

Can Graph Neural Networks Learn Language with Extremely Weak Text Supervision?

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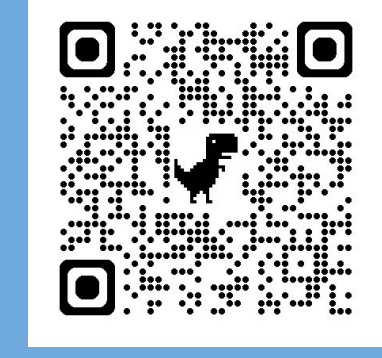
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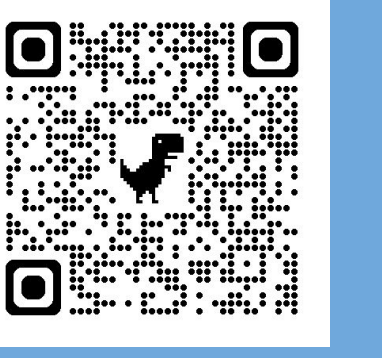
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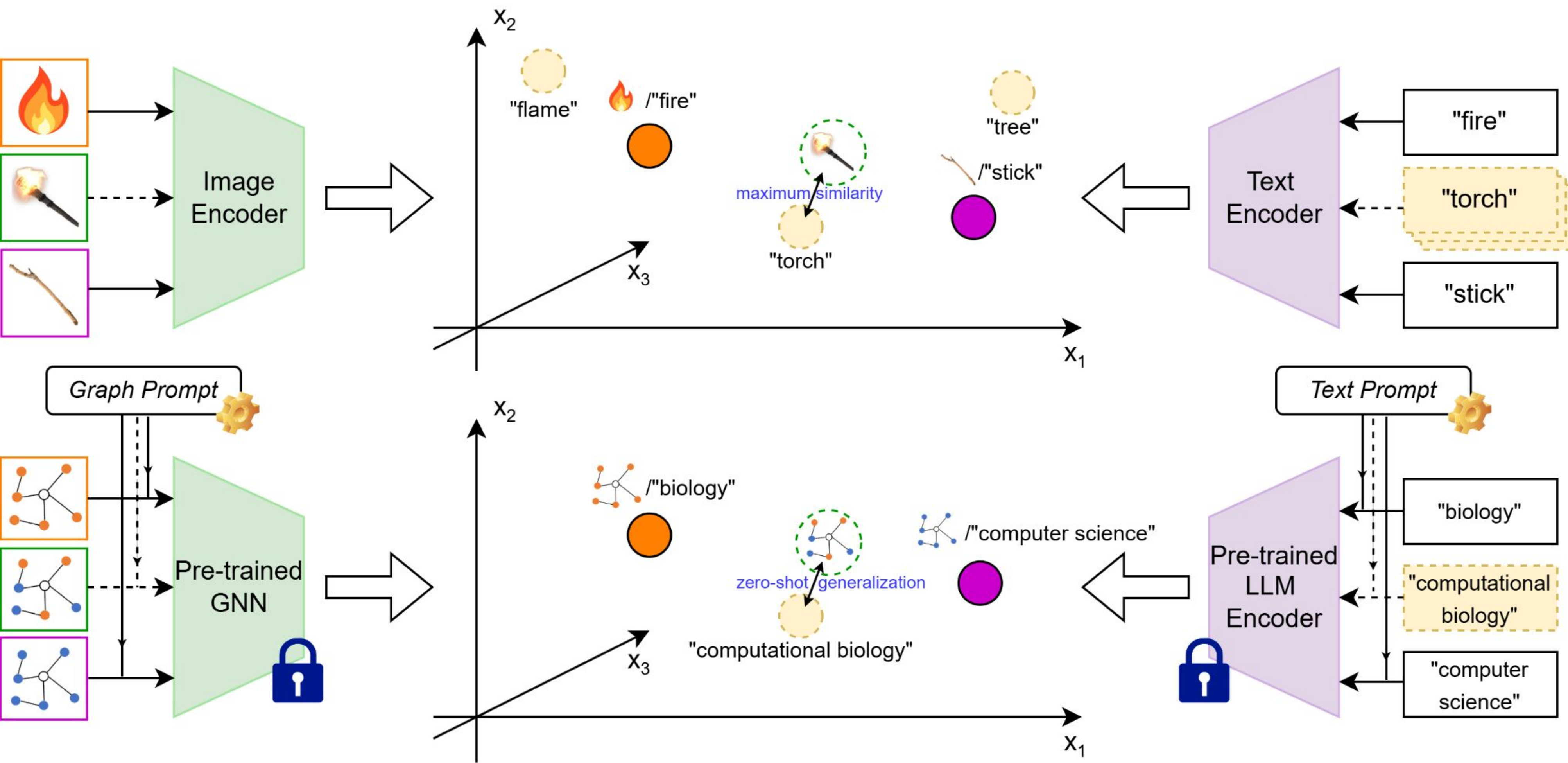


paper



author (open for
internship in USA)

Vision: CLIP in graph domain for foundational graph representation learning



Challenges:

- graph data is very scarce and the text supervision is extremely weak (v.s., million-scale image-text pairs in CLIP)
- Conceptual gap between different graph domains (v.s., language tokens and visual objects retain their concepts)
- Multiple task space: node-level, edge-level, graph-level

Observations:

- We don't need joint-pretraining. we already have pre-trained LLMs and many GNN pretraining methods
- When data is limited, prompt learning usually provides better option

Let's try *co-adapting GNN and LLM with prompt learning!*

Multi-modal Prompt Learning for Graph Neural Networks

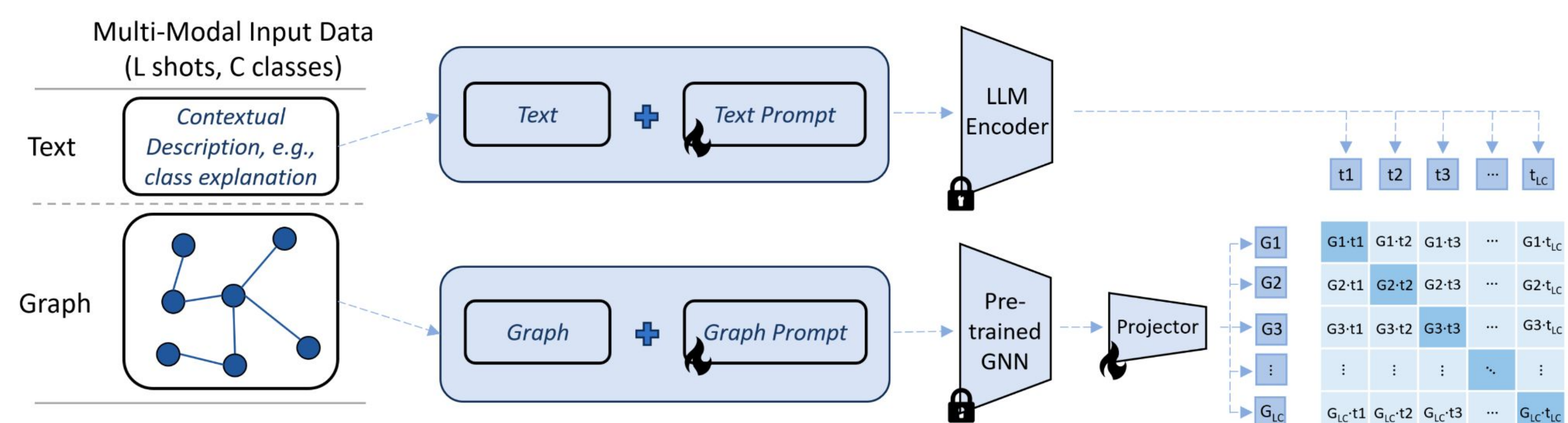


Figure 2: Similar to CLIP backbone, Morpher adapts the graph representations to semantic space through multi-modal prompt learning, even if the GNN and LLM are not jointly trained and are kept frozen.

Improved graph prompts by cross-connection pruning

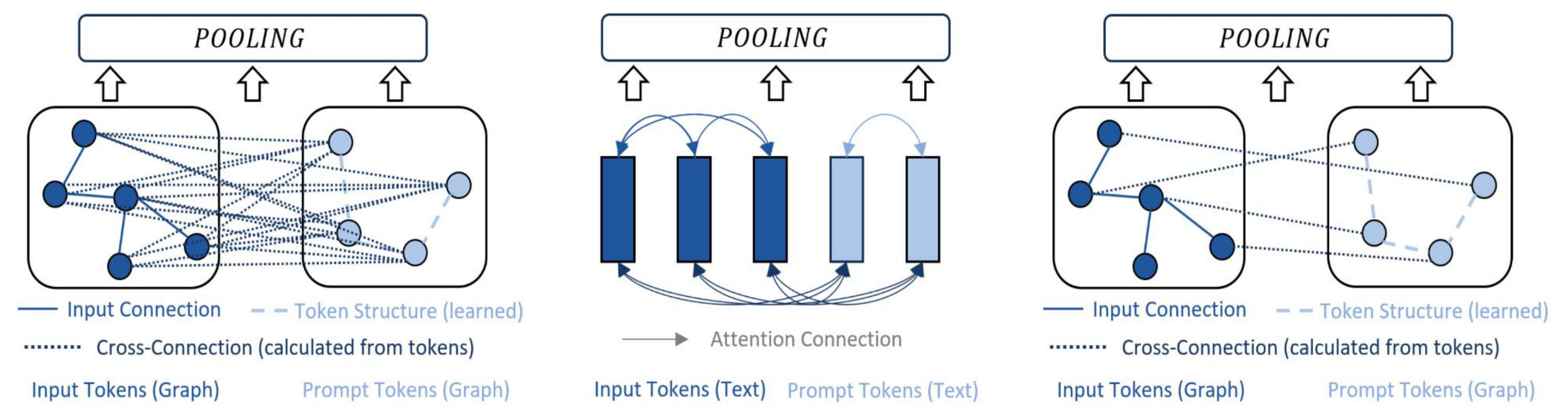


Figure 1: Cross-connections overwhelm inner-connections in current graph prompt design, which may be unstable during training (left); attention in NLP where $3 \times 2 = 6$ cross-connections and $3 + 1 = 4$ inner-connections are balanced (middle); and our balanced graph prompt design (right). **The cross-connections between input and prompt should have a consistent scale with the input connections.**

Main Results: few-shot classification

Training schemes	GNN pretraining	MUTAG		ENZYMES		PROTEINS		MSRC_21C	
		Acc	F1	Acc	F1	Acc	F1	Acc	F1
Supervised	N/A + GCN	66.00	66.67	16.67	8.68	65.89	60.77	38.85	35.32
	N/A + GAT	66.00	65.69	16.45	4.65	64.75	64.08	41.14	39.86
	N/A + GT	66.66	66.26	15.62	4.22	62.81	57.12	38.28	41.62
Pre-train + Fine-tune	GraphCL+GCN	70.00	70.23	17.91	11.82	65.89	61.23	40.00	43.89
	GraphCL+GAT	70.00	69.73	17.91	10.46	65.16	63.92	44.57	45.74
	GraphCL+GT	68.00	67.81	17.70	8.99	63.28	56.41	41.71	43.73
	SimGRACE+GCN	66.67	67.27	17.29	8.78	66.82	64.70	40.57	43.84
	SimGRACE+GAT	70.67	69.10	16.87	7.18	65.42	63.65	42.85	42.37
AIO (Sun et al., 2023a)	SimGRACE+GT	69.33	69.77	16.24	6.08	65.98	62.31	39.42	40.78
	GraphCL+GCN	64.67	39.27	17.50	4.97	61.35	44.93	3.59	10.09
	GraphCL+GAT	64.67	39.27	17.50	4.97	59.21	37.19	14.37	3.11
	GraphCL+GT	73.33	72.06	18.33	9.09	40.79	28.97	17.96	8.30
	SimGRACE+GCN	64.67	39.27	16.04	4.61	67.42	60.87	34.73	18.16
GPF-plus (Fang et al., 2023)	SimGRACE+GAT	64.67	39.27	16.04	4.61	59.21	37.19	7.78	1.79
	SimGRACE+GT	36.00	27.26	17.50	8.15	50.56	49.34	32.34	15.13
	GraphCL+GCN	68.67	67.27	16.88	15.48	64.75	61.45	47.42	29.02
	GraphCL+GAT	68.67	62.84	16.45	13.23	65.89	60.07	47.42	26.28
	GraphCL+GT	69.33	67.87	18.12	15.56	59.66	37.37	41.71	21.35
Gprompt (Liu et al., 2023d)	SimGRACE+GCN	65.33	39.52	18.96	15.83	65.16	58.80	45.71	23.32
	SimGRACE+GAT	69.33	66.72	18.54	12.58	63.28	53.50	42.85	21.40
	SimGRACE+GT	70.00	67.31	17.91	14.69	64.83	52.97	34.13	20.13
	GraphCL+GCN	73.33	66.93	17.91	8.44	61.01	60.01	1.80	0.21
	GraphCL+GAT	64.67	62.63	17.08	14.18	50.56	50.55	1.80	0.22
Morpher (Ours)	GraphCL+GT	70.67	70.02	17.91	9.64	63.28	58.65	1.80	0.21
	SimGRACE+GCN	65.33	39.52	17.29	14.48	52.70	52.68	1.80	0.21
	SimGRACE+GAT	67.33	65.88	16.25	11.31	59.10	58.72	1.80	0.21
	SimGRACE+GT	73.33	67.84	16.87	13.54	64.75	62.37	1.80	0.223
	GraphCL+GCN	77.33	77.74	18.13	11.98	65.89	65.97	42.85	45.91
Improved AIO (Ours)	GraphCL+GAT	74.67	75.51	18.33	11.26	65.76	66.05	46.85	51.39
	GraphCL+GT	74.67	74.67	19.16	9.04	68.12	68.18	42.85	43.54
	SimGRACE+GCN	68.00	69.01	17.91	9.02	66.82	66.40	44.57	49.24
	SimGRACE+GAT	77.33	77.20	18.75	9.39	66.91	65.49	45.14	42.31
	SimGRACE+GT	71.33	72.06	18.95	11.25	68.59	68.84	40.57	42.82
Morpher (Ours)	GraphCL+GCN	78.67	78.09	20.41	15.20	67.47	66.40	45.14	49.62
	GraphCL+GAT	79.33	79.15	23.12	18.01	70.89	70.30	50.85	54.48
	GraphCL+GT	76.00	76.51	19.58	13.28	73.53	72.48	45.71	48.41
	SimGRACE+GCN	69.33	70.27	19.79	14.94	67.10	66.15	45.71	51.24
	SimGRACE+GAT	78.00	77.65	20.21	16.27	68.12	67.26	45.71	51.13
IMP of ImprovedAIO	SimGRACE+GT	74.00	74.84	19.16	14.29	71.76	71.75	44.00	48.16
	IMP of Morpher	2.00 ↑	5.01 ↑	0.52 ↑	4.41 ↓	2.01 ↑	4.37 ↑	0.28 ↓	2.50 ↑
IMP of Morpher		4.00 ↑	6.73 ↑	2.36 ↑	0.60 ↑	4.81 ↑	6.61 ↑	2.66 ↑	7.14 ↑

Table 14: Few-shot graph classification performance (%). IMP (%): the average improvement (absolute value) compared to the **best result** among all the baseline methods.

Multi-task and domain-transfer performance

Dataset	Methods	Cora		CiteSeer	
		Acc	F1	Acc	F1
Node Level	Supervised	52.83	47.73	63.91	64.82
	Fine-tune	56.37	55.04	64.87	66.42
	AIO (Sun et al., 2023a)	14.69	7.10	18.93	6.92
	ImprovedAIO	58.46	55.10	66.44	66.53
	Morpher	61.26	62.36	68.20	68.56
Edge Level	Supervised	51.78	50.62	52.14	50.81
	Fine-tune	52.50	51.00	52.50	51.12
	AIO (Sun et al., 2023a)	50.00	33.33	50.00	33.33
	ImprovedAIO	54.64	54.57	53.92	53.55
	Morpher	55.71	55.05	55.35	55.05

Table 2: Node-level, edge-level performance. Best results are bolded and second-best results are underlined.

Target Domain	Target Task	MUTAG		PubMed	
		graph-level	node-level	graph-level	node-level
ENZYMES (graph-level)	Supervised	66.00	56.67	47.57	36.07
	Fine-tune	68.00	55.04	47.57	36.07
	AIO	64.00	54.50	44.85	34.13
	ImprovedAIO	70.67	64.07	50.28	50.51
	Morpher	72.67	73.29	54.42	53.96
CiteSeer (node-level)	Supervised	66.00	56.67	47.57	36.07
	Fine-tune	71.33	62.19	48.71	40.66
	AIO	65.33	57.20	45.71	34.39
	ImprovedAIO	74.00	73.76	52.57	51.29
	Morpher	76.67	77.04	58.29	57.54

Table 13: Domain Transfer Performance. Best results are bolded and second-best results are underlined.

Compatibility

Table 7: Few-shot graph classification performance (%) of Morpher with ELBERTA (Clark et al., 2020) as language encoder. Other experiment settings are identical to the main experiment.

GNN pretraining	MUTAG		ENZYMES		PROTEINS		MSRC_21C	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1
GraphCL+GCN	78.00	78.17	20.41	15.79	67.38	65.66	43.42	47.19
GraphCL+GAT	76.67	75.75	20.41	11.37	66.26	65.66	44.57	49.01
GraphCL+GT	76.67	77.04	19.16	14.68	73.36	72.70	42.28	44.99
SimGRACE+GCN	70.00	70.99	19.79	12.41	68.96	67.77	45.71	48.44
SimGRACE+GAT	77.33	77.51	18.12	13.31	68.96	67.78	44.00	49.43
SimGRACE+GT	72.67	73.55	18.33	15.76	70.18	70.28	41.14	44.50

Table 9: Few-shot graph classification performance (%) of Morpher with the GNN pre-trained by GraphMAE (Hou et al., 2022). Other experiment settings are identical to the main experiment.

GNN pretraining	MUTAG		ENZYMES		PROTEINS		MSRC_21C	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1
Pre-train + Fine-tune	71.33	71.41	16.04	12.14	65.86	65.32	39.42	40.30
ImprovedAIO	76.67	76.95	19.58	12.59	66.36	65.30	42.28	46.81
Morpher	78.67	78.67	20.20	16.95	67.38	65.66	45.71	48.49

On AI4Science tasks (with more graph-language pairs)

Table 11: AUC-ROC (↑) on MoleculeNet (bace, tox21, hiv). Morpher-K denotes K shots.

Dataset	KVPLM	MoMu	Galactica-1.3B	GIMLET-64M-50-shots	GAT-IM-supervised	Morpher-10	Morpher-20	Morpher-50
bace	0.5126	0.6656	0.5648	0.729	0.697	0.6231	0.6513	0.6858
tox21	0.4917	0.5757	0.4946	0.652	0.754	0.6769	0.7275	0.7459
hiv	0.6120	0.5026	0.3385	0.721	0.729	0.5742	0.7034	0.7283

The performance of Our Morpher paradigm is comparable to much larger models

GNN zero-shot prototype (“reasoning over graph representations”)

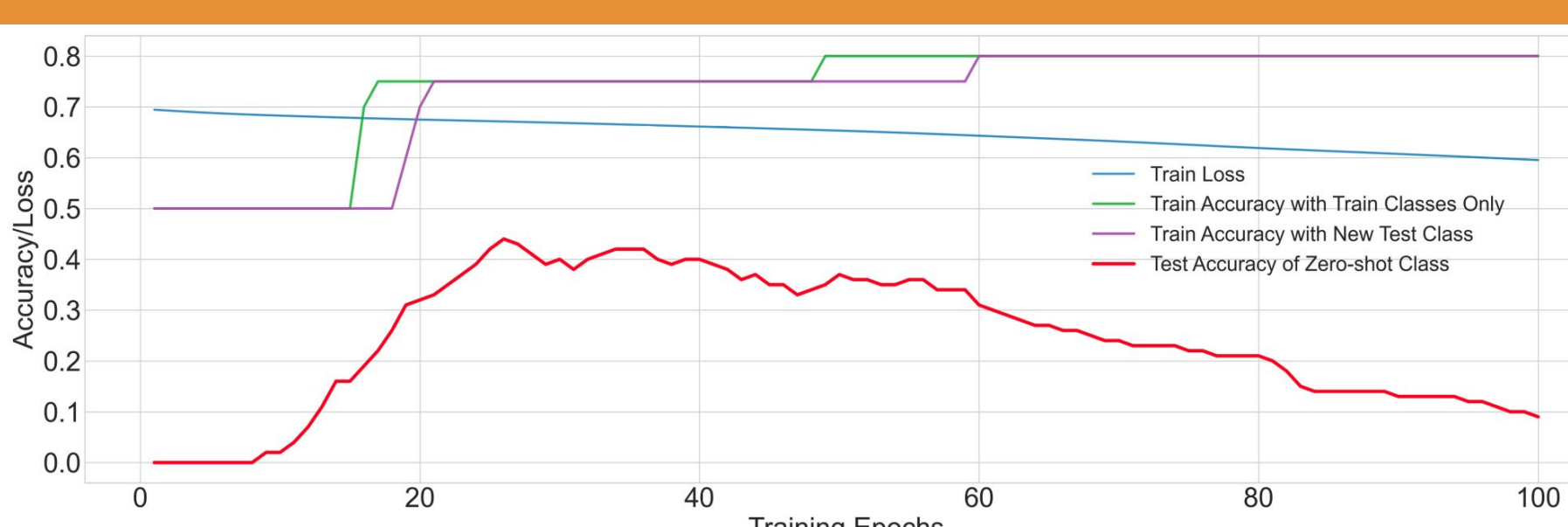


Figure 7: Novel class generalization result for our ZERO-CiteSeer dataset.

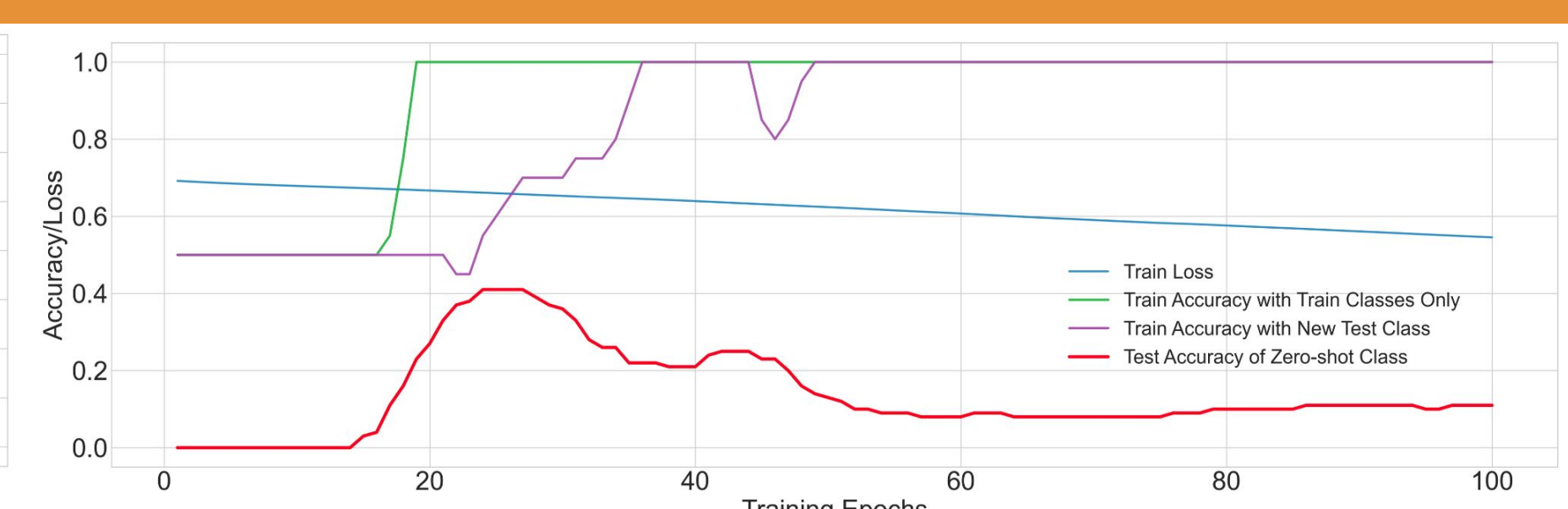


Figure 8: Novel class generalization result for our ZERO-PubMed dataset.