Towards Unsupervised Open-Set Graph Domain Adaptation via Dual Reprogramming

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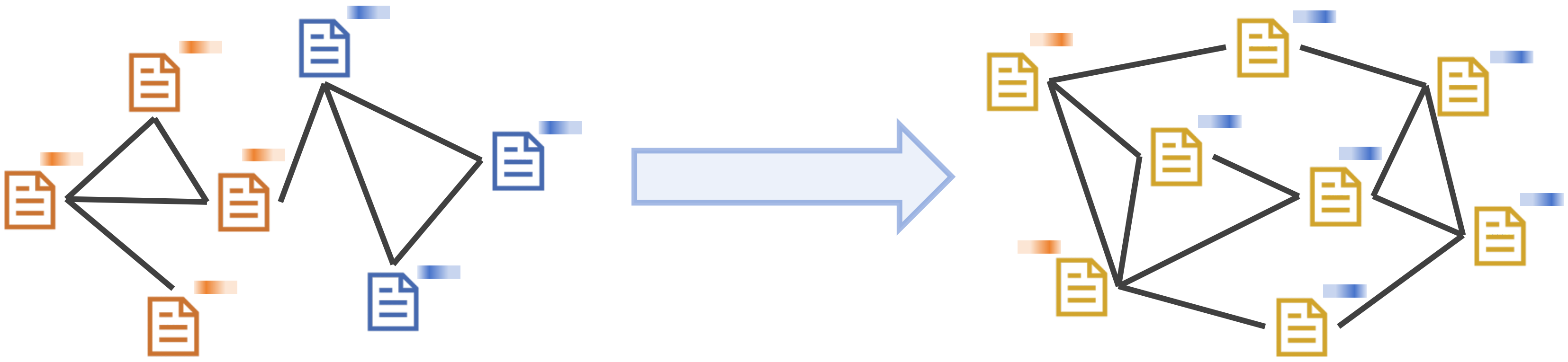
Background

- **Unsupervised Graph Domain Adaptation has become a promising paradigm for transferring knowledge from a fully labeled source graph to an unlabeled target graph**

- **Existing graph domain adaptation models primarily focus on the *closed-set setting*, where the source and target domains share the same label spaces**



ACM Citation Network

Source Graph: 2 Classes

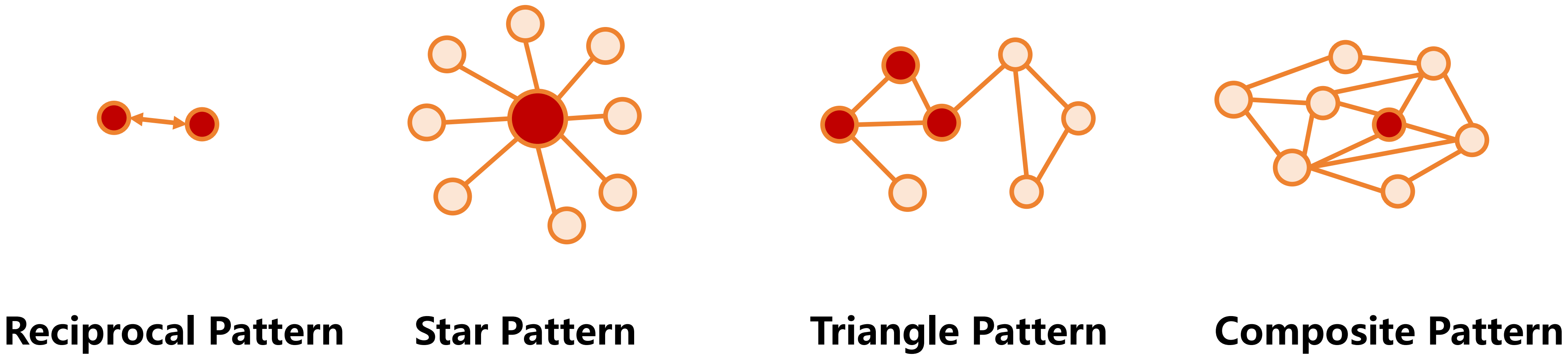
DBLP Citation Network

Target Graph: 2 Classes

Background

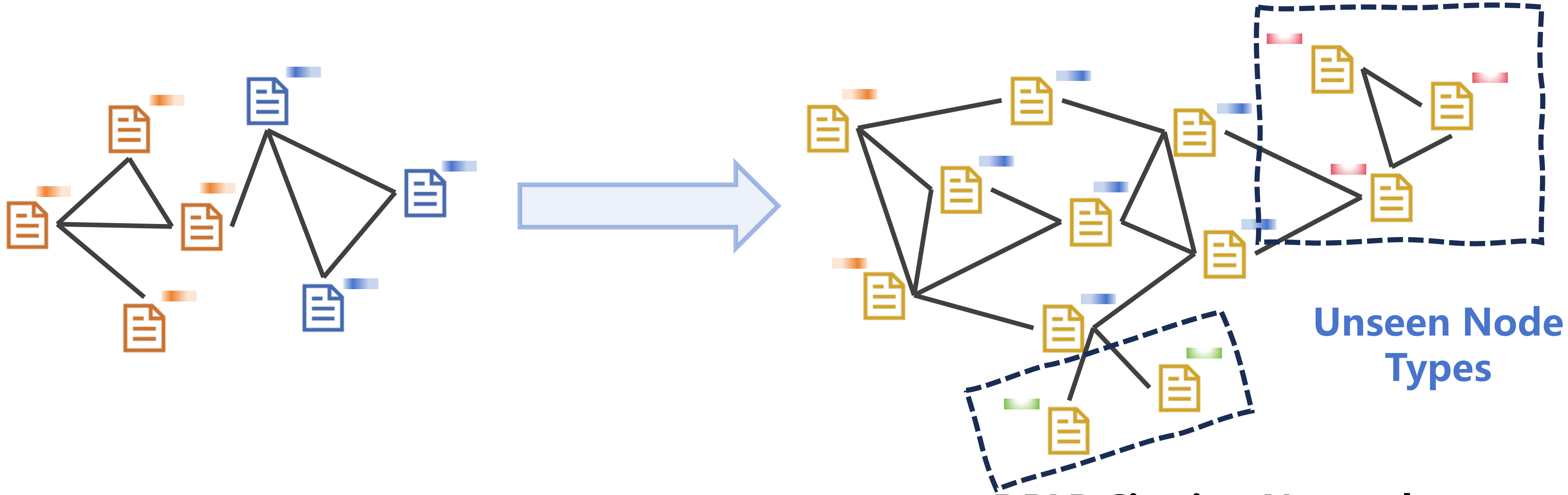
- However, such a strict assumption is unrealistic in real-world applications, since the target domain might introduce new classes that are absent from the source domain, leading to significant challenges in identifying unseen samples

- Examples: fraud schemes are *continually evolving* with fraudsters frequently developing new tactics



Background

- In this paper, we investigate the problem of unsupervised ***open-set*** graph domain adaptation, where the goal is to not only correctly classify target nodes into the known classes, but also recognize previously unseen node types into the unknown class



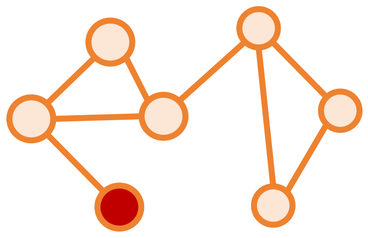
ACM Citation Network
Source Graph: 2 Classes

DBLP Citation Network
Target Graph: 4 Classes

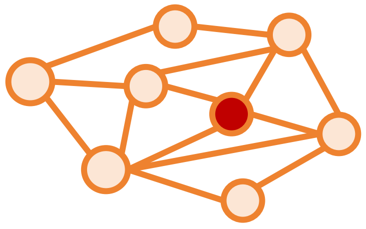
Related Work

- Recent models utilize a *threshold* to designate low-confidence samples as unknown, while aligning the source domain with the known portion of the target domain via adversarial training

- While promising, these methods depend heavily on manually set threshold and *one threshold cannot fit all*, which makes them difficult to adapt to different distributions



Threshold: 0.25 ✅



Threshold: 0.25 ❌
Threshold: 0.40 ✅

Method

- **To effectively distinguish between known and unknown groups and facilitate open-set recognition, it is essential to promote a clearer separation between these two groups**

- **We propose to perform dual reprogramming from the graph and the model perspectives**

  - ***Model Reprogramming:*** **pruning domain-specific parameters to reduce bias towards the source graph while preserving parameters that capture transferable patterns across graphs**

  - ***Graph Reprogramming:*** **modifying target graph structure and node features, which facilitates better separation of known and unknown classes**

Model Reprogramming

- **Motivated by the lottery ticket hypothesis, which demonstrates that only a subset of parameters is crucial for generalization, we propose to reprogram the graph neural network $f_w(\cdot)$ by *selectively masking its weights***

$$Z^l = f_w\left(G, \widetilde{W}^l\right) = \sigma(\widetilde{D}^{\frac{1}{2}}\widetilde{A}\widetilde{D}^{\frac{1}{2}}Z^{l-1}(W^l \odot M^l))$$

- **We calculate its gradient $\nabla \mathrm{M}^l$ with respect to the loss function to quantify the importance of each weight element**

- **We set the lowest ρ percent of gradient values in M^l to zero, leaving the remaining elements at 1. These sparse masks are then applied to prune W^l, resulting in the reprogrammed sparse model**

Graph Reprogramming

- We modify the target ***graph's structure*** and ***node features*** to better align with the source domain, while differentiating the known and unknown groups within the target domain

$$\hat{X}_t = \psi_x(X_t) = X_t + \nabla X_t$$
$$\hat{A}_t = \psi_a(A_t) = A_t \oplus \nabla A_t$$

- $\psi_x(\cdot)$ represents the transformation function applied to update node features, and $\psi_a(\cdot)$ denotes the function for modifying the graph structure by adding or removing edges

- We choose two simple, direct transformation strategies described above

Method

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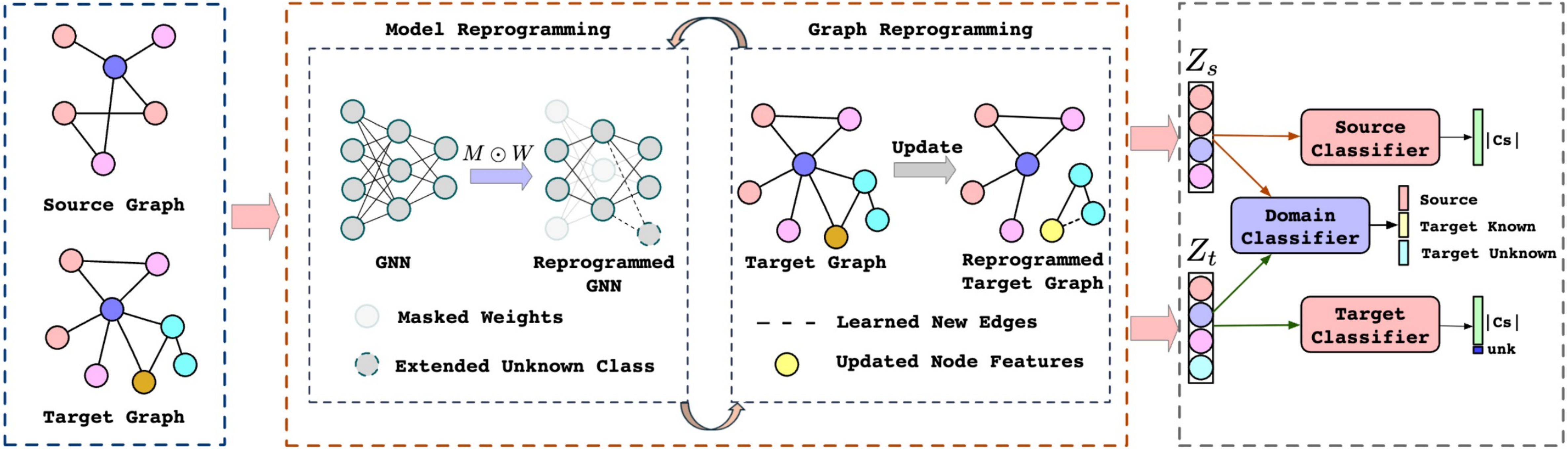
➢ We present an overview of the proposed **GraphRTA** framework



Training

- We model the entropy of instances as being generated by a mixture of two Beta distributions to capture the overall characteristics of the target graph

$$p(e_i) = \mu_{tk} \cdot p(e_i|tk) + \mu_{tu} \cdot p(e_i|tu)$$

- After estimating the probability of each target instance belonging to either the target-known or target-unknown group, we can classify all the instances into three distinct domains for the domain adversarial learning framework

- The domain discriminator $d_\theta(\cdot)$ is optimized by minimizing the cross-entropy loss to effectively classify three domains
  - ***Source, Target-known, and Target-unknown***

Experiments

- Datasets: we conduct experiments using three categories of publicly available datasets

- Three key category baselines:
  - *Graph Neural Networks*
    - GCN, SAGE, GAT
  - *Closed-set GDA*
    - UDAGCN, A2GNN, etc.
  - *Open-set GDA*
    - DANCE, SDA, UAGA, etc.

Datasets	#Nodes	#Edges	#Feat	#Class
DBLPv7	5,484	8,117	6,775	5
Citationv1	8,935	15,098		
ACMv9	9,360	15,556		
ogbn-arxiv	169,343	1,166,243	128	40
Cornell	183	298	1,703	5
Texas	183	325		
Wisconsin	251	515		

Experiments

- **Our proposed GraphRTA consistently demonstrates superior performance across a variety of scenarios**

H-score: $HS = \frac{2 \times Acc_{tk} \times Acc_{tu}}{Acc_{tk} + Acc_{tu}}$

Models	ACMv9→Citationv1		ACMv9→DBLPv7		Citationv1→ACMv9		Citationv1→DBLPv7		DBLPv7→ACMv9		DBLPv7→Citationv1	
	Acc	HS	Acc	HS	Acc	HS	Acc	HS	Acc	HS	Acc	HS
GCN	40.64±0.98	41.02±2.11	45.84±1.06	50.20±1.26	47.10±0.49	49.05±0.74	51.48±0.42	56.13±0.22	43.90±1.50	44.47±2.80	39.26±0.70	37.96±1.34
SAGE	38.24±0.80	36.89±2.10	41.77±1.05	45.20±1.41	43.90±1.56	45.63±2.18	47.14±0.82	51.65±0.83	41.66±0.47	42.04±1.32	39.62±0.22	40.32±0.40
GAT	32.01±0.73	21.51±2.36	34.84±1.25	32.90±2.66	36.38±0.66	30.67±1.66	34.56±0.64	32.22±1.53	35.85±1.91	25.66±5.30	32.87±1.41	20.91±3.92
UDAGCN	44.78±4.12	20.94±6.21	55.07±1.03	50.05±7.90	53.38±1.53	53.56±6.00	62.36±4.19	43.21±4.08	47.28±1.49	39.21±1.16	52.38±1.18	46.92±6.26
GRADE	57.23±1.06	59.49±1.16	56.12±0.65	58.14±1.07	57.86±0.29	60.41±0.26	61.94±0.38	64.21±0.48	54.93±0.40	57.73±0.41	54.60±0.64	57.36±0.55
SpecReg	51.31±5.60	36.70±1.49	58.17±2.06	60.15±0.41	56.58±1.22	56.36±0.86	63.68±5.82	59.62±0.59	53.30±4.05	53.12±6.84	55.72±2.43	49.43±7.41
StruRW	46.47±4.63	42.36±4.25	46.91±1.95	46.08±3.60	51.91±0.60	45.38±0.13	56.19±0.10	54.08±1.19	48.86±0.62	43.85±1.74	51.08±0.91	43.25±1.29
A2GNN	42.53±2.07	41.66±3.69	60.43±0.52	62.74±0.82	57.21±1.03	57.12±0.63	63.45±0.31	65.37±0.59	57.64±1.82	**60.68±2.27**	41.09±1.20	43.52±1.24
DANCE	57.77±0.64	60.94±0.76	58.01±0.47	61.31±0.62	58.76±0.36	61.33±0.55	62.97±0.65	65.42±1.20	55.97±0.62	58.90±0.60	55.77±0.56	58.95±0.70
OpenWGL	49.98±0.62	5.57±1.56	52.43±0.62	7.86±0.69	48.37±0.50	4.07±0.99	55.68±0.35	3.49±0.76	48.04±1.08	25.13±4.89	49.52±0.68	22.05±2.29
PGL	54.42±1.04	57.86±1.12	48.43±1.12	53.15±1.23	51.87±0.69	54.71±0.72	53.83±0.66	59.01±0.75	49.27±0.80	51.74±0.83	52.82±0.87	56.16±0.93
OpenWRF	53.53±2.59	31.05±4.57	48.16±1.63	35.45±3.62	47.01±3.32	33.08±6.46	52.81±1.43	31.96±1.24	47.27±1.54	19.38±4.03	57.31±1.14	34.06±9.77
G2Pxy	59.75±0.49	54.47±1.33	56.26±0.73	49.63±2.41	58.49±1.03	58.56±1.36	61.42±0.47	59.13±0.54	54.48±0.58	54.82±0.78	56.36±0.69	54.02±1.75
SDA	58.23±4.67	59.97±6.74	59.06±4.75	56.34±1.23	57.33±6.22	58.85±8.58	63.55±0.91	65.53±2.00	**57.66±0.61**	60.54±1.20	57.27±2.72	59.73±3.87
UAGA	53.37±6.72	61.34±1.16	52.11±2.96	**67.50±2.95**	52.25±4.81	60.59±5.95	52.73±5.13	64.81±4.50	48.14±1.47	55.73±3.98	47.97±9.24	52.16±2.18
GraphRTA	**66.26±0.93**	**66.33±1.69**	**62.33±0.68**	64.42±1.10	**60.93±2.63**	**62.89±2.46**	**63.87±1.97**	**65.99±1.87**	56.91±2.50	59.41±2.22	**60.11±1.98**	**62.33±1.53**

Experiments

- H-score provides a more comprehensive evaluation metric than accuracy
- Several baselines *achieve high accuracy scores but suffer from low H-scores*, reflecting their difficulty in accurately identifying open-set instances

Models	Arxiv I→Arxiv II		Arxiv I→Arxiv III		Arxiv II→Arxiv III		Cornell→Wisconsin		Texas→Cornell		Texas→Wisconsin	
	Acc	HS	Acc	HS	Acc	HS	Acc	HS	Acc	HS	Acc	HS
GCN	44.82±0.20	41.08±0.74	41.57±0.22	41.05±0.66	45.65±0.37	41.04±0.89	21.19±0.17	0.20±0.45	38.46±8.43	25.19±11.0	21.83±6.29	13.32±9.15
SAGE	44.95±0.15	37.83±0.71	42.75±0.15	38.63±0.64	49.60±0.12	38.11±0.49	18.56±2.86	10.30±10.7	34.75±3.31	11.66±4.91	24.22±10.7	14.48±9.01
GAT	44.81±0.13	34.31±1.39	42.05±0.30	34.97±0.76	46.49±0.17	36.35±0.78	20.96±0.21	0.40±0.54	27.97±3.00	15.89±9.15	9.48±2.31	8.08±2.24
UDAGCN	31.90±2.27	33.68±3.48	27.71±0.86	28.37±1.63	35.09±1.29	39.53±1.56	19.28±6.57	5.94±5.51	29.18±1.87	7.35±5.28	22.78±5.19	3.93±4.12
GRADE	43.01±0.20	47.18±0.29	39.28±0.37	44.19±0.41	42.80±0.17	46.09±0.21	17.05±11.5	12.52±1.26	28.96±7.54	21.52±11.5	24.46±7.32	23.84±4.67
SpecReg	37.80±1.90	31.76±1.64	28.14±4.59	29.03±3.87	46.60±0.29	31.70±4.27	20.79±3.24	19.93±3.12	31.69±3.34	13.53±9.15	19.20±4.72	10.28±6.14
StruRW	37.47±1.93	40.67±2.09	36.17±0.27	40.54±0.45	42.10±0.44	43.62±0.50	16.57±2.26	16.22±3.72	42.02±7.51	**40.98±7.86**	16.01±2.47	11.46±6.17
A2GNN	42.07±0.14	45.00±0.24	38.92±0.16	43.14±0.17	42.26±0.53	45.18±0.17	19.12±2.56	17.40±3.32	44.37±0.71	31.59±6.44	14.98±0.77	6.22±2.58
DANCE	OOM	OOM	OOM	OOM	OOM	OOM	21.52±23.4	3.11±0.49	20.77±0.00	0.00±0.00	4.22±0.21	1.65±1.50
OpenWGL	32.58±0.58	1.45±0.40	32.99±1.49	1.31±0.37	35.46±2.61	0.04±0.08	16.57±2.49	14.09±2.30	33.22±5.77	28.99±5.65	10.51±4.80	8.76±3.56
PGL	41.50±0.25	46.32±0.28	38.38±0.14	43.31±0.16	40.28±0.24	45.43±0.27	18.24±7.16	0.00±0.00	21.20±0.45	0.00±0.00	28.45±5.93	0.00±0.00
OpenWRF	32.58±0.58	1.45±0.40	32.99±1.49	1.31±0.37	35.46±2.61	0.04±0.08	26.29±7.11	6.84±5.81	21.64±3.81	4.58±5.03	26.93±11.4	5.99±4.65
G2Pxy	31.13±4.55	28.45±1.13	24.79±1.49	16.28±3.25	34.93±3.03	37.27±6.75	-	-	-	-	-	-
SDA	39.77±0.34	42.60±0.15	36.37±0.21	39.44±0.21	41.53±0.20	46.03±0.18	-	-	-	-	-	-
UAGA	32.92±0.16	23.69±0.16	32.24±0.13	22.98±0.13	39.16±0.39	29.79±0.41	-	-	-	-	-	-
GraphRTA	**47.70±1.39**	**50.79±2.79**	**45.52±2.00**	**46.25±0.40**	**52.37±1.49**	**48.42±1.94**	**33.46±4.43**	**34.36±1.76**	**52.18±0.38**	35.64±0.83	**29.34±1.21**	**30.08±2.96**

Conclusion

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- **We study *unsupervised open-set graph domain adaptation*, an under-explored area in the graph community, where the target graph introduces new classes that are not present in the source graph**

- **We propose a novel framework named GraphRTA that conducts *dual reprogramming* at the model as well as the graph levels**

- **Experiments further show that our proposed GraphRTA consistently *outperforms or matches* the performance of recent state-of-the-art models**

Thanks
Q&A

Code and Data