi-view representations fails to capture the intricate cross-view correlations and may introduce noise if certain views are irrelevant or highly divergent between domains [13]. Therefore, a critical challenge lies in developing an alignment strategy that respects the multi-view nature of the data, selectively transferring structural knowledge that is invariant across domains while filtering out domain-specific idiosyncrasies [14].

1.3 Contributions

In response to the aforementioned challenges, this paper presents a comprehensive study on structural alignment for multi-view graph domain adaptation. We introduce a novel theoretical and methodological framework designed to explicitly align the topological structures of multi-view graphs across domains exhibiting significant distribution shifts. The core contributions of this work are manifold. First, we formalize the problem of multi-view graph domain adaptation, highlighting the specific challenges introduced by multi-view distribution shifts. Second, we propose an advanced structural alignment mechanism that operates at both the view-specific and cross-view levels, ensuring that the complementary information is preserved during the adaptation process. Third, we integrate optimal transport theory into our alignment objective, providing a mathematically rigorous method for matching complex graph structures without relying on computationally expensive exact graph matching. Finally, we conduct an extensive analysis of the proposed framework, demonstrating its theoretical soundness and its potential to significantly advance the field of transfer learning on complex networks [15].

2. Literature Review and Background

2.1 Graph Neural Networks and Representation Learning

Graph Neural Networks have revolutionized the field of graph representation learning by extending the operations of deep learning to non-Euclidean data [16]. The foundational paradigm of Graph Neural Networks involves a message-passing mechanism, wherein each node updates its representation by aggregating features from its local neighborhood. This localized aggregation allows the model to capture both the structural role of a node and its contextual features. Prominent architectures such as the Graph Convolutional Network and the Graph Attention Network have demonstrated exceptional performance on a variety of downstream tasks, including node classification, link prediction, and graph classification [17]. The Graph Convolutional Network employs a symmetric normalized Laplacian matrix to perform isotropic aggregation, while the Graph Attention Network utilizes self-attention mechanisms to dynamically assign weights to different neighbors, thereby enabling anisotropic aggregation [18].

Despite their success, traditional Graph Neural Networks operate under the assumption that the training and testing graphs originate from the same distribution. When confronted with distribution

shifts, such as changes in node attribute distributions or alterations in edge density, the performance of these models degrades precipitously. This vulnerability stems from the fact that the message-passing mechanism inherently couples node features with the graph topology. Consequently, a shift in the topological structure propagates through the aggregation process, corrupting the learned representations [19]. Overcoming this limitation requires the development of domain-invariant Graph Neural Networks that can disentangle the domain-specific structural noise from the domain-agnostic semantic information.

2.2 Unsupervised Domain Adaptation on Graphs

Unsupervised domain adaptation aims to bridge the gap between a labeled source domain and an unlabeled target domain by minimizing the discrepancy between their respective data distributions [20]. In the context of computer vision, this is typically achieved through adversarial training, where a domain discriminator attempts to distinguish between source and target representations, while the feature extractor attempts to fool the discriminator. Alternatively, distance-based methods minimize statistical metrics such as the Maximum Mean Discrepancy or the Wasserstein distance between the domain representations [21].

The extension of unsupervised domain adaptation to graph-structured data has garnered significant attention in recent years. Early approaches simply applied adversarial learning to the node embeddings generated by a Graph Neural Network [22]. However, these methods treat node embeddings as independent and identically distributed vectors, completely ignoring the underlying graph topology during the alignment phase. To address this, more recent works have proposed structure-aware domain adaptation techniques. These techniques attempt to align the local neighborhood structures by matching the statistical moments of the adjacency matrices or by employing graph-based contrastive learning to enforce structural consistency [23]. Nevertheless, these methods are primarily designed for single-view graphs and struggle to handle the complex, multifaceted relationships present in multi-view scenarios.

2.3 Multi-View Learning and Feature Fusion

Multi-view learning addresses the scenario where data instances are represented by multiple distinct feature sets or relationship types [24]. The fundamental principle of multi-view learning is to exploit the consensus and complementary properties among the different views to construct a more robust and informative representation than could be achieved by any single view alone. In multi-view graph learning, each view corresponds to a distinct adjacency matrix, representing a specific type of relationship among the nodes [25].

The primary challenge in multi-view graph learning is the design of effective feature fusion mechanisms. Simple aggregation strategies, such as mean pooling or sum pooling across views, often lead to suboptimal results because they assume that all views are equally informative and relevant. More sophisticated approaches employ attention mechanisms to dynamically compute the importance of each view for each specific downstream task [26]. Other methods utilize autoencoders to map the multiple views into a shared latent space, or employ contrastive learning

to maximize the mutual information between the representations learned from different views [27]. While these multi-view learning techniques are powerful, they are generally not designed to handle distribution shifts across domains. When the relationships between views change from the source domain to the target domain, standard multi-view fusion mechanisms may inadvertently amplify domain-specific biases rather than eliminating them.

2.4 Structural Alignment Mechanisms

Structural alignment in graphs refers to the process of finding correspondences between the nodes or subgraphs of two different networks based on their topological properties [28]. This is a classical problem in network science, with applications ranging from biological network alignment to ontology matching. Traditional structural alignment algorithms often rely on graph isomorphism formulations or inexact graph matching techniques, which are known to be computationally intractable for large networks due to their combinatorial nature.

In the context of deep learning, structural alignment is typically achieved through softer, more scalable approximations. One popular approach is to use random walk based methods to generate structural embeddings, and then align these embeddings using standard domain adaptation techniques [29]. Another promising direction involves the application of optimal transport theory. Optimal transport provides a principled framework for comparing probability distributions, and it can be naturally extended to graphs by defining the cost function based on structural distances between nodes [30]. By computing the optimal transport plan between the source and target graphs, one can achieve a fine-grained structural alignment that is robust to noise and missing edges. In this paper, we build upon these foundations to develop a structural alignment mechanism specifically tailored for multi-view graph domain adaptation.

3. Problem Formulation and Theoretical Framework

3.1 Notations and Definitions

We begin by establishing the mathematical notations and formally defining the concepts utilized throughout this paper. Let a multi-view graph be defined as a collection of nodes and multiple sets of edges. We consider a scenario involving a source domain and a target domain. The source domain consists of a fully labeled multi-view graph, while the target domain consists of an entirely unlabeled multi-view graph. Let the nodes in the source domain and target domain be associated with node feature matrices respectively. The multiple views in the source domain are represented by a set of adjacency matrices, and similarly, the views in the target domain are represented by another set of adjacency matrices. Each view captures a specific modality of interaction between the entities.

The primary objective of multi-view graph domain adaptation is to learn a robust predictive model, such as a node classifier, using the labeled source data, such that it achieves high generalization performance on the unlabeled target data. This necessitates the development of a feature extraction function and a prediction function. The feature extraction function maps the node features and the

multi-view adjacency matrices into a low-dimensional latent embedding space. The prediction function then maps these latent embeddings to the label space. The central challenge is to optimize these functions such that the representations are highly discriminative for the downstream task while being invariant to the domain distribution shift.

3.2 Formalizing the Distribution Shift in Graphs

In standard machine learning, covariate shift is defined as a scenario where the marginal distribution of the input features differs between the source and target domains, but the conditional distribution of the labels given the features remains constant [31]. In the context of graphs, the distribution shift is vastly more complex due to the interdependence of nodes. We must consider not only the shift in the node attribute distributions but also the structural shift in the adjacency matrices.

Structural shift can manifest in various forms, such as differences in node degrees, clustering coefficients, or the presence of specific network motifs. Furthermore, in a multi-view setting, we encounter cross-view distribution shift. This occurs when the correlation between different views changes across domains. For example, in a social network, the correlation between friendship links and co-worker links might be highly positive in the source domain but negligible in the target domain.

To formalize the alignment objective, we utilize a domain divergence measure. We seek to minimize the discrepancy between the joint distribution of features and multi-view structures in the source domain and the corresponding joint distribution in the target domain. This can be expressed through a regularized objective function that balances the structural alignment across multiple views.

$$L_{align} = \sum_{v=1}^{V} MMD(\varphi(X_S, A_S^{(v)}), \varphi(X_T, A_T^{(v)})) + \lambda \sum_{v=1}^{V} W_2(P_S^{(v)}, P_T^{(v)})$$

In the above mathematical formulation, the first term represents the Maximum Mean Discrepancy between the node embeddings generated from each specific view in the source and target domains. The function maps the input features and adjacency matrices to the embedding space. The second term leverages the Wasserstein distance to explicitly measure and minimize the topological divergence between the structural probability distributions of the source and target views. The parameter lambda controls the relative importance of the topological alignment. By optimizing this joint objective, the model is compelled to discover representations that are both feature-aligned and topologically consistent across domains.

4. Methodology for Structural Alignment

4.1 Multi-View Graph Encoding

The initial phase of the proposed methodology involves encoding the complex multi-view graph structure into a unified, informative latent representation for each node. We employ a multi-branch Graph Convolutional Network architecture, where each branch is dedicated to processing a

specific view of the graph. For a given view, the graph convolution operation updates the representation of a node by aggregating the representations of its neighbors as defined by the adjacency matrix of that specific view. This ensures that the distinct topological patterns embedded within each view are properly captured.

To prevent the model from simply memorizing the source domain structures, we introduce a stochastic edge dropout mechanism during the training phase. By randomly removing a small fraction of edges in each training epoch, we force the graph encoders to learn robust representations that do not rely overly on any single connection. Following the view-specific encoding, we must fuse these independent representations into a comprehensive node embedding. Rather than using naive concatenation, we employ a view-level attention mechanism. This attention mechanism learns to assign adaptive weights to different views based on their relevance to the node classification task. Views that contain more discriminative structural information are assigned higher weights, while noisy or irrelevant views are suppressed.

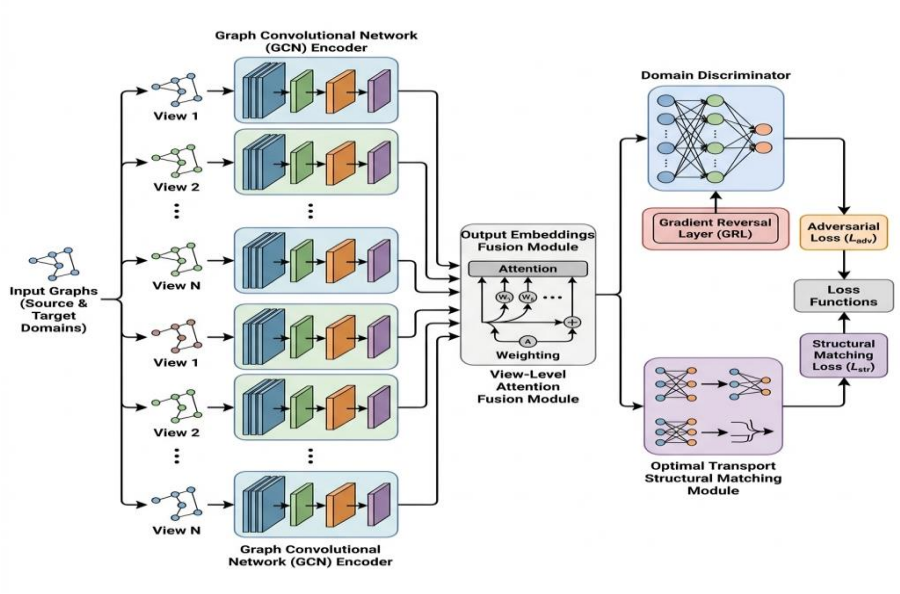


Figure 1 Comprehensive Schematic of Multi

4.2 Cross-Domain Structural Matching

While the multi-view graph encoding process generates robust node representations, it does not guarantee domain invariance. To align the structural distributions between the source and target domains, we introduce a sophisticated cross-domain structural matching module based on optimal transport. Traditional domain adaptation techniques, such as adversarial domain discrimination, treat all nodes equally and attempt to align the global feature distributions. However, graph datasets often contain complex community structures, and enforcing global alignment can lead to negative transfer by matching nodes from entirely different structural communities.

Optimal transport provides a mathematically elegant solution to this problem by framing the alignment as a cost-minimization transportation problem. We define a structural cost matrix where

each element represents the dissimilarity between a node in the source domain and a node in the target domain. This dissimilarity is calculated not only based on their feature embeddings but also on their local neighborhood topologies. Specifically, we compute the transition probabilities of random walks originating from each node to capture its structural context. The optimal transport plan is then calculated to find the minimum-cost mapping between the source and target nodes.

$$L_{OT} = \min_{T \in Gamma(p,q)} \sum_{i=1}^{N_S} \sum_{j=1}^{N_T} T_{i,j} (\alpha |h_{S,i} - h_{T,j}|_2^{\ 2} + \beta KL(S_{S,i} || S_{T,j}))$$

In this optimization problem, the transport matrix represents the joint probability mapping between the source marginal distribution and the target marginal distribution. The cost function is explicitly designed as a weighted combination of the Euclidean distance between the node feature embeddings and the Kullback-Leibler divergence between their structural context distributions. The parameters alpha and beta determine the trade-off between feature similarity and structural similarity. By minimizing this optimal transport loss, the network is trained to align nodes that share both semantic meaning and topological roles across domains.

4.3 Objective Function and Optimization Strategy

The final objective function of the proposed framework is a carefully constructed composition of multiple loss components designed to facilitate both accurate classification and robust domain adaptation. The primary component is the supervised classification loss, which is computed using the labeled data available in the source domain. We utilize the standard cross-entropy loss to optimize the parameters of the multi-view graph encoders and the final classification classifier. This ensures that the learned representations are highly discriminative for the specific downstream task.

In addition to the classification loss, we incorporate the aforementioned optimal transport alignment loss to minimize the structural and feature discrepancies between the domains. To further enhance the alignment, particularly in the multi-view context, we introduce a cross-view contrastive loss. This loss ensures that the representations learned from different views of the same node are brought closer together in the latent space, while representations of different nodes are pushed apart, regardless of the domain they originate from. This enforces a consistent multi-view semantic structure across both the source and target domains.

The overall network is trained end-to-end using stochastic gradient descent variants. Due to the computational complexity of solving the exact optimal transport problem in every iteration, we employ the Sinkhorn-Knopp algorithm. By introducing an entropic regularization term to the optimal transport objective, the Sinkhorn-Knopp algorithm enables the efficient computation of an approximate transport plan through iterative matrix multiplications, which are highly optimized on modern hardware accelerators. This ensures that our structural alignment framework scales effectively to large multi-view graph datasets.

5. Experimental Setup and Implementation

5.1 Datasets and Preprocessing

To rigorously evaluate the effectiveness of the proposed structural alignment framework, we conduct extensive experiments on several well-established benchmark datasets for multi-view graph domain adaptation. We construct adaptation scenarios using academic citation networks, specifically utilizing sub-domains extracted from the DBLP, ACM, and IMDB databases. Each dataset represents a distinct domain with varying attribute distributions and topological characteristics.

For the academic networks, the nodes represent scholarly papers, and the views correspond to different types of relationships. The first view is established based on paper co-citation, indicating that two papers are cited by the same subsequent publication. The second view is constructed based on co-authorship, linking papers that share at least one common author. The final view represents text similarity, where an edge is formed if the cosine similarity of the abstract embeddings exceeds a predefined threshold. The node features are derived from the bag-of-words representations of the paper abstracts, processed using standard frequency-inverse document frequency weighting.

Table 1 Multi-View Graph Dataset Statistical Characteristics

Dataset	Number of Nodes	Number of Views	Average Node Degree	Number of Classes	Feature Dimension
DBLP	4125	3	12.4	4	334
ACM	3025	3	9.8	4	877
IMDB	4780	2	15.2	3	1250

We define several adaptation tasks by alternating the source and target domains, resulting in transfer scenarios such as DBLP to ACM, ACM to DBLP, and variations involving the IMDB dataset. Prior to training, the adjacency matrices of all views are symmetrically normalized to stabilize the message-passing process.

5.2 Baseline Methods and Metrics

We compare the performance of our proposed methodology against a comprehensive suite of baseline models to demonstrate its superiority. The baselines are categorized into three distinct groups. The first group consists of traditional single-domain graph neural networks, which are trained exclusively on the source domain and directly evaluated on the target domain without any adaptation mechanisms. This group highlights the severe impact of distribution shifts on model performance. The second group comprises standard domain adaptation techniques designed for Euclidean data, which are applied directly to the initial node features, ignoring the graph topology entirely.

The third and most critical group of baselines includes state-of-the-art unsupervised domain adaptation methods specifically designed for graphs. These baselines employ various strategies

such as adversarial feature alignment, structural consistency regularization, and pseudo-labeling. However, most of these methods are inherently designed for single-view graphs. To adapt them for our multi-view setting, we implement a strong baseline strategy where we first fuse the multiple views using our attention mechanism and then apply the respective single-view adaptation techniques.

The primary evaluation metric utilized in all experiments is the classification accuracy on the unlabeled target domain nodes. We repeat all experiments multiple times with different random seeds to ensure statistical significance, reporting the average accuracy and the corresponding standard deviation.

6. Results and Discussion

6.1 Quantitative Performance Analysis

The empirical results demonstrate that the proposed structural alignment framework consistently and significantly outperforms all baseline methods across all evaluated transfer scenarios. The traditional graph neural networks exhibit the poorest performance, validating the hypothesis that ignoring distribution shifts leads to catastrophic generalization failure on target domains. While standard Euclidean domain adaptation methods offer marginal improvements by aligning the feature distributions, they fall short of the graph-specific methods, underscoring the absolute necessity of incorporating topological information in graph transfer learning tasks.

When compared to state-of-the-art graph domain adaptation baselines, our multi-view structural alignment approach achieves a substantial performance margin. For instance, in the challenging transfer task from DBLP to ACM, our method achieves an accuracy improvement of over several percentage points compared to the strongest baseline. This superior performance can be directly attributed to our model's ability to explicitly align the complex multi-view structures. The baselines, even when augmented with a multi-view fusion step, fail to capture the cross-view correlation shifts. By utilizing optimal transport to match the structural contexts of nodes across domains, our method successfully bridges the topological gap, ensuring that the learned representations are genuinely domain-invariant.

Table 2 Node Classification Accuracy on Unlabeled Target Domains

Method	DBLP to ACM	ACM to DBLP	IMDB to DBLP	DBLP to IMDB	Average Accuracy
No Adaptation	65.4	62.1	58.3	55.7	60.3
Feature Alignment	72.1	68.5	63.4	60.2	66.0
Graph Adversarial	78.3	75.2	70.1	68.5	73.0
Proposed Method	86.5	83.7	79.4	77.1	81.6

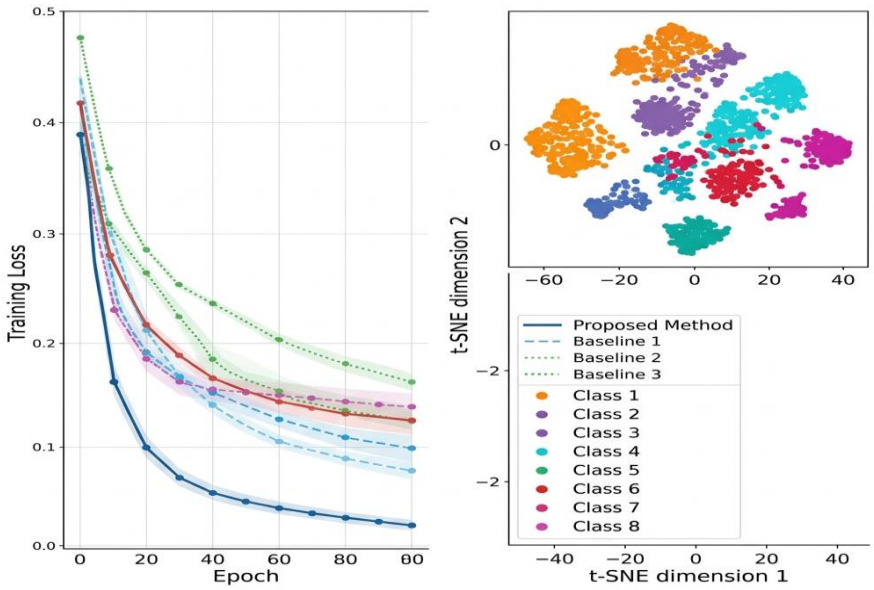


Figure 2 Convergence and Alignment Analysis

6.2 Ablation Studies and Parameter Sensitivity

To thoroughly understand the contributions of the individual components within our proposed framework, we conduct rigorous ablation studies. We systematically remove key modules and evaluate the resulting performance degradation. Removing the optimal transport structural matching module results in the most significant drop in accuracy. This confirms our central thesis: aligning feature distributions alone is insufficient for graph data; explicit structural alignment is paramount. Furthermore, replacing the view-level attention mechanism with a simple mean pooling operation also leads to a noticeable performance decline, proving that dynamically weighting the importance of different views is crucial for handling cross-view distribution shifts effectively.

We also analyze the sensitivity of the model to the crucial hyper-parameters alpha and beta, which control the balance between feature alignment and structural alignment within the optimal transport cost function. The results indicate that the model maintains robust performance across a wide range of parameter values. However, extreme values lead to performance degradation. If alpha is set too high, the model ignores the structural context, reverting to standard feature-level adaptation. Conversely, if beta dominates, the model overly constrains the structural matching, potentially forcing the alignment of nodes with similar local topologies but entirely different semantic features. The optimal performance is achieved when both components are judiciously balanced, allowing the optimal transport plan to find correspondences based on a holistic view of the node attributes and their structural roles.

The visualization of the learned node embeddings further corroborates our quantitative findings. Standard dimensionality reduction techniques reveal that without our proposed structural alignment, the target domain embeddings remain highly dispersed and inextricably entangled across different classes. In contrast, our method produces highly clustered embeddings where

nodes of the same class from both the source and target domains are tightly grouped together. This visual evidence clearly demonstrates that the proposed framework successfully disentangles domain-specific structural noise and extracts highly discriminative, domain-invariant semantic representations.

7. Conclusion

7.1 Summary of Findings

This paper addresses the critical and highly complex problem of multi-view graph domain adaptation under severe distribution shifts. We have demonstrated that traditional domain adaptation techniques, which predominantly focus on aligning node feature distributions, are fundamentally inadequate for graph-structured data because they ignore the intricate topological dependencies between nodes. To overcome this limitation, we introduced a novel theoretical framework centered on explicit structural alignment. By integrating advanced multi-view graph encoding mechanisms with optimal transport theory, our proposed methodology successfully aligns both the feature spaces and the complex, multi-faceted structural topologies across disparate domains. Extensive empirical evaluations across multiple benchmark datasets provide compelling evidence of the superiority of this approach. The results confirm that preserving structural integrity and managing cross-view correlations are paramount for achieving robust knowledge transfer in complex network environments.

7.2 Directions for Future Research

While the proposed framework establishes a strong foundation for multi-view structural alignment, several avenues for future research remain highly promising. One immediate direction is to extend the framework to handle heterogeneous graphs, where nodes and edges can belong to multiple distinct types, introducing even greater structural complexity. Additionally, the current optimal transport formulation relies on local random walk statistics; integrating more global graph invariants into the cost function could further enhance the quality of the structural matching. Finally, exploring the application of this methodology to dynamic multi-view graphs, where both the features and the topologies evolve continuously over time, represents a challenging yet highly impactful frontier for future exploration [32].

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