Appendix

A Distribution Shift in Graph-Structured Data

Distribution shift appears when the joint distribution differs between source domain and target domain [7, 69]. Assuming that the relationship between the input and class variables is unchanged, there are two kinds of distribution shift, i.e., covariate shift and label shift (prior probability shift) [70].

A.1 Covariate Shift

Covariate shift [71] refers to changes in the distribution of the input variables, which can be defined formally as follows:

Definition 1 (Covariate Shift)**.** Covariate shift appears when $\mathbb{P}_S(G) \neq \mathbb{P}_T(G)$ with the assumption of $\mathbb{P}_S(Y|G) = \mathbb{P}_T(Y|G)$, where $\mathbb{P}_S$ and $\mathbb{P}_T$ are the probability distributions of the source and target domains, respectively.

To deal with covariate shift, it is essential to align $\mathbb{P}_S(Y|H)$ and $\mathbb{P}_T(Y|H)$, where H is the representation after data attributes passing through the encoder. However, in graph-structured data, node representation is not only affected by the data attributes but also graph structure. Thus, covariate shift in graph data can be decoupled as feature shift and structure shift [26].

Definition 2 (Feature Shift)**.** Given the joint distribution of the node attributes and node labels $\mathbb{P}_T(X, Y)$, the feature shift is then defined as $\mathbb{P}_S(X, Y) \neq \mathbb{P}_T(X, Y)$ with the assumption of $\mathbb{P}_S(Y|G) = \mathbb{P}_T(Y|G)$.

Definition 3 (Structure Shift)**.** Given the joint distribution of the adjacency matrix and node labels $\mathbb{P}_T(A, Y)$, the structure shift is then defined as $\mathbb{P}_S(A, Y) \neq \mathbb{P}_T(A, Y)$ with the assumption of $\mathbb{P}_S(Y|G) = \mathbb{P}_T(Y|G)$.

A.2 Label Shift

Label shift refers to changes in the distribution of the class variable Y. It also appears with different names in the literature and the definitions have slight differences between them.

Definition 4 (Label Shift)**.** Label shift occurs when the distribution of labels changes across two domains, which is defined as $\mathbb{P}_S(Y) \neq \mathbb{P}_T(Y)$ where $\mathbb{P}_S(G|Y) = \mathbb{P}_T(G|Y)$.

In all, structure shift is unique to graph data due to the non-IID nature caused by node interconnections. Moreover, the learning of node representations implemented by the GNN will mix the feature shift, sutructure shift and label shift [32].

B Detailed Description of Datasets

In this section, we provide additional details about the datasets used in our benchmark.

B.1 Dataset Description

- **Airport**[2]: The Airport datasets consist of three separate collections corresponding to Brazil (B), Europe (E), and the USA (U). In these datasets, nodes represent airports and edges denote flight connections between them. The labels categorize airports by activity levels, measured in terms of flights or passenger numbers.
- **Blog**[3]: Blog1 and Blog2 are disjoint social networks derived from the BlogCatalog dataset. In these networks, nodes correspond to bloggers, and edges reflect friendships among them. The attributes for each node consist of keywords from the blogger's self-description, and each node is assigned a label denoting its group affiliation. Given that both Blog1 and Blog2 originate from the same underlying network, their data distributions are nearly identical.

[2]https://github.com/GentleZhu/EGI/tree/main/data

[3]https://github.com/shenxiaocam/ACDNE/tree/master/ACDNE_codes/input

Table 7: Dataset Statistics.

Dataset	# Domains	# Nodes	# Edges	# Homo	# Avg Degree	# Feat Dims	# Labels
Airport	USA (U)	1,190	27,198	0.6978	22.86	241	4
	BRAZIL (B)	131	2,148	0.4683	16.40		
	EUROPE (E)	399	11,990	0.4048	30.05		
Blog	Blog1 (B1)	2,300	66,942	0.3991	29.11	8,189	6
	Blog2 (B2)	2,896	107,672	0.4002	37.18		
ArnetMiner	DBLPv7 (D)	5,484	16,234	0.8198	2.96	6,775	5
	ACMv9 (A)	9,360	31,112	0.7998	3.32		
	Citationv1 (C)	8,935	30,196	0.8598	3.38		
Twitch	England (EN)	7,126	35,324	0.5560	4.96	3,170	2
	Germany (DE)	9,498	153,138	0.6322	16.14		
	France (FR)	6,549	112,666	0.5595	17.20		
	Russia (RU)	4,385	37,304	0.6176	8.51		
	Spain (ES)	4,648	59,382	0.5800	12.78		
	Porutgal (PT)	1,912	31,299	0.5708	16.40		
MAG	China (CN)	101,952	285,991	0.5307	2.81	128	20
	Germany (DE)	43,032	127,704	0.5311	2.97		
	France (FR)	29,262	79,182	0.5732	2.71		
	Janpan (JP)	37,498	91,412	0.5645	2.44		
	Russia (RU)	32,833	68,294	0.7682	2.08		
	USA (US)	132,558	702,482	0.5174	5.30		

- **ArnetMiner**[4]: These datasets comprise paper citation networks sourced from three distinct origins as provided by ArnetMiner [72]: "ACMv9" (A), "Citationv1" (C), and "DBLPv7" (D). Each dataset's nodes symbolize papers, while edges reflect their citation relationships. Specifically, "ACMv9" (A) includes papers from ACM spanning 2000 to 2010, "Citationv1" (C) consists of papers from the Microsoft Academic Graph up to 2008, and "DBLPv7" (D) contains papers from DBLP collected between 2004 and 2008. The aim is to categorize all papers into five specific research areas: Databases, Artificial Intelligence, Computer Vision, Information Security, and Networking.
- **Twitch**[5]: Twitch gamer networks from six regions—Germany (DE), England (EN), Spain (ES), France (FR), Portugal (PT), and Russia (RU)—comprise nodes representing users and connections that signify friendships among them. Node features include data on users' preferred games, geographical location, and streaming habits, among others. Users within these networks are categorized into two groups based on their use of explicit language.
- **MAG**[6]: The MAG dataset, a subset of the Microsoft Academic Graph, is a heterogeneous network featuring four distinct types of entities: papers (736,389 nodes), authors (1,134,649 nodes), institutions (8,740 nodes), and fields of study (59,965 nodes). It includes four varieties of directed relationships linking pairs of entity types: an author's affiliation with an institution, an author's authorship of a paper, paper citations, and papers' association with fields of study. Each paper node is enriched with a 128-dimensional word2vec feature vector, while the other entities lack input node features. The primary task within this dataset involves predicting the publication venue (conference or journal) for each paper, leveraging information about its content, cited references, authors, and the affiliations of these authors. Following PairAlign [26], we split the original dataset into six countries.

B.2 Shift Statistics of Datasets

According to dataset statistics, shown in Table 7 and Figure 4, we measure the degree of domain shift exhibited in the datasets for each tasks using statistical methods. We use MMD [41], CSS [26], Kullback-Leibler Divergence to characterize the degree of feature shift, structure shift and label shift. The results of each tasks is shown in Table 13. We take the average results of all tasks as the shift statistics for the datasets, shown in Table 8. The 74 tasks compiled by the five carefully selected datasets can cover all combinations of domain shift scenarios.

[4]https://github.com/yuntaodu/ASN/tree/main/data
[5]http://snap.stanford.edu/data/twitch-social-networks.html
[6]https://zenodo.org/records/10681285

Table 8: Domain shifts statistics of GDABench datasets.

Dataset	Size	Feature Shift	Structure Shift	Label Shift	Domain Num
Blog	S	0.0132	0.0802	0.2532	2
Airport	S	0	0.2769	0.0351	3
ArnetMiner	M	0.0241	0.2074	1.1519	3
Twitch	M	0.0468	0.3264	8.6949	6
MAG	L	0.0499	0.3960	25.7725	6

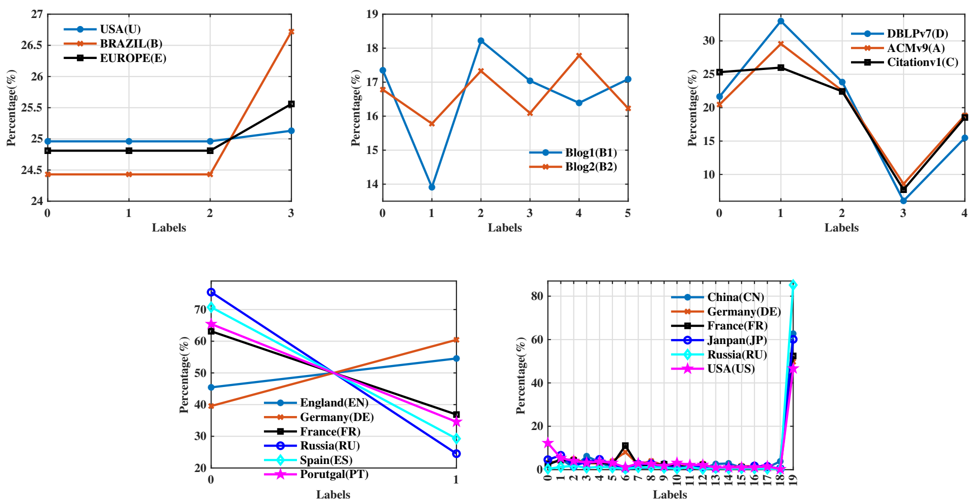


Figure 4: Label distribution of GDABench datasets.

- **Feature shift determined**: Tasks ES → PT, PT→ES, EN→DE, ED→EN, FR→ES, FR→PT, ES→FR, PT→FR, RU→ES, ES→RU, RU→PT, PT→RU, RU→FR and FR→RU in Twitch. Tasks JP→US, US→JP, JP→CN and CN→JP in MAG.
- **Sturcture shift determined**: Tasks E→B, B→E, U→B, B→U, U→E and E→U in Airport. Tasks GP→DE and US→DE in MAG. Tasks FR→DE, RU→EN, RU→DE, ES→DE, EN→RU, DE→RU, DE→ES and DE→PT in Twitch.
- **Lable shift determined**: Task FR→DE in MAG.
- **Determined by both feature and structure shift**: Tasks D→A, D→C, A→D and C→D in ArmetMiner. Tasks FR→EN, EN→FR, PT→EN, EN→PT, DE→FR, FR→DE, PT→DE and EN→ES in Twitch. Tasks JP→FR, RU→PT, RU→CN and DE→JP in MAG.
- **Determined by both feature and label shift**: Tasks EN→US, US→EN in MAG.
- **Determined by both structure and label shift**: Tasks DE→US, FR→US, US→FR, FR→RU in MAG.
- **All shifts effects**: Tasks B1→B2 and B2→B1 in Blog. Tasks A→C and C→A in ArnetMiner. Tasks DE→FR, CN→FR, JP→RU, RU→FR, CN→RU, FR→JP, RU→DE, CN→DE, RU→US, DE→CN, FR→CN, DE→RU and US→RU in MAG.

C GDA Baselines

MLP, GCN [47], GAT [49], and GIN [50] are classical GNN models. We directly adopt the implementation from Pytorch Geometric. The publicly available implementations of baselines can be found at the following URLs:

- **DANE** [10] uses shared weight GCNs to get node representations and then handles distribution shift via least square generative adversarial network. The source code is available at `https://github.com/Jerry2398/DANE-Simple-implementation`.

Figure 5: The compared performance of vanilla DA with 6 GNN variants.

- **ACDNE** [11] utilizes two feature extractors to jointly preserve attributed affinity and topological proximities as deep network embedding module and incorporates a domain classifier to make node representations label-discriminative. The source code is available at `https://github.com/shenxiaocam/ACDNE`.
- **UDAGCN** [12] develops a dual graph convolutional network with attention mechanism to jointly exploit local and global consistency for effective graph representation learning. The source code is available at `https://github.com/GRAND-Lab/UDAGCN`.
- **ASN** [44] separates domain-private and domain-shared information and combines local and global consistency to capture network topology information. The source code is available at `https://github.com/yuntaodu/ASN`.
- **AdaGCN** [13] leverages GCN to integrate network topology and combines adversarial domain adaptation with graph convolution. The source code is available at `https://github.com/daiquanyu/AdaGCN_TKDE`.
- **StruRW** [17] investigates different types of distribution shifts of graph-structured data and reweights edges in the source graph to reduces the conditional shift of neighborhoods. The source code is available at `https://github.com/Graph-COM/StruRW`.
- **GRADE** [15] introduces graph subtree discrepancy as a metric to measure the graph distribution shift by connecting GNNs with WL subtree kernel [45]. The source code is available at `https://github.com/jwu4sml/GRADE`.
- **SpceReg** [16] finds the OT-based bound for graph is closely coupled with the Lipschitz constant of GNN and proposes spectral regularization to modulate the Lipschitz constant to restrict the target risk bound. The source code is available at `https://github.com/Shen-Lab/GDA-SpecReg`.
- **A2GNN** [25] further investigates the GNN's underlying generalization capability behind its architecture and finds propagation operation plays a pivotal role. Based on this observation, A2GNN proposes a simple yet effective GNN which stacks more propagation layers on target branch. The source code is available at `https://github.com/Meihan-Liu/24AAAI-A2GNN`.
- **JHGDA** [18] designs a hierarchical pooling model to extract meaningful and adaptive hierarchical structures and jointly minimizes marginal and class conditional distribution shifts on each hierarchical level. The source code is available at `https://github.com/Skyorca/JHGDA`.
- **KBL** [19] redefines the aggregate mechanism as learning a knowledge-enhanced posterior distribution for target domains, which learns the scope of knowledge transfer by connecting knowledgeable samples between domains. The source code is available at `https://github.com/wendongbi/Bridged-GNN`.
- **DMGNN** [21] employs a GNN encoder with dual feature extractors to separate ego-embedding learning from neighbor-embedding learning and then a label propagation node classifier is employed

Table 9: We evaluated the Micro-F1 score on Airport and ArnetMiner.

Models	Airport				ArnetMiner			
	B → E	B → U	E → B	U → B	A → C	A → D	C → D	D → C
DANE	33.00	41.23	41.98	39.44	64.40	62.52	66.13	71.30
ACDNE	46.45	56.30	55.73	64.12	79.07	74.27	75.47	79.06
UDAGCN	43.78	35.49	45.29	37.91	78.21	72.98	76.14	72.15
ASN	53.05	46.58	62.34	49.36	78.68	72.02	75.57	77.58
AdaGCN	50.63	43.47	60.56	61.32	73.87	66.91	72.56	71.20
DMGNN	33.92	29.92	35.37	34.10	81.59	76.62	76.77	80.65
CWGCN	46.37	46.58	58.78	44.27	80.00	74.29	76.23	76.95
SAGDA	35.51	37.76	47.33	48.35	77.5	70.56	74.03	59.49
DGDA	49.71	33.56	44.02	49.36	64.48	57.85	63.29	57.98
StruRW	56.06	43.36	65.65	61.32	77.24	67.51	74.37	73.96
KBL	45.28	45.52	51.40	33.84	77.71	69.16	74.48	74.62
JHGDA	48.87	40.59	65.14	43.51	73.74	69.13	71.71	71.59
PairAlign	39.93	42.18	51.91	54.96	68.29	61.80	62.89	63.28
GRADE	52.88	49.22	75.83	49.62	74.09	69.18	72.57	73.12
SpecReg	48.87	44.20	63.36	40.97	80.81	73.16	74.60	71.96
A2GNN	53.13	54.54	62.34	59.29	82.64	77.43	78.13	81.54
SimGDA	55.64	53.11	60.31	62.60	79.91	75.16	75.95	77.31
SimGDA+	58.40	57.56	72.14	67.18	82.97	76.60	77.50	82.09

to refine label prediction. The source code is available at `https://github.com/shenxiaocam/DM_GNN`.

- **CWGCN** [22] puts forward a two-step correntropy-induced Wasserstein GCN, which first suppresses the noisy nodes in the source graph and then learns the target GCN based on extending the Wasserstein distance. The source code is available at `https://github.com/CocoLab-2022/CW-GCN`.
- **SAGDA** [23] proposes a spectral augmentation module to enhance the node representation learning, which combines the target domain spectral information within the source domain. Since the authors did not release the source code, we try our best to reproduce their results.
- **DGDA** [24] addresses graph domain adaptation in a generative view, which disentangles the generation process into the semantic latent variables, the domain latent variables, and the random latent variables. The source code is available at `https://github.com/rynewu224/GraphDA`.
- **PairAlign** [26] not only uses edge weights to recalibrate the influence among neighboring nodes to handle conditional structure shift but also adjusts the classification loss with label weights to handle label shift. The source code is available at `https://github.com/Graph-COM/Pair-Align`.

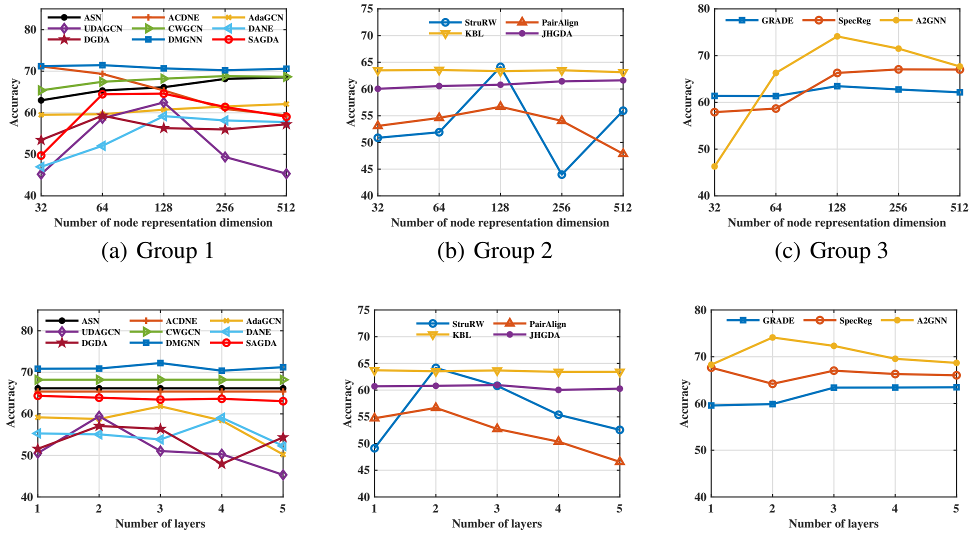
D Other Information in GDABench

We implement our GDABench library in PyTorch [73] and provide an infrastructure to run all the experiments to generate corresponding results. We have stored all models and logged all hyperparameters to facilitate reproducibility. Our framework can be easily extended to include new algorithms.

D.1 Metrics

Following previous works [44, 12], we present the experiment performance on target domain. We select Area Under the Receiver Operating Characteristic Curve (AUROC) for Twitch, Micro-F1 for Airport, Blog and ArnetMiner and Macro-F1 for MAG.

- **AUROC** measures how well a model can distinguish between positive and negative classes by looking at the area under the ROC curve. This curve shows the true positive rate versus the false positive rate at various thresholds. An AUROC score of 1 means perfect distinction, while a score of 0.5 indicates the model does no better than guessing randomly.
- **Macro-F1** calculates the F1 score for each category independently and then taking the average of these scores. This method treats all categories equally, regardless of their frequency in the dataset.



(a) Group 1 (b) Group 2 (c) Group 3

(d) Group 1 (e) Group 2 (f) Group 3

Figure 6: The impact of node representation dimension and the number of layers on ArnetMiner dataset (D→A). We classify all baselines into three groups: DA incorporated node embedding methods (Group 1), structure shift directed alignment (Group 2) and domain adaptive message passing (Group 3). The first row illustrates the impact of node representation dimension, while the second row presents the effect of the number of layers.

It is particularly useful when you want to understand the model's performance across smaller or less frequent categories, ensuring that performance on rare categories has as much weight as performance on more common ones.

- **Micro-F1** computes the average F1 score. This is achieved by summing up the true positives, false positives, and false negatives of the model across all categories and then calculating the F1 score using these totals. As a result, Micro-F1 gives a higher weight to the performance on more frequent categories, making it a useful metric when you're interested in understanding how the model performs on the majority of cases or the overall dataset.

D.2 Additional Experimental Details

- **Hardware Specifications.** The experiments were conducted on a Linux server equipped with an Intel(R) Xeon(R) Platinum 8163 CPU operating at 2.50GHz, running Ubuntu 18.04.5 LTS. For GPU resources, we utilized a single NVIDIA Tesla V100 graphics card with 32GB of memory. The Python libraries employed for implementing our experiments include Python 3.8, PyTorch 1.13.1, PyTorch Geometric 2.4.0, PyTorch Sparse 0.6.15, and PyTorch Scatter 2.1.0.
- **Hyperparameter Settings.** To control the effect of hyperparameter selection and ensure fairness, we standardize the evaluation process with hyperparameter tuning. We utilize grid search to form the predefined search space for each models. We use all the source nodes and target nodes for model training. The experiments are repeated three times, and we report the mean performance. Table 14 provides a comprehensive list of all hyperparameters used in our grid search.
- **More Experimental Results.** In accordance with Table 2 and 3, we provide the performance for all tasks of each model in Table 9, 11 and 12. In accordance with Figure 3, we provide the compared performance of vanilla DA with 6 GNN variants in Figure 5.
- **Exploration of Hyperparameter Impact.** We investigate how various hyperparameters in common modules influence the performance of different UGDA methods on ArnetMiner dataset (task D → A). We focus on two key aspects: the number of GNN layers and the representation dimensions. Results are shown in Figure 6.
- **Running Time and Memory Consumption.** We also demonstrate the running time and memory consumption of each model on S/M/L datasets respectively. For time consumption, we evaluate the

efficiency of baselines by measuring the time it takes to converge. As shown in Figure 7, we can observe that some algorithms (e.g. A2GNN) can achieve relatively good performance with less complexity.

D.3 The PyGDA Library

PyGDA is a Python library for Graph Domain Adaptation built upon PyTorch and PyG to easily train graph domain adaptation models in a sklearn style. PyGDA includes 15+ graph domain adaptation models. See examples with PyGDA below!

Graph Domain Adaptation Using PyGDA with 5 Lines of Code

```
from pygda.models import A2GNN

# choose a graph domain adaptation model
model = A2GNN(in_dim=num_features, hid_dim=args.nhid,
num_classes=num_classes, device=args.device)

# train the model
model.fit(source_data, target_data)

# evaluate the performance
logits, labels = model.predict(target_data)
```

PyGDA is featured for:

- Consistent APIs and comprehensive documentation.
- Cover 15+ graph domain adaptation models.
- Scalable architecture that efficiently handles large graph datasets through mini-batching and sampling techniques.
- Seamlessly integrated data processing with PyG, ensuring full compatibility with PyG data structures.

E Experiments on Graph Classification

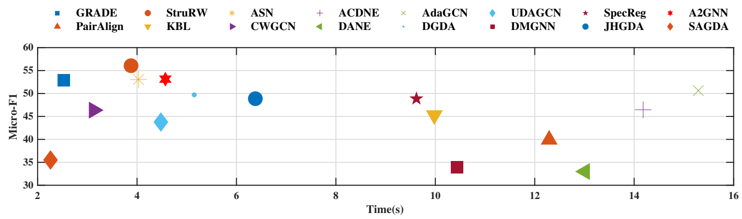
To expand our research scope, we take graph-level shifts into consideration and add a pooling layer to evaluate capabilities of baselines in graph-level domain adaptation. We employ three TUdatasets: Proteins, Mutagenicity, and Frankenstein, partitioning each dataset into 2 equally sized disjoint groups based on density shifts. Detailed statistics are shown in Table 10.

Table 10: Statistics of graph-level datasets in GDABench.

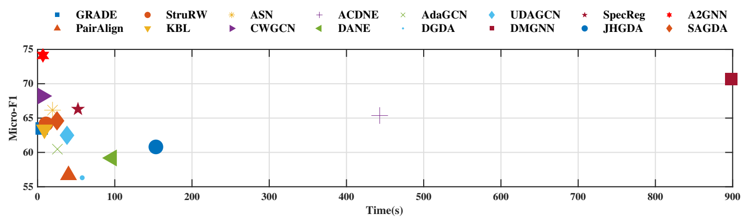
Dataset	# Nodes	# Edges	# Feature	# Class	Num of graphs
Proteins	39.06	72.82	4	2	1,113
Mutagenicity	30.32	30.77	14	2	4,337
Frankenstein	16.90	17.88	780	2	4,337

The results are detailed in Table 15 and Table 16. Among the methods, GRADE and A2GNN are domain adaptive message passing methods and the remaining are DA incorporated node embedding methods. Key observations are as follows:

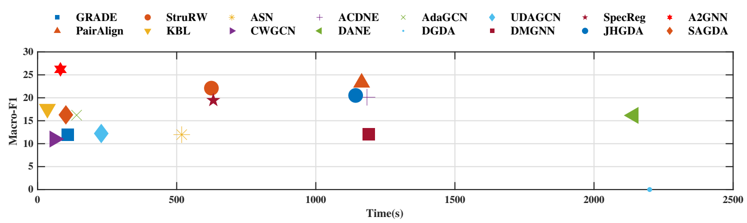
DA incorporated node embedding methods shows task-inconsisteny across node and graph-level tasks. For example, DANE performs averagely in node-level tasks, but its performance improves significantly in graph-level tasks. This disparity highlights a challenge in predicting the performance of unsupervised graph domain adaptation (UGDA) models in real-world applications. The inconsistency suggests that models optimized for node-level tasks may not generalize well to graph-level tasks and



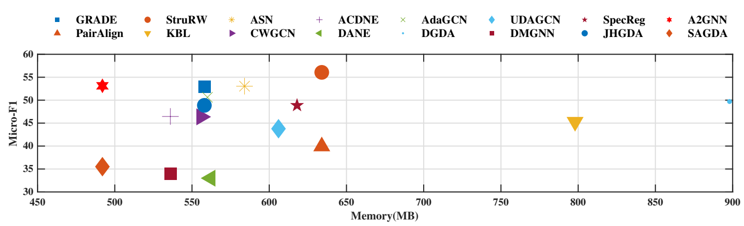
(a) Running time of B → U in Airport.



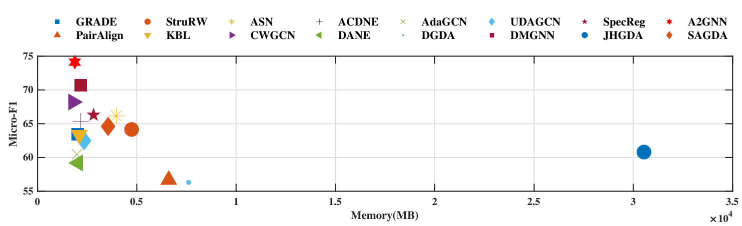
(b) Running time of D → A in ArnetMiner.



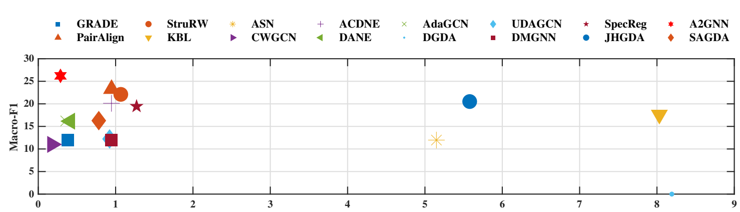
(c) Running time of FR → JP in MAG.



(d) Memory consumption of B → U in Airport.



(e) Memory consumption of D → A in ArnetMiner.



(f) Memory consumption of FR → JP in MAG.

Figure 7: Running time and memory consumption of baselines.

Table 11: We evaluated the AUROC score on Twitch.

Models	DE → EN	DE → FR	EN → DE	EN → ES	EN → FR	EN → PT	EN → RU	ES → DE	ES → EN
DANE	56.95	59.67	67.10	60.67	62.29	62.11	53.64	64.37	58.96
ACDNE	51.29	53.61	52.78	52.83	53.45	52.52	50.65	56.21	55.96
UDAGCN	54.70	54.51	56.95	53.80	54.64	51.55	50.76	55.35	56.58
ASN	51.00	51.79	55.17	53.95	50.64	54.56	51.01	56.96	54.64
AdaGCN	51.64	57.33	56.28	53.05	52.37	56.23	50.52	59.02	56.34
DMGNN	53.08	51.44	53.94	53.70	51.09	52.09	50.46	51.90	52.41
CWGCN	54.85	52.81	60.47	56.97	51.14	60.09	52.52	65.00	56.66
SAGDA	54.39	53.58	54.82	51.99	54.75	52.57	50.95	54.48	53.34
DGDA	56.67	52.63	62.77	60.47	56.37	57.75	52.25	62.64	54.00
StruRW	51.31	56.26	51.87	58.65	51.68	59.41	52.92	58.60	53.90
KBL	52.01	63.93	66.43	60.34	61.01	52.48	55.42	68.86	61.87
JHGDA	57.50	59.04	62.43	57.67	56.96	56.85	51.16	52.22	53.36
PairAlign	51.05	52.12	52.13	51.93	51.62	51.52	50.56	59.86	53.18
GRADE	53.66	57.61	52.31	50.77	53.04	54.60	50.49	62.48	57.54
SpecReg	54.67	54.55	58.35	51.94	54.88	50.70	51.02	59.18	55.43
A2GNN	53.84	51.17	53.45	59.31	51.15	53.43	52.64	52.42	53.24
SimGDA	58.64	57.91	59.21	58.48	55.97	57.73	52.95	60.03	53.98
SimGDA+	58.64	59.97	63.01	60.34	59.44	60.06	53.67	63.61	57.69

Models	ES → FR	ES → PT	ES → RU	FR → DE	FR → EN	FR → ES	FR → PT	FR → RU	PT → DE
DANE	55.36	62.22	51.71	65.58	57.48	58.45	53.49	50.43	57.66
ACDNE	52.55	53.61	51.74	54.68	53.91	52.76	54.33	51.57	52.82
UDAGCN	52.49	62.08	52.49	56.71	56.52	59.47	58.27	54.37	53.78
ASN	53.02	55.38	51.68	55.55	53.03	53.49	51.39	51.20	55.38
AdaGCN	53.82	62.24	52.93	59.52	57.47	61.22	56.42	51.37	57.82
DMGNN	50.07	50.71	51.06	51.72	52.51	51.86	50.76	51.21	51.65
CWGCN	50.92	61.59	51.83	62.45	56.55	58.15	60.44	52.87	58.30
SAGDA	53.42	52.36	50.70	54.34	54.69	51.25	52.66	50.92	55.11
DGDA	54.95	51.72	50.95	62.74	57.39	61.17	60.90	52.12	59.19
StruRW	53.70	53.74	52.17	56.96	53.62	56.29	51.23	51.38	55.85
KBL	63.05	62.26	55.29	64.37	60.01	63.02	62.08	54.03	66.22
JHGDA	51.62	53.98	51.01	57.57	53.98	56.94	55.36	50.92	51.35
PairAlign	54.07	50.95	52.60	53.88	53.81	53.28	51.93	52.05	54.10
GRADE	57.72	60.46	53.56	59.25	56.58	55.08	55.71	50.34	57.54
SpecReg	55.00	50.81	51.52	59.58	55.50	54.05	50.89	51.08	56.18
A2GNN	51.39	54.59	50.34	53.38	54.05	53.89	53.91	50.63	52.27
SimGDA	54.05	61.91	60.35	61.09	56.00	65.66	60.93	62.65	59.47
SimGDA+	59.73	62.07	60.37	62.99	58.08	65.96	61.57	62.85	61.23

Models	PT → EN	PT → ES	PT → FR	PT → RU	RU → DE	RU → EN	RU → ES	RU → FR	RU → PT
DANE	55.74	53.11	51.90	52.46	68.75	59.79	59.34	57.42	66.34
ACDNE	54.34	54.46	52.51	51.52	52.46	51.32	53.05	50.96	50.78
UDAGCN	53.01	57.08	51.63	51.19	54.74	51.32	51.30	53.21	55.47
ASN	52.13	52.03	52.80	51.71	51.97	52.87	51.86	51.24	51.77
AdaGCN	51.80	58.28	53.98	51.23	58.35	54.78	57.76	54.35	57.23
DMGNN	52.63	51.89	50.20	50.83	52.21	52.69	52.43	50.34	51.29
CWGCN	52.39	55.46	54.98	51.58	61.25	57.48	54.90	50.46	62.36
SAGDA	53.92	51.58	53.92	50.37	54.84	53.62	51.41	53.83	52.67
DGDA	54.64	50.74	55.66	52.51	62.34	57.31	60.86	56.15	60.88
StruRW	52.78	53.50	53.96	50.77	52.27	51.77	52.73	50.67	51.03
KBL	56.53	64.56	52.92	53.16	59.17	55.15	59.35	58.15	59.23
JHGDA	51.38	54.64	52.12	51.36	55.20	51.37	51.12	55.43	54.31
PairAlign	53.97	53.79	54.42	50.88	52.29	50.94	52.87	50.90	50.80
GRADE	54.52	57.04	55.15	50.14	50.22	53.90	60.48	57.54	55.08
SpecReg	53.12	53.34	51.71	50.13	58.77	53.59	52.17	55.42	51.01
A2GNN	50.49	53.80	50.99	51.21	51.54	52.15	54.70	51.60	53.53
SimGDA	55.48	60.17	63.02	54.20	51.16	51.43	55.31	52.64	62.27
SimGDA+	57.57	61.29	63.07	55.20	61.96	56.14	59.17	56.47	62.78

Table 12: We evaluated the Macro-F1 score on MAG. OOM indicates out of memory.

Models	CN → DE	CN → FR	CN → JP	CN → RU	CN → US	DE → CN	DE → FR	DE → JP	DE → RU
DANE	OOM	12.56	19.50	11.04	OOM	OOM	23.44	22.53	14.84
ACDNE	12.18	10.41	10.08	8.57	13.40	16.08	20.99	18.07	13.95
UDAGCN	12.84	6.85	10.69	7.32	12.23	15.01	23.26	21.82	14.48
ASN	9.52	OOM	OOM	OOM	10.64	14.67	24.08	22.60	13.99
AdaGCN	7.63	10.51	12.36	10.65	9.30	10.75	14.79	12.85	10.47
DMGNN	OOM	7.64	11.18	6.99	OOM	12.11	17.82	11.52	11.43
CWGCN	OOM	10.62	10.58	10.20	OOM	11.00	13.95	12.63	9.59
SAGDA	OOM	6.14	9.05	6.09	OOM	OOM	OOM	OOM	OOM
DGDA	OOM	OOM	OOM	OOM	OOM	OOM	19.66	18.70	11.94
StruRW	3.32	3.54	3.75	4.59	7.69	10.55	4.94	6.08	4.63
KBL	15.79	14.03	16.53	11.69	16.98	13.14	19.51	17.26	12.60
JHGDA	OOM	OOM	OOM	OOM	OOM	OOM	25.10	21.69	12.52
PairAlign	10.52	20.90	18.70	12.13	9.33	11.53	17.61	13.80	12.45
GRADE	11.72	11.06	13.18	10.14	12.54	11.21	17.30	14.06	10.43
SpecReg	19.42	12.11	13.85	11.64	22.23	23.22	30.80	28.13	17.89
A2GNN	22.59	18.44	22.22	13.37	25.23	19.75	24.15	24.16	12.19
SimGDA	12.20	11.42	13.83	11.40	14.09	14.55	19.53	17.53	13.28
SimGDA+	21.28	18.25	22.50	13.96	23.16	18.50	25.39	24.60	15.47

Models	DE → US	FR → CN	FR → DE	FR → RU	FR → US	JP → CN	JP → DE	JP → US	RU → CN
DANE	OOM	15.77	22.11	12.92	16.38	16.59	20.21	OOM	7.35
ACDNE	18.04	14.20	20.47	14.60	14.79	14.89	15.79	15.96	6.73
UDAGCN	25.24	16.27	25.97	8.47	24.25	17.34	21.31	18.57	8.70
ASN	23.11	15.22	25.62	10.92	21.22	15.36	22.27	20.77	8.88
AdaGCN	10.48	9.27	12.73	12.34	9.17	9.99	9.97	9.63	4.36
DMGNN	12.65	11.52	16.84	9.89	12.94	11.62	14.45	11.39	4.10
CWGCN	10.78	OOM	0.19	11.16	10.33	9.93	9.39	9.44	4.74
SAGDA	OOM	OOM	OOM	2.98	OOM	OOM	OOM	OOM	OOM
DGDA	OOM	OOM	15.80	OOM	OOM	OOM	12.51	OOM	OOM
StruRW	12.16	15.67	15.27	14.65	25.45	8.30	6.59	20.05	5.65
KBL	13.94	14.08	18.06	13.88	13.39	14.61	16.24	17.40	12.49
JHGDA	OOM	OOM	24.23	12.88	OOM	OOM	21.96	0.00	0.00
PairAlign	13.44	8.67	15.78	12.49	11.65	12.99	12.49	12.87	4.51
GRADE	12.52	10.92	16.94	9.56	12.57	11.98	11.64	13.95	4.09
SpecReg	29.09	22.49	31.57	14.33	28.01	25.54	28.97	30.30	17.65
A2GNN	27.67	20.95	28.57	16.13	28.51	21.71	25.53	27.14	18.91
SimGDA	16.84	13.53	18.83	12.51	16.01	14.21	14.66	15.04	6.36
SimGDA+	26.37	17.72	28.91	15.09	26.35	19.99	25.43	24.22	15.05

Models	RU → DE	RU → FR	RU → JP	RU → US	US → CN	US → DE	US → FR	US → JP	US → RU
DANE	7.75	6.17	8.47	6.57	OOM	OOM	22.27	OOM	OOM
ACDNE	5.98	6.12	7.42	5.93	20.63	22.48	19.65	23.90	14.86
UDAGCN	8.42	7.96	8.92	8.38	19.01	28.24	25.17	25.80	15.37
ASN	9.69	9.73	8.99	10.88	15.99	24.52	21.09	22.93	12.27
AdaGCN	3.59	3.73	4.25	3.26	14.80	15.95	14.40	18.34	10.99
DMGNN	3.69	4.34	4.42	3.22	OOM	OOM	OOM	OOM	OOM
CWGCN	3.32	3.76	4.60	4.61	15.11	15.54	13.41	16.85	11.59
SAGDA	OOM	5.61	OOM	OOM	0.00	0.00	0.00	0.00	0.00
DGDA	4.17	4.52	6.98	OOM	0.00	0.00	0.00	0.00	0.00
StruRW	4.88	3.44	4.31	4.79	8.44	10.61	3.44	6.37	7.44
KBL	11.52	9.35	12.92	11.49	16.62	19.67	17.90	19.25	12.69
JHGDA	19.85	16.67	19.15	OOM	OOM	OOM	OOM	OOM	OOM
PairAlign	3.61	4.21	4.60	3.51	16.12	17.85	16.66	19.28	11.93
GRADE	3.32	3.47	4.01	3.18	16.30	16.28	17.02	21.42	11.83
SpecReg	18.66	16.51	21.35	16.02	26.23	31.82	28.81	30.12	16.23
A2GNN	22.67	20.36	20.90	22.24	21.47	27.42	25.29	25.43	13.06
SimGDA	6.09	6.21	7.48	6.33	18.37	11.31	10.59	22.19	14.31
SimGDA+	20.35	16.84	20.06	20.65	21.17	26.94	24.23	25.58	15.62

Table 13: Domain shifts statistics of each task.

Dataset	Source	Target	Feature Shift	Structure Shift	Label Shift
Blog	Blog1	Blog2	0.0140	0.0802	0.253
	Blog2	Blog1	0.0137	0.0802	0.258
Airport	USA	BRAZIL	0.0514	0.2331	0.065
	USA	EUROPE	0.0913	0.3983	0.005
	BRAZIL	USA	0.0523	0.2331	0.066
	BRAZIL	EUROPE	0.0549	0.1993	0.035
	EUROPE	USA	0.1000	0.3983	0.005
	EUROPE	BRAZIL	0.0582	0.1993	0.034
ArnetMiner	DBLPv7	ACMv9	0.0312	0.2327	0.997
	DBLPv7	Citationv1	0.0245	0.1965	1.643
	ACMv9	DBLPv7	0.0305	0.2327	1.062
	ACMv9	Citationv1	0.0163	0.1931	0.780
	Citationv1	DBLPv7	0.0244	0.1965	1.624
	Citationv1	ACMv9	0.0166	0.1931	0.805
Twitch	EN	DE	0.0493	0.1486	0.715
	EN	FR	0.0440	0.3148	6.449
	EN	RU	0.0368	0.5960	20.578
	EN	ES	0.0530	0.3836	13.883
	EN	PT	0.0790	0.3374	8.330
	DE	EN	0.0478	0.1486	0.707
	DE	FR	0.0408	0.4635	11.403
	DE	RU	0.0387	0.7446	28.985
	DE	ES	0.0283	0.5323	20.866
	DE	PT	0.0391	0.4860	13.871
	FR	EN	0.0463	0.3148	6.315
	FR	DE	0.0383	0.4635	11.302
	FR	RU	0.0503	0.2811	3.754
	FR	ES	0.0432	0.0688	1.335
	FR	PT	0.0733	0.0226	0.115
	RU	EN	0.0369	0.5960	18.693
	RU	DE	0.0355	0.7446	26.658
	RU	FR	0.0542	0.2811	3.479
	RU	ES	0.0426	0.2124	0.562
	RU	PT	0.0551	0.2586	2.363
	ES	EN	0.0525	0.3836	13.080
	ES	DE	0.0282	0.5323	19.901
	ES	FR	0.0406	0.0688	1.284
	ES	RU	0.0460	0.2124	0.583
	ES	PT	0.0320	0.0462	0.640
	PT	EN	0.0776	0.3374	8.080
	PT	DE	0.0407	0.4860	13.620
	PT	FR	0.0713	0.0226	0.114
	PT	RU	0.0554	0.2586	2.526
	PT	ES	0.0311	0.0462	0.660
MAG	CN	DE	0.0750	0.3608	33.807
	CN	FR	0.0773	0.3902	26.427
	CN	JP	0.0451	0.2775	16.382
	CN	RU	0.0779	0.5454	30.058
	CN	US	0.0781	0.2858	28.992
	DE	CN	0.0727	0.3608	46.271
	DE	FR	0.0213	0.2041	2.316
	DE	JP	0.0464	0.3278	22.811
	DE	RU	0.0419	0.4778	48.632
	DE	US	0.0179	0.3561	16.266
	FR	CN	0.0702	0.3902	46.780
	FR	DE	0.0196	0.2041	2.241
	FR	JP	0.0508	0.3815	30.343
	FR	RU	0.0382	0.5091	49.558
	FR	US	0.0187	0.4210	23.644
	JP	CN	0.0486	0.2775	14.352
	JP	DE	0.0391	0.3278	12.240
	JP	FR	0.0467	0.3815	13.597
	JP	RU	0.0513	0.4968	27.544
	JP	US	0.0540	0.2893	8.235
	RU	CN	0.0776	0.5454	18.701
	RU	DE	0.0442	0.4778	31.345
	RU	FR	0.0416	0.5091	28.260
	RU	JP	0.0524	0.4968	18.269
	RU	US	0.0517	0.6171	35.979
	US	CN	0.0832	0.2858	35.273
	US	DE	0.0206	0.3561	14.702
	US	FR	0.0197	0.4210	19.245
	US	JP	0.0431	0.2893	10.104
	US	RU	0.0567	0.6171	60.803

Table 14: Parameter search space list.

Dataset	Models		Hyperparameter	Search Space
Airport	SimGDA+	SimGDA	learning rate	[0.0001, 0.0005, 0.001, 0.005]
			weight decay	[0.0001, 0.0005, 0.001, 0.005]
			momentum	[0.01, 0.99]
			backbone	gcn
			backbone layers	[1, 3, 4, 5]
			dropout ratio	0.5
			feature dimension	128
			alpha	[0.5, 1]
			epochs	200
		SimGDA + IM	beta	[0, 0.05, 0.1, 0.5]
			epochs	200
		SimGDA + AE	beta	[0, 0.05, 0.1, 0.5]
			decoder dropout	0.1
		SimGDA + CL	beta	[0, 0.05, 0.1, 0.5]
			epochs	500
			augment dropout	[0.1, 0.9]
			temperature	[0.1, 0.9]
	GDABench Baselines		learning rate	[0.0001, 0.001, 0.003]
			weight decay	[0.0001, 0.001, 0.003, 0.01]
			backbone layers	[1, 2, 3, 4, 5]
			dropout ratio	[0.1, 0.2, 0.3, 0.4, 0.5]
			feature dimension	128
			epochs	[100, 200, 400]
Blog	SimGDA+	SimGDA	learning rate	[0.0001, 0.0005]
			weight decay	[0.001, 0.005]
			momentum	[0.01, 0.99]
			backbone	gcn
			backbone layers	[1, 2, 3, 4, 5]
			dropout ratio	0.5
			feature dimension	128
			alpha	[0.5, 1]
			epochs	200
		SimGDA + AE	beta	[0, 0.05]
			decoder dropout	0.1
	GDABench Baselines		learning rate	[0.0001,0.0003, 0.001]
			weight decay	[0.001, 0.003, 0.01]
			backbone layers	[1, 2, 3, 4]
			dropout ratio	[0.1, 0.2, 0.3, 0.4, 0.5]
			feature dimension	128
			epochs	[200, 300, 400]
ArnetMiner	SimGDA+	SimGDA	learning rate	[0.0001, 0.0005, 0.001, 0.005]
			weight decay	[0.0005, 0.001, 0.005]
			momentum	[0.01, 0.99]
			backbone	gcn
			backbone layers	[1, 2, 3, 4, 5]
			dropout ratio	0.5
			feature dimension	128
			alpha	[0.5, 1]
			epochs	200
		SimGDA + IM	beta	[0.5, 1]
			epochs	200
	GDABench Baselines		learning rate	[0.0001, 0.001, 0.003, 0.01]
			weight decay	[0.0001, 0.001, 0.003, 0.01]
			backbone layers	[1, 2, 3, 4, 5]
			dropout ratio	[0.1, 0.2, 0.3, 0.4, 0.5]
			feature dimension	128
			epochs	[100, 200, 400, 800]
Twitch	SimGDA+	SimGDA	learning rate	[0.0001, 0.0005, 0.001, 0.005]
			weight decay	[0.0001, 0.0005, 0.001, 0.005]
			momentum	[0.01, 0.99]
			backbone	gcn
			backbone layers	[1, 2, 3, 4, 5]
			dropout ratio	0.5
			feature dimension	128
			alpha	[0.5, 1]
			epochs	200
		SimGDA + AE	beta	[0, 0.05, 0.1, 0.2, 0.5]
			decoder dropout	[0.1, 0.9]
		SimGDA + CL	beta	[0, 0.05, 0.1, 0.5, 1, 1.5]
			epochs	500
			augment dropout	[0.1, 0.9]
			temperature	[0.1, 0.9]
	GDABench Baselines		learning rate	[0.0001, 0.001, 0.003]
			weight decay	[0.0001, 0.001, 0.003, 0.01]
			backbone layers	[1, 2, 3, 4, 5]
			dropout ratio	[0.1, 0.2, 0.3, 0.4, 0.5]
			feature dimension	128
			epochs	[100, 200, 400]
MAG	SimGDA+	SimGDA	learning rate	[0.0001, 0.0005, 0.001, 0.005]
			weight decay	[0.0001, 0.0005, 0.001, 0.005]
			momentum	[0.01, 0.99]
			backbone	gcn
			backbone layers	[1, 2, 3, 4, 5]
			dropout ratio	0.5
			feature dimension	128
			alpha	[0.5, 1]
			epochs	200
	GDABench Baselines		learning rate	[0.0001, 0.001, 0.003]
			weight decay	[0.0001, 0.001, 0.003]
			backbone layers	[1, 2, 3]
			dropout ratio	[0.1, 0.2, 0.3, 0.4, 0.5]
			feature dimension	300
			epochs	[200, 400, 600, 800]

Table 15: To evaluate the baselines on graph-level shifts, we compared the Micro-F1 scores of each model on the Proteins, Mutagenicity, and Frankenstein datasets. The best results are highlighted in **bold**, and the second-best results are underlined.

Models	Proteins		Mutagenicity		Frankenstein	
	P1 → P2	P2 → P1	M1 → M2	M2 → M1	F1 → F2	F2 → F1
DANE	**60.14** ± 3.58	75.66 ± 0.98	67.25 ± 0.14	**76.92** ± 0.35	54.77 ± 0.53	56.96 ± 2.89
UDAGCN	53.50 ± 2.42	73.14 ± 4.29	58.11 ± 0.58	65.34 ± 0.55	52.48 ± 0.32	52.37 ± 1.38
AdaGCN	52.60 ± 0.78	**78.12** ± 0.37	58.89 ± 0.06	56.18 ± 0.02	56.28 ± 0.75	53.01 ± 3.63
CWGCN	50.45 ± 4.81	44.84 ± 8.20	55.60 ± 1.27	56.72 ± 0.67	49.76 ± 0.27	51.92 ± 0.71
SAGDA	53.14 ± 4.80	46.22 ± 2.99	57.06 ± 3.54	56.00 ± 8.85	50.35 ± 0.26	51.01 ± 8.37
GRADE	43.93 ± 0.31	76.80 ± 0.29	**69.00** ± 0.22	76.57 ± 0.31	**57.54** ± 1.09	**58.39** ± 4.57
A2GNN	51.70 ± 1.54	69.65 ± 4.21	56.83 ± 0.19	58.88 ± 1.23	50.43 ± 0.69	48.99 ± 3.97

Table 16: To evaluate the baselines on graph-level shifts, we compared the Macro-F1 scores of each model on the Proteins, Mutagenicity, and Frankenstein datasets. The best results are highlighted in **bold**, and the second-best results are underlined.

Models	Proteins		Mutagenicity		Frankenstein	
	P1 → P2	P2 → P1	M1 → M2	M2 → M1	F1 → F2	F2 → F1
DANE	**59.14** ± 3.06	56.30 ± 6.09	67.11 ± 0.17	**76.50** ± 0.35	52.24 ± 1.02	54.94 ± 2.13
UDAGCN	53.15 ± 2.74	50.19 ± 1.20	56.71 ± 0.61	63.35 ± 0.56	50.06 ± 0.64	52.32 ± 1.40
AdaGCN	49.33 ± 1.62	57.99 ± 2.82	58.00 ± 0.10	35.97 ± 0.10	55.99 ± 0.94	51.76 ± 4.43
CWGCN	40.57 ± 3.13	42.75 ± 6.01	39.00 ± 4.96	37.32 ± 1.66	39.46 ± 0.22	51.68 ± 0.67
SAGDA	46.65 ± 6.14	33.42 ± 1.01	56.26 ± 3.74	54.95 ± 8.22	36.89 ± 4.93	38.03 ± 6.81
GRADE	32.23 ± 0.86	50.52 ± 1.77	**68.98** ± 0.21	76.32 ± 0.26	**56.93** ± 1.80	**54.98** ± 2.62
A2GNN	47.71 ± 3.22	**58.85** ± 1.16	55.42 ± 0.10	50.17 ± 1.59	46.97 ± 0.96	43.33 ± 1.87

vice versa. Consequently, this variability complicates the task of assessing how well these models will perform when deployed in diverse and complex real-world scenarios where both node-level and graph-level information may be critical.

Domain adaptive message passing methods demonstrate superior and consistency performance across a wide range of datasets and tasks. As shown in Table 3, 9, 16 and 15, methods designed based on the inherent properties of GNN achieves the top-three best performance in 8 tasks out of 12 node-level tasks and top-two best performance in 5 tasks out of 6 graph-level tasks. This observation verified our findings that establishing domain adaptation principles by leveraging inherent properties of GNN can result in an effective and efficient approach to addressing the challenges of domain variability in graph datasets.

To summarize, our observations underscore the importance of leveraging the intrinsic properties of GNNs to devise effective domain adaptation strategies, which not only enhances performance but also ensures consistency in real-world applications.

F Discussion

F.1 How these findings generalize to real-world scenarios

Our benchmark includes a range of datasets with varying characteristics to capture different aspects of graph domain adaptation. This diversity aims to provide a broad perspective on the applicability of our methods. In real-world scenarios, applying graph adaptation methods effectively involves several key considerations: Firstly, it is imperative to develop tailored strategies specifically designed to address the structural shifts observed in graphs. For example, if a graph is dynamic and changing overtime, it is crucial to accord greater attention to its evolving structure. Secondly, recognizing the importance of the aggregation scope and aggregation architecture in GNNs' transferability within unsupervised graph domain adaptation (UGDA) are crucial. In real-world graphs, noise is inevitable, hence, strategically selecting effective neighbors not only improve performance but also avoid noise.

Thirdly, by leveraging the properties of GNNs that make them inherently adaptable to changes in graph structure and data distribution, we can develop simple yet highly effective models.

F.2 A broader discussion on DA problem and other related UGDA scenarios

UDA vs UGDA. Unsupervised domain adaptation (UDA) entails transferring knowledge from a labeled source domain to an unlabeled target domain. A prevalent strategy in domain adaptation is to reduce domain discrepancies while learning domain-invariant representations, a method that has seen considerable success in the fields of computer vision and natural language processing. However, these techniques typically operate under the assumption that inputs are independently and identically distributed (IID), making them unsuitable for tasks involving non-IID data, such as node classification in graph-structured datasets.

UGDA vs muti-domain UGDA. Muti-domain UGDA extends the concept of domain adaptation to situations where there are multiple source domains and a single target domain. This approach aims to learn a model that can generalize well across multiple source domains, and then adapt it to perform well on the target domain. Compared to standard UGDA, multi-domain UGDA can enhance generalization by leveraging the diversity of multiple source domains. However, it may require more complex models and additional computational resources.

UGDA vs source-free UGDA. Source-free UGDA advances domain adaptation by tackling the challenge of adapting models without access to labeled data from the source domains. This setting is more challenging as it involves learning to transfer knowledge without explicit supervision. Source-free UGDA methods often employ techniques such as self-training or consistency regularization to adapt the model to the target domain. Compared to UGDA, source-free UGDA may be more sensitive to domain shift and require careful selection of adaptation techniques.