Would prompt work for graph learning?
An exploration of few-shot learning on graphs

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VALSE Webinar

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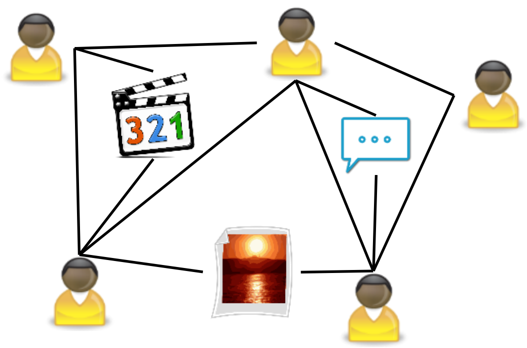
Outline

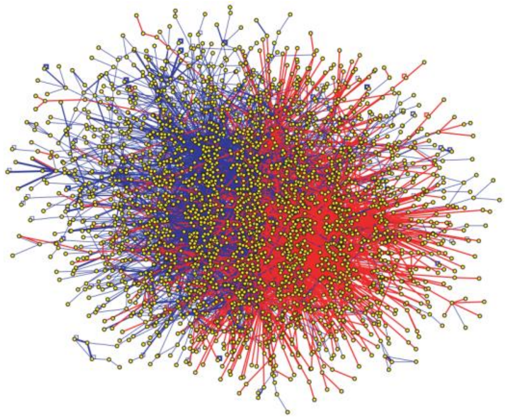
- **Introduction: Data and problems**
- Overview of few-shot methodologies
- Can prompt work on graph + text?
- Can prompt work on graph alone?
- Conclusion

Complex big data as graphs

Social networks

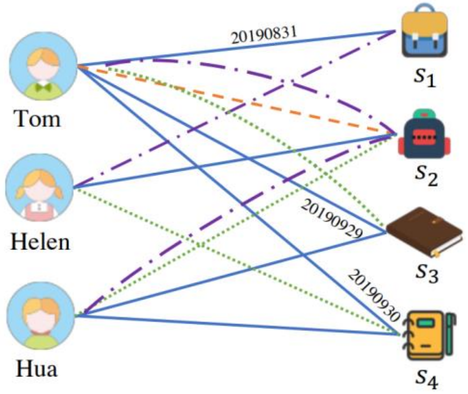


Biology



[Image from RVH05]

E-commerce

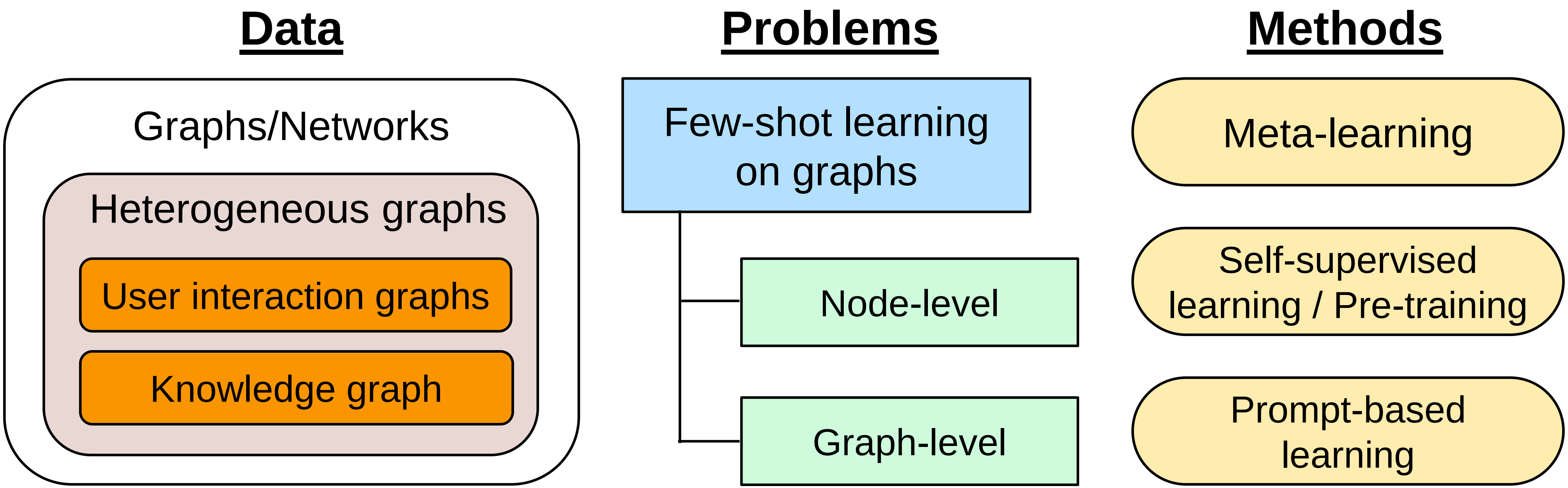


Knowledge graph

[Image from Microsoft]

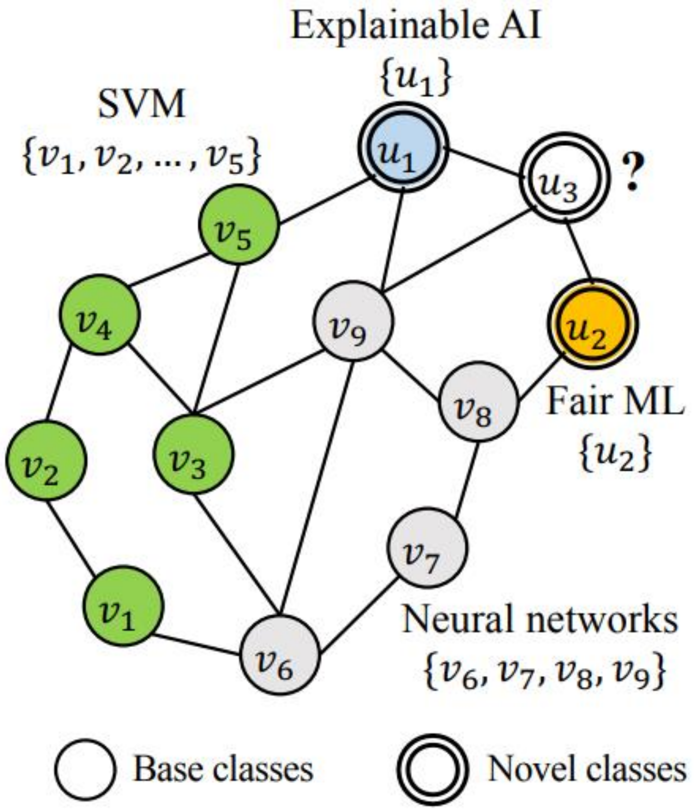
[RVH05] Towards a proteome-scale map of the human protein–protein interaction network. J. Rual, *et al*. Nature: 437(7062), 2005.

Data, Problems and Methods

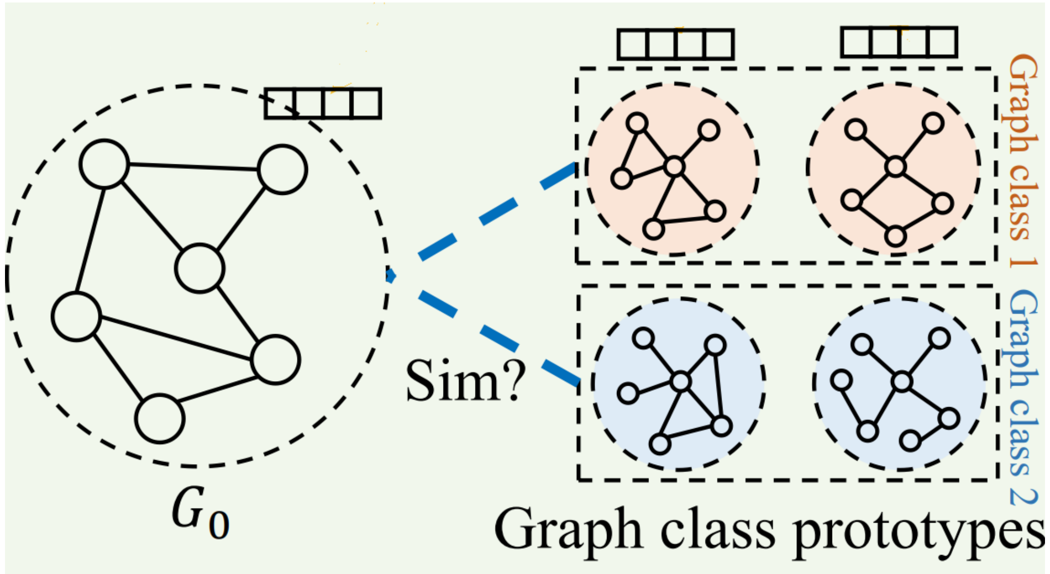


Few-shot problems on graphs

Node classification



Graph classification



[AAAI21] Z. Liu, Y. Fang, C. Liu and S. C. H. Hoi. *Relative and Absolute Location Embedding for Few-Shot Node Classification on Graph.*

[WWW23] Z. Liu, X. Yu, Y. Fang and X. Zhang. *GraphPrompt: Unifying Pre-Training and Downstream Tasks for Graph Neural Networks.*

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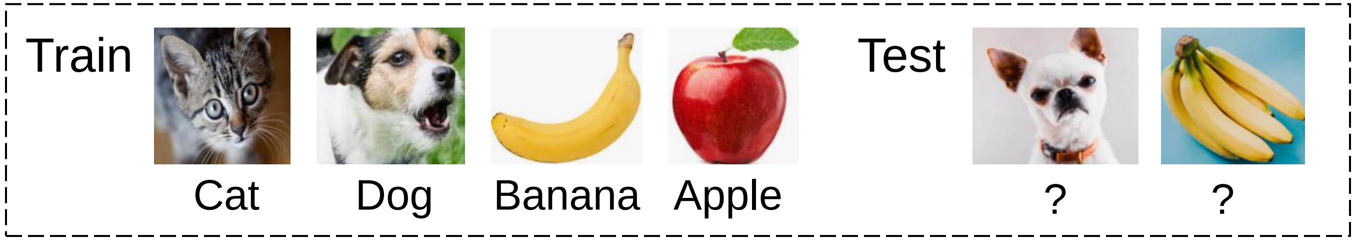
Why supervised learning does not work?

Supervised learning



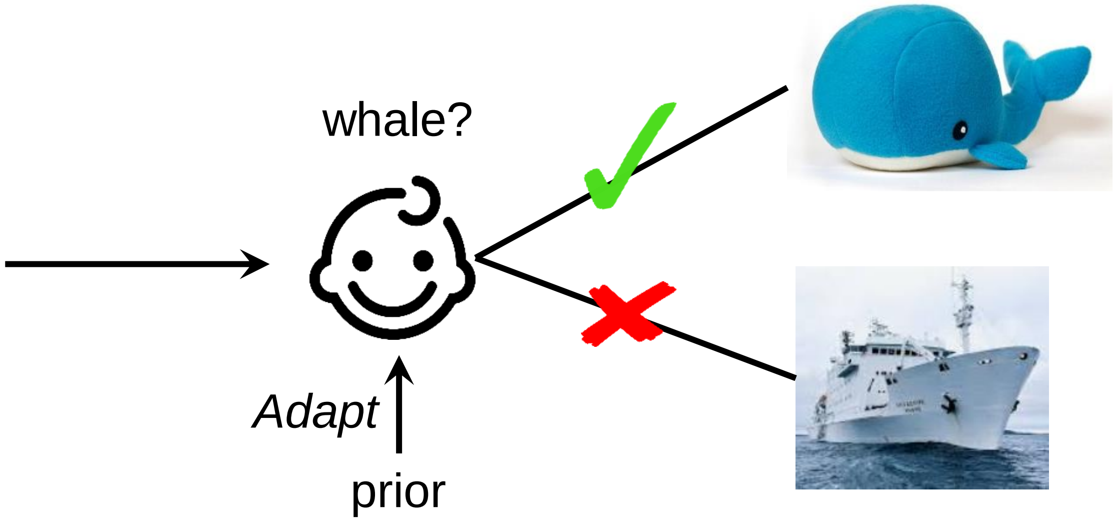
Learn a classifier

$f_\theta($  $) \rightarrow \text{dog}$

Need many, many labelled data!
Hard to deal with novel classes.

How humans learn?

One example of toy whale



Even toddlers can learn novel classes very quickly with one/few examples…by generalizing from prior knowledge.

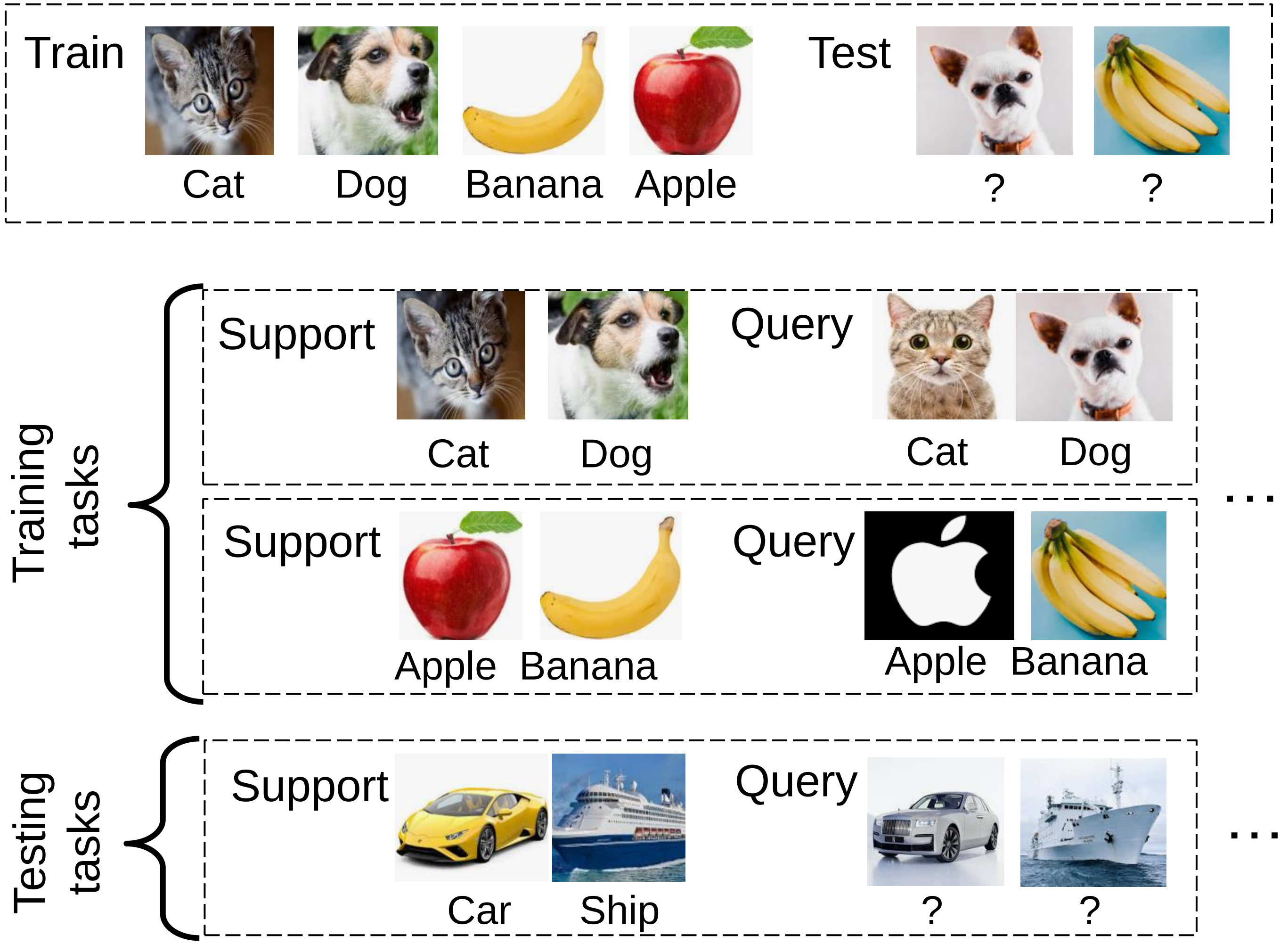
[Images from the Web]

From supervised learning to meta-learning

Supervised learning

Meta-learning

(MAML [FAL17])



Learn a classifier

$f_\theta($  $) \rightarrow \text{dog}$

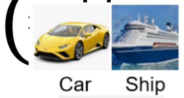
Need many, many labelled data!

Hard to deal with novel classes.

Learn a prior ϕ from the training tasks

Adapt

support

$g_\phi($  $) \rightarrow f_{\phi'}$

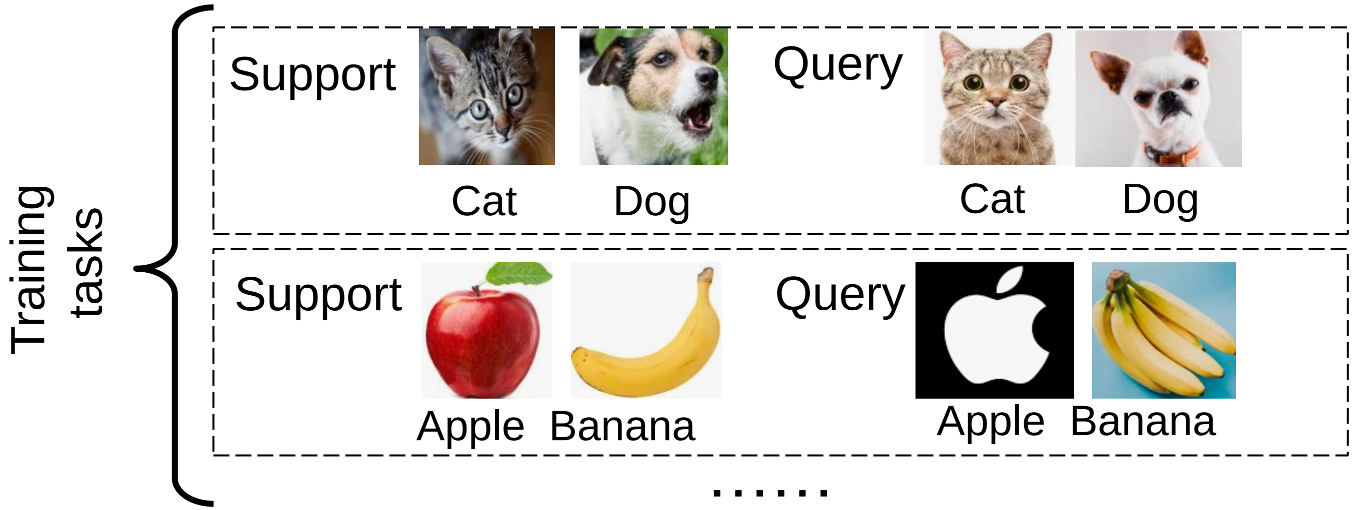
$f_{\phi'}($  $) \rightarrow \text{car}$

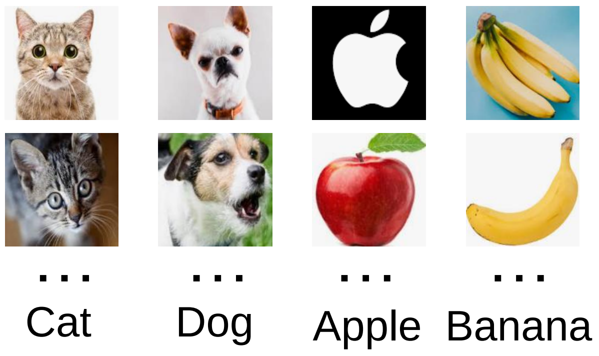
"Learn to learn"

[FAL17] Model-Agnostic Meta-Learning for Fast Adaptation of Deep Networks. C. Finn *et al*. ICML 2017.

Self-supervised learning

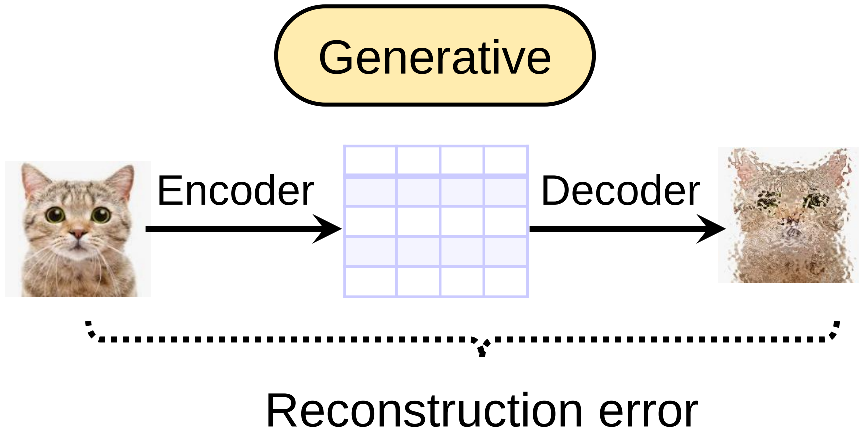
Meta-learning

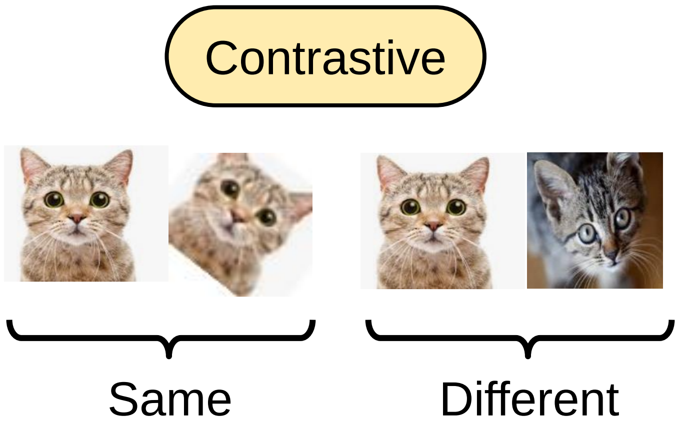




Still require many labels on these base classes to form training tasks

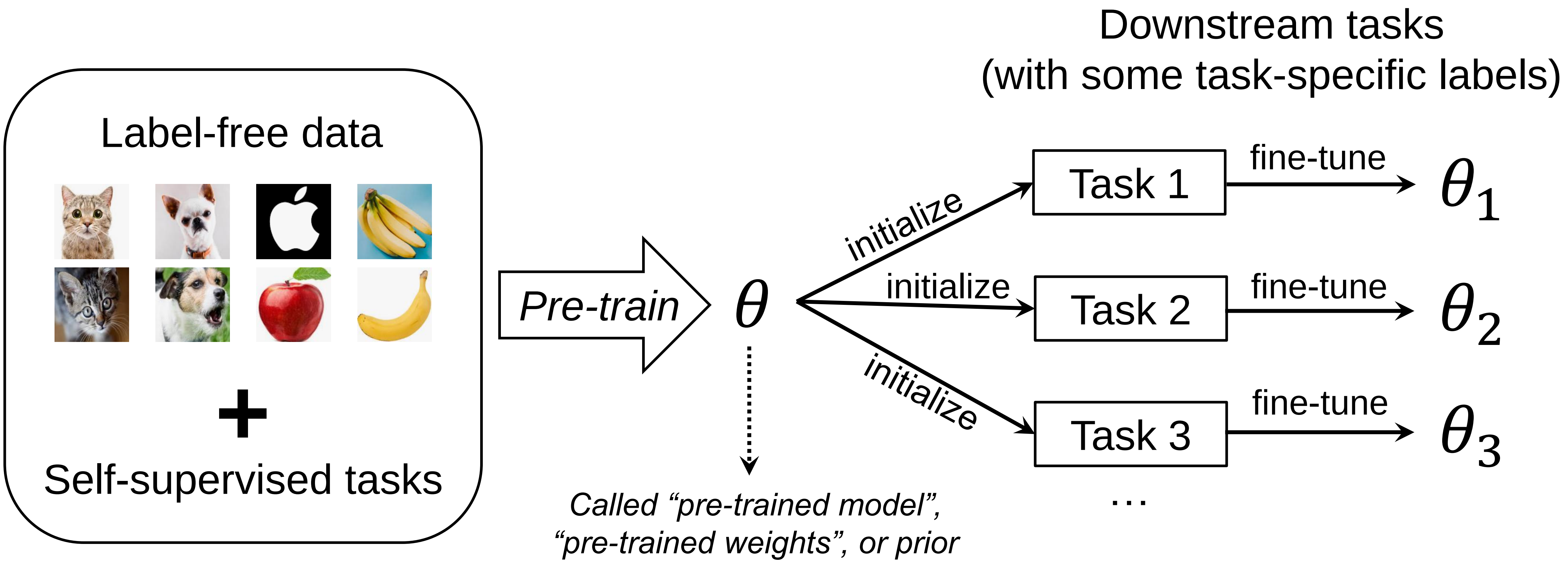
Self-supervised learning





“Free” supervision, no annotation cost!

Self-supervised learning / Pre-training

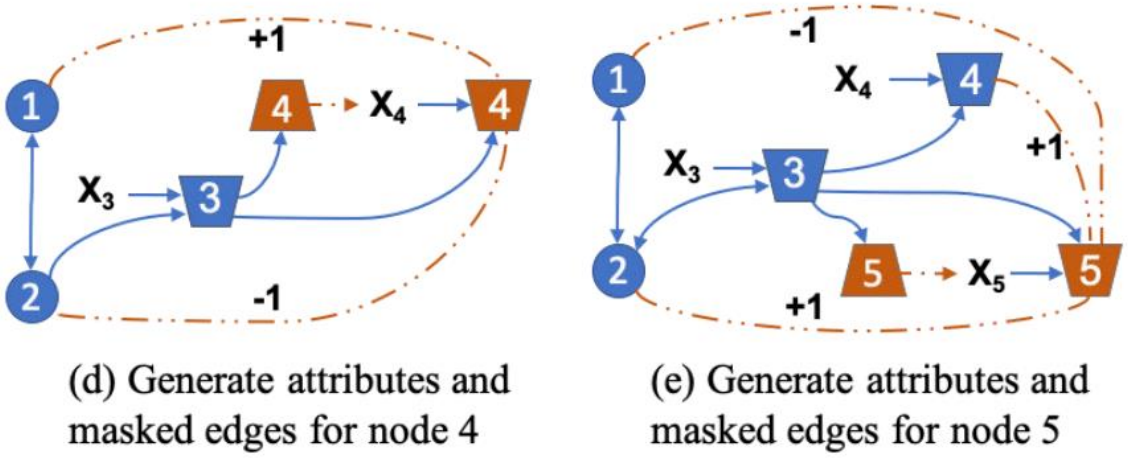


Graph pre-training: Generative vs. contrastive

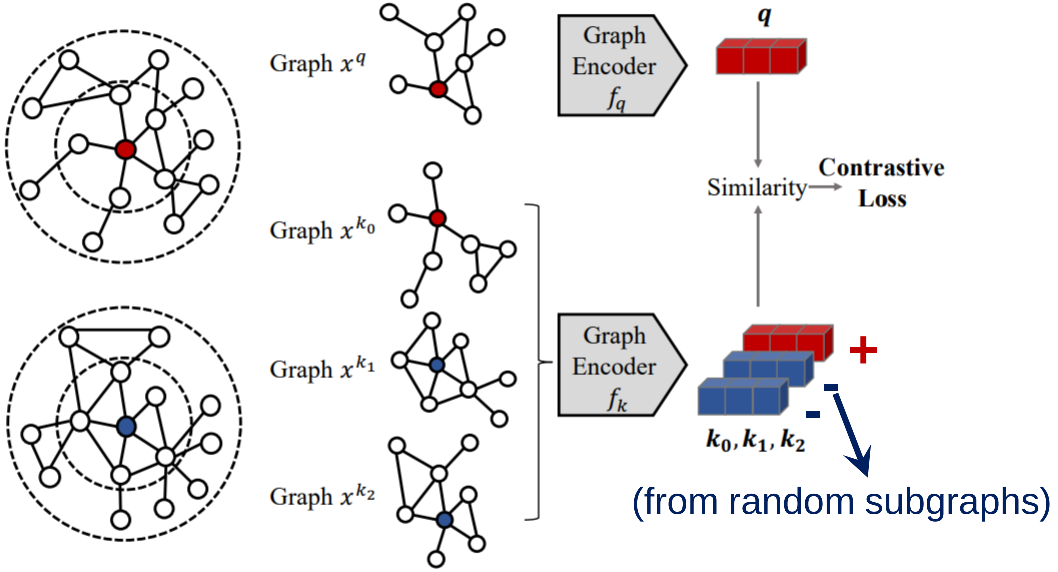
- Key: Design self-supervised pre-training tasks on graphs

Generative

Contrastive



[Image from HDW20]



[Image from QCD20]

[HDW20] GPT-GNN: Generative Pre-Training of Graph Neural Networks. Z. Hu *et al*. KDD 2020
[QCD20] GCC: Graph Contrastive Coding for Graph Neural Network Pre-Training. J. Qiu *et al*. KDD 2020

Graph pre-training: Spatial vs. Spectral

Spatial

Explicit (local) structures and node features

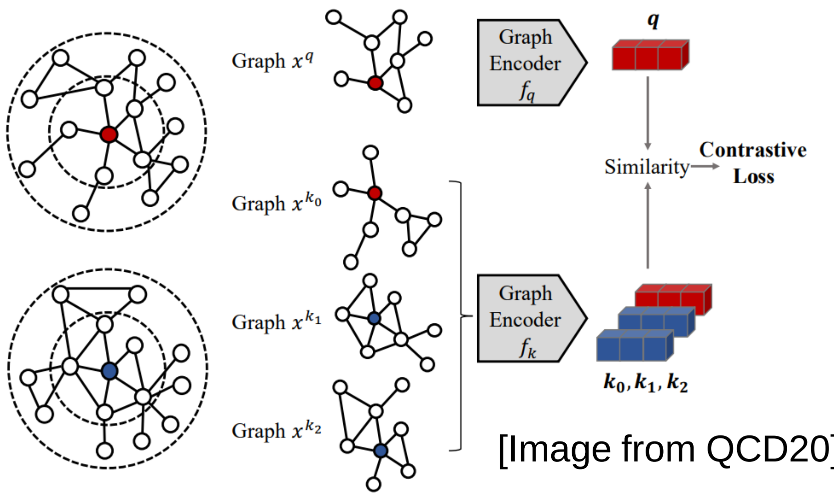
$$\mathbf{H}_a = f(\mathbf{A}, \mathbf{X})$$

Contrast

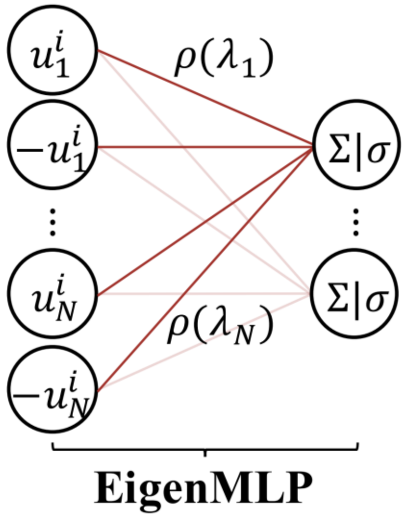
Spectral

Implicit node (global) positions on graph topology

$$\mathbf{H}_e = g(\mathbf{\Lambda}, \mathbf{U})$$



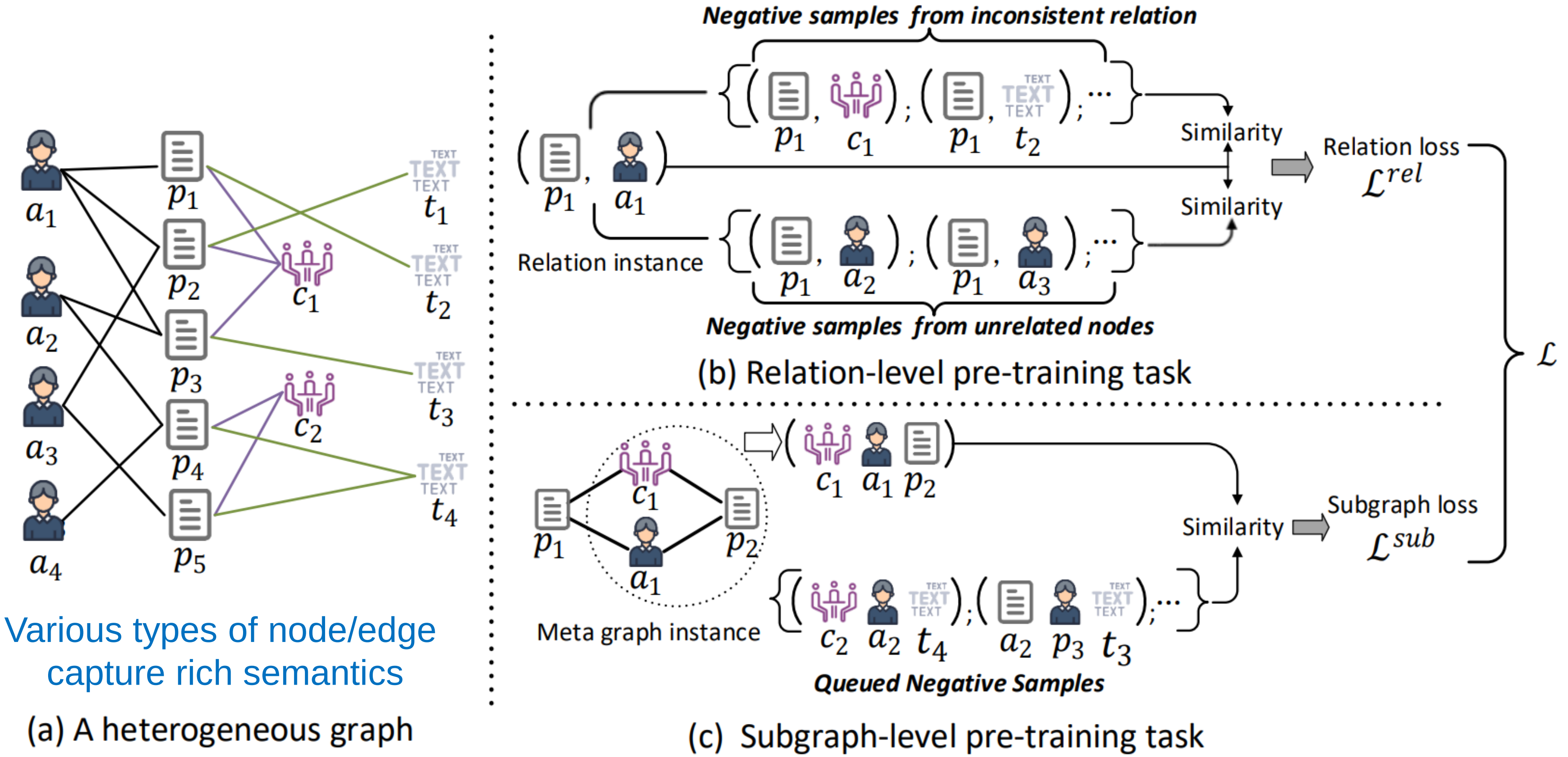
[Image from QCD20]



[NeurIPS23] Deyu Bo, Yuan Fang, Yang Liu, Chuan Shi. *Graph Contrastive Learning with Stable and Scalable Spectral Encoding*

Pre-training on heterogeneous graphs

- Pre-training tasks to capture relation- and subgraph-level semantics

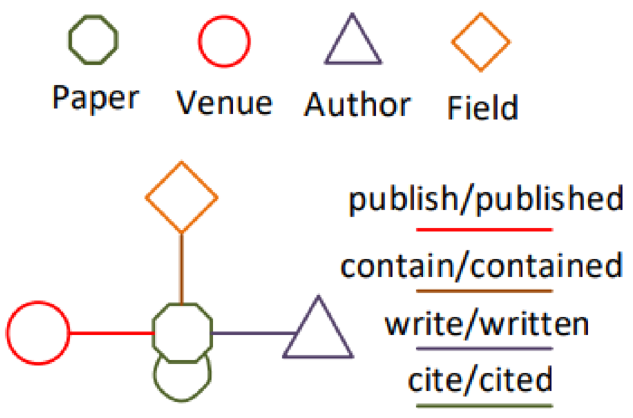


[CIKM21] X. Jiang, Y. Lu, Y. Fang and C. Shi. *Contrastive Pre-training of GNNs on Heterogeneous Graphs*

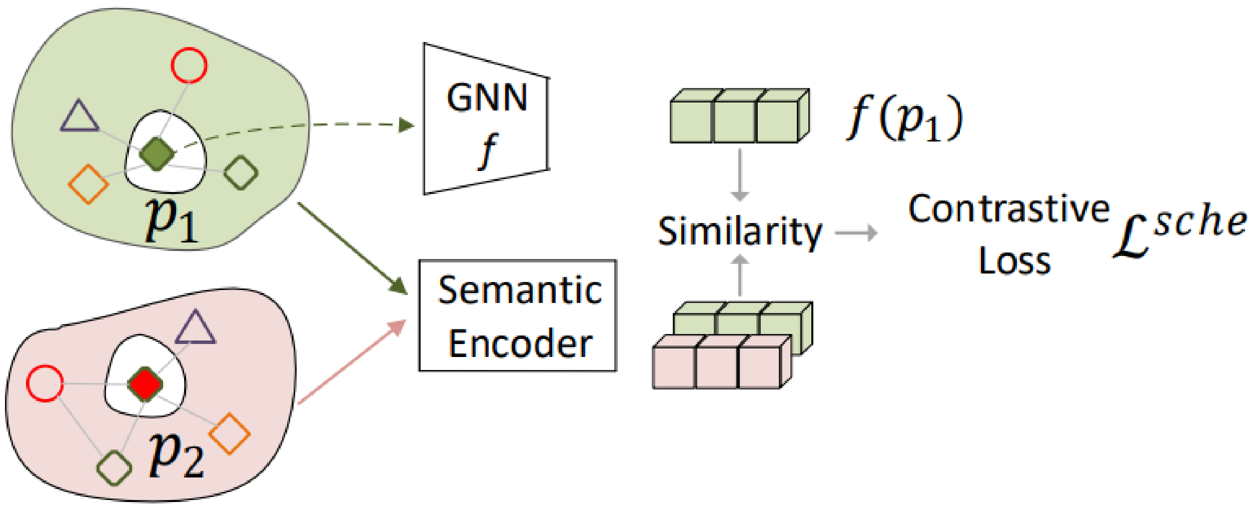
Pre-training on heterogeneous graphs

- Pre-training tasks to capture schema-level semantics

Schema



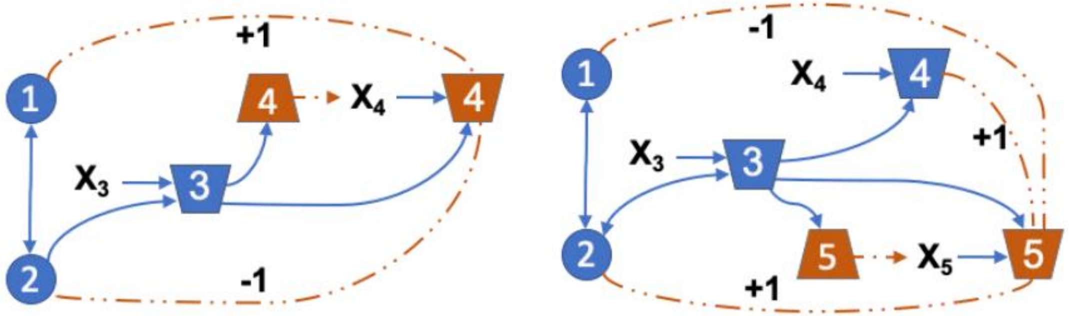
Schema-level task



[KDD21] X. Jiang, T. Jia, C. Shi, Y. Fang, Z. Lin and H. Wang. *Pre-training on Large-Scale Heterogeneous Graph.*

Problem with pre-training approaches

- The gap between pre-training and downstream objectives



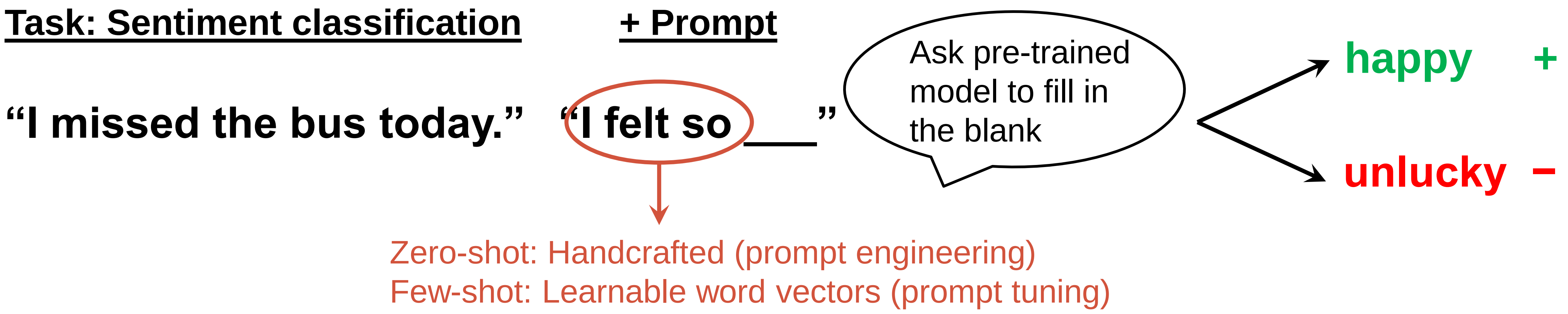
(d) Generate attributes and masked edges for node 4

(e) Generate attributes and masked edges for node 5

- And the fine-tuning step..
  - Can be expensive for large pre-trained models
  - may overfit if there are very few labels from downstream tasks

Bridging the gap: Pre-train, prompt

- **Problem:** Gap between pre-training and downstream tasks
- **Prompt** [LYF23]**:** an alternative to "pre-train, fine-tune"
  - Originated in NLP, an instruction to reformulate the original task to unify with pre-trained model (e.g., masked language modeling)



[LYF23] Pre-train, Prompt, and Predict: A Systematic Survey of Prompting Methods in Natural Language Processing. P. Liu, *et al*. ACM Computing Surveys: 55(9), 2023.

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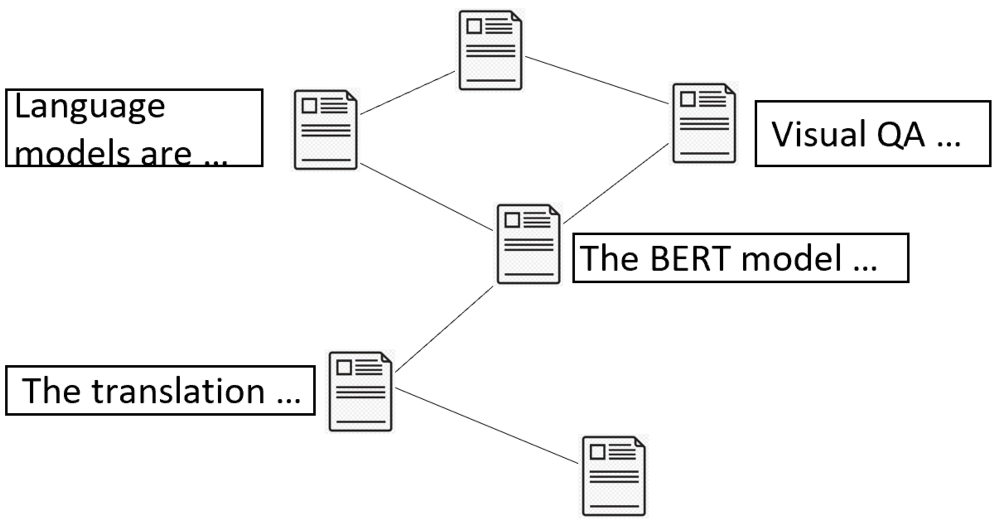
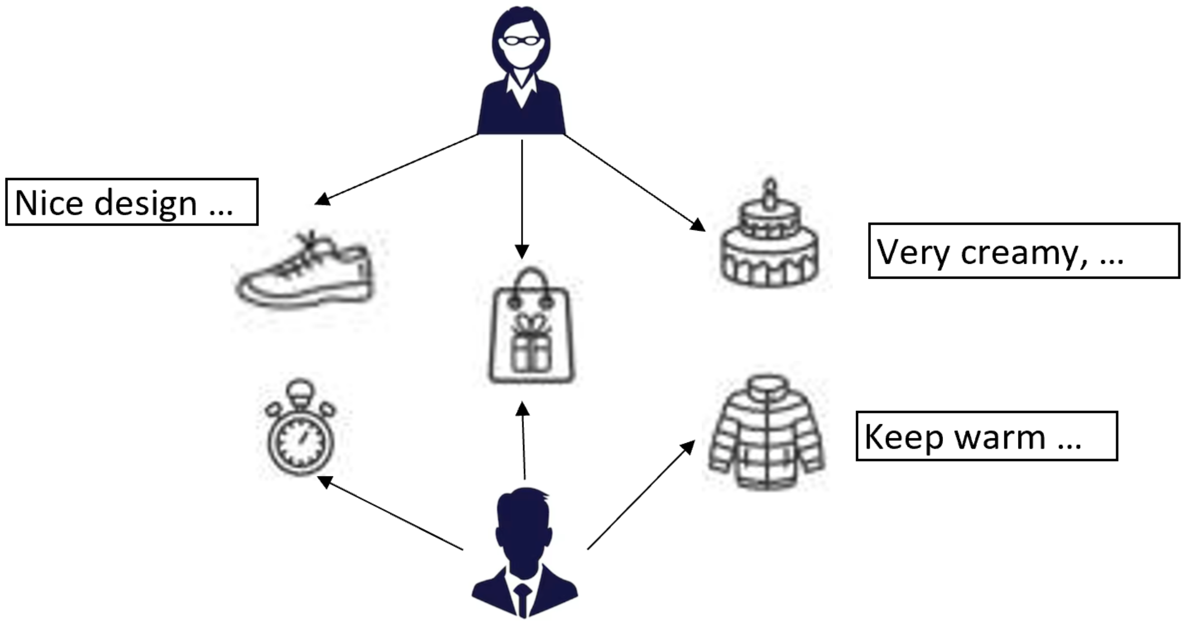
Graph data often associate with texts



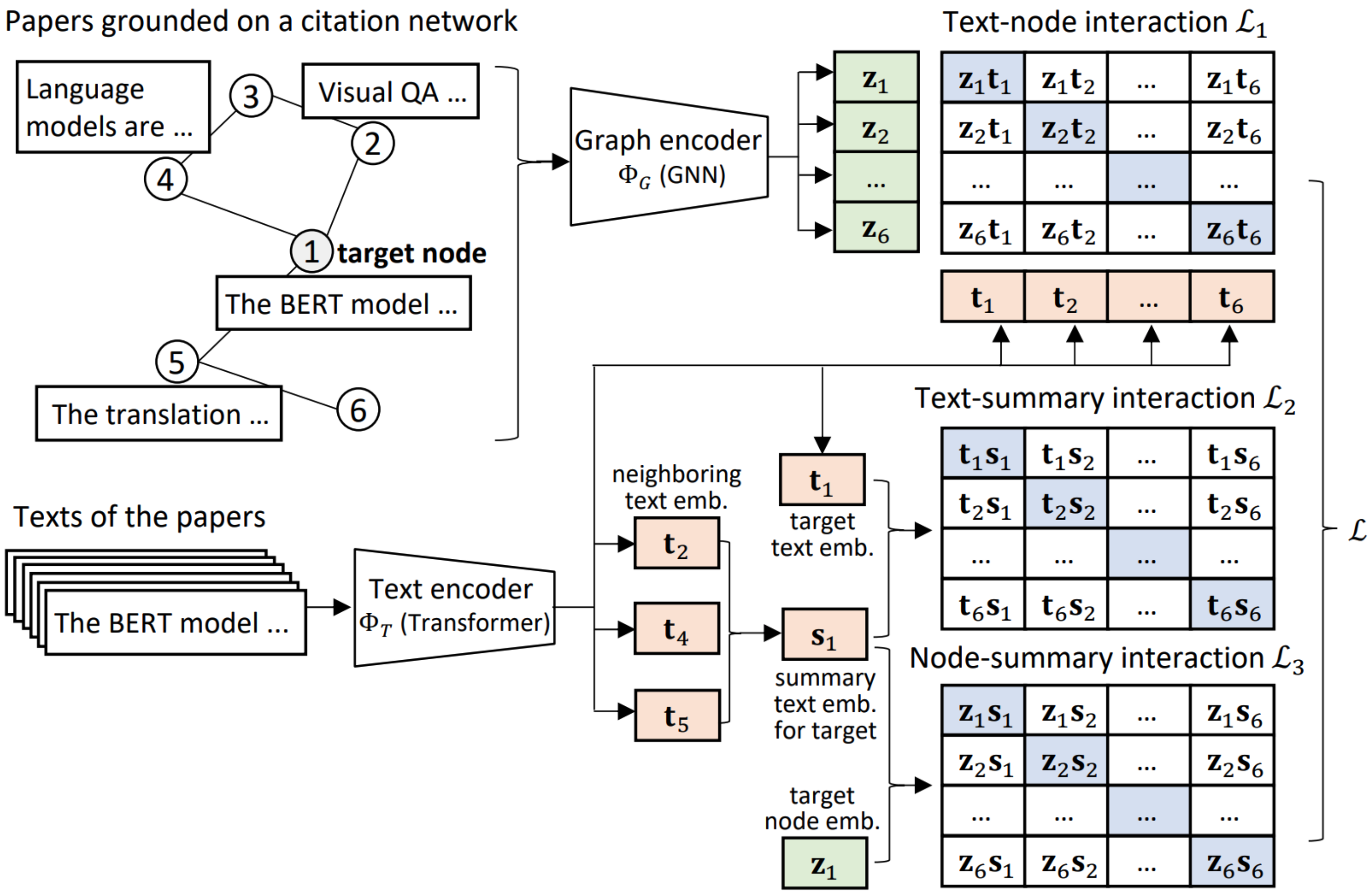
Citation graph for online articles



E-commerce item review graph

So, if there is a **jointly pre-trained graph-text model**, we can easily apply natural language-based prompts to graphs.

Graph-grounded **pre-training** and prompting (G2P2)



(a) Graph-grounded contrastive pre-training

Learns a dual-modal embedding space by jointly training a **text encoder** and **graph encoder**

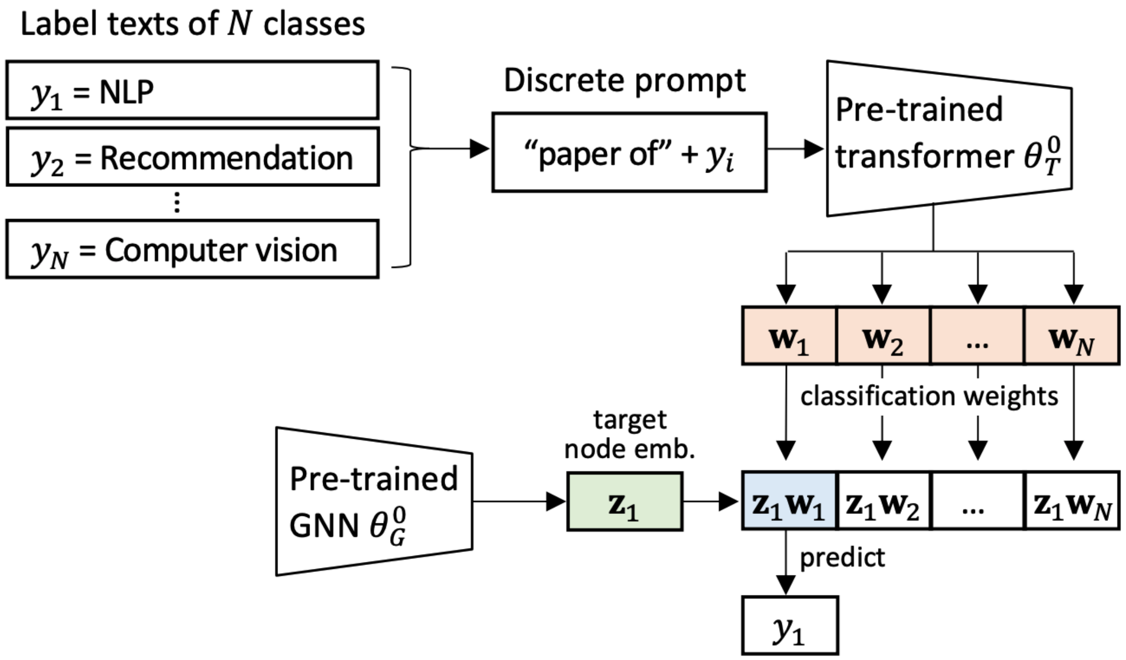
Exploits **three contrastive strategies**

- Text-node contrast
- Text-summary contrast
- Node-summary contrast

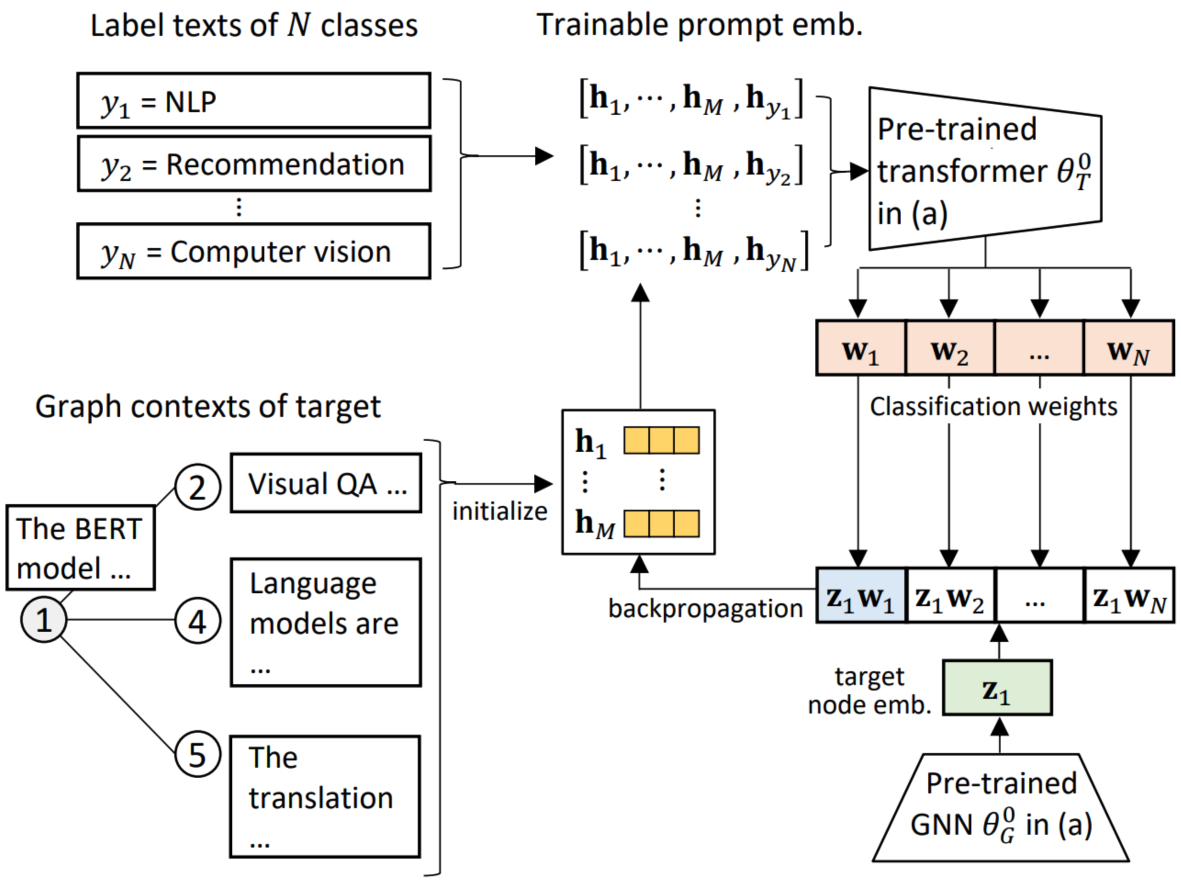
[SIGIR23] Z. Wen and Y. Fang. *Augmenting Low-Resource Text Classification with Graph-Grounded Pre-training and Prompting.*

Graph-grounded pre-training and **prompting** (G2P2)

Zero-shot node classification with discrete prompts

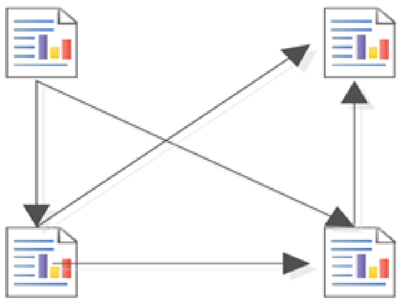


Few-shot node classification with continuous prompt tuning

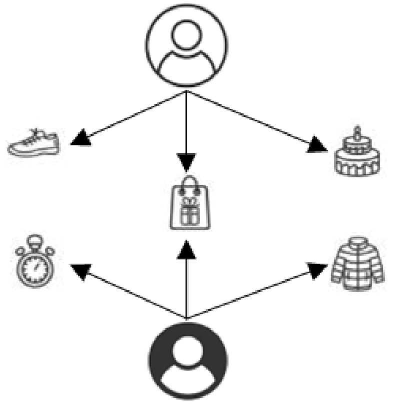


Datasets to evaluate G2P2

Dataset	Cora	Art	Industrial	M.I.
# Documents	25,120	1,615,902	1,260,053	905,453
# Links	182,280	4,898,218	3,101,670	2,692,734
# Avg. doc length	141.26	54.23	52.15	84.66
# Avg. node deg	7.26	3.03	2.46	2.97
# Classes	70	3,347	2,462	1,191



Cora is a collection of research papers with citation links



Art, **Industrial** and **Music Instruments** (M.I.) are three Amazon review datasets

Empirical performance of G2P2

Group	Method	Cora Accuracy	Cora Macro-F1	Art Accuracy	Art Macro-F1	Industrial Accuracy	Industrial Macro-F1	M.I. Accuracy	M.I. Macro-F1
End-to-end GNN	GCN	41.15±2.41	34.50±2.23	22.47±1.78	15.45±1.14	21.08±0.45	15.23±0.29	22.54±0.82	16.26±0.72
	SAGE_{sup}	41.42±2.90	35.14±2.14	22.60±0.56	16.01±0.28	20.74±0.91	15.31±0.37	22.14±0.80	16.69±0.62
	TextGCN	59.78±1.88	55.85±1.50	43.47±1.02	32.20±1.30	53.60±0.70	45.97±0.49	46.26±0.91	38.75±0.78
Pre-trained GNN	GPT-GNN	76.72±2.02	72.23±1.17	65.15±1.37	52.79±0.83	62.13±0.65	54.47±0.67	67.97±2.49	59.89±2.51
	DGI	78.42±1.39	74.58±1.24	65.41±0.86	53.57±0.75	52.29±0.66	45.26±0.51	68.06±0.73	60.64±0.61
	$\text{SAGE}_{\text{self}}$	77.59±1.71	73.47±1.53	76.13±0.94	65.25±0.31	71.87±0.61	65.09±0.47	77.70±0.48	70.87±0.59
Pre-trained Transformers	BERT	37.86±5.31	32.78±5.01	46.39±1.05	37.07± 0.68	54.00±0.20	47.57±0.50	50.14±0.68	42.96±1.02
	BERT*	27.22±1.22	23.34±1.11	45.31±0.96	36.28±0.71	49.60±0.27	43.36±0.27	40.19±0.74	33.69±0.72
	RoBERTa	62.10±2.77	57.21±2.51	72.95±1.75	62.25±1.33	76.35±0.65	70.49±0.59	70.67±0.87	63.50±1.11
	RoBERTa*	67.42±4.35	62.72±3.02	74.47±1.00	63.35±1.09	77.08±1.02	71.44±0.87	74.61±1.08	67.78±0.95
Prompt tuning	P-Tuning v2	71.00±2.03	66.76±1.95	76.86±0.59	66.89±1.14	79.65±0.38	74.33±0.37	72.08±0.51	65.44±0.63
	G2P2-p	79.16±1.23	74.99±1.35	79.59±0.31	68.26±0.43	80.86±0.40	74.44±0.29	81.26±0.36	74.82±0.45
	G2P2	**80.08***±1.33	**75.91***±1.39	**81.03***±0.43	**69.86***±0.67	**82.46***±0.29	**76.36***±0.25	**82.77***±0.32	**76.48***±0.52
	(improv.)	(+2.12%)	(+1.78%)	(+5.43%)	(+4.44%)	(+3.53%)	(+2.7%)	(+6.53%)	(+7.92%)

G2P2 outperforms the best baseline by around 3–7%.

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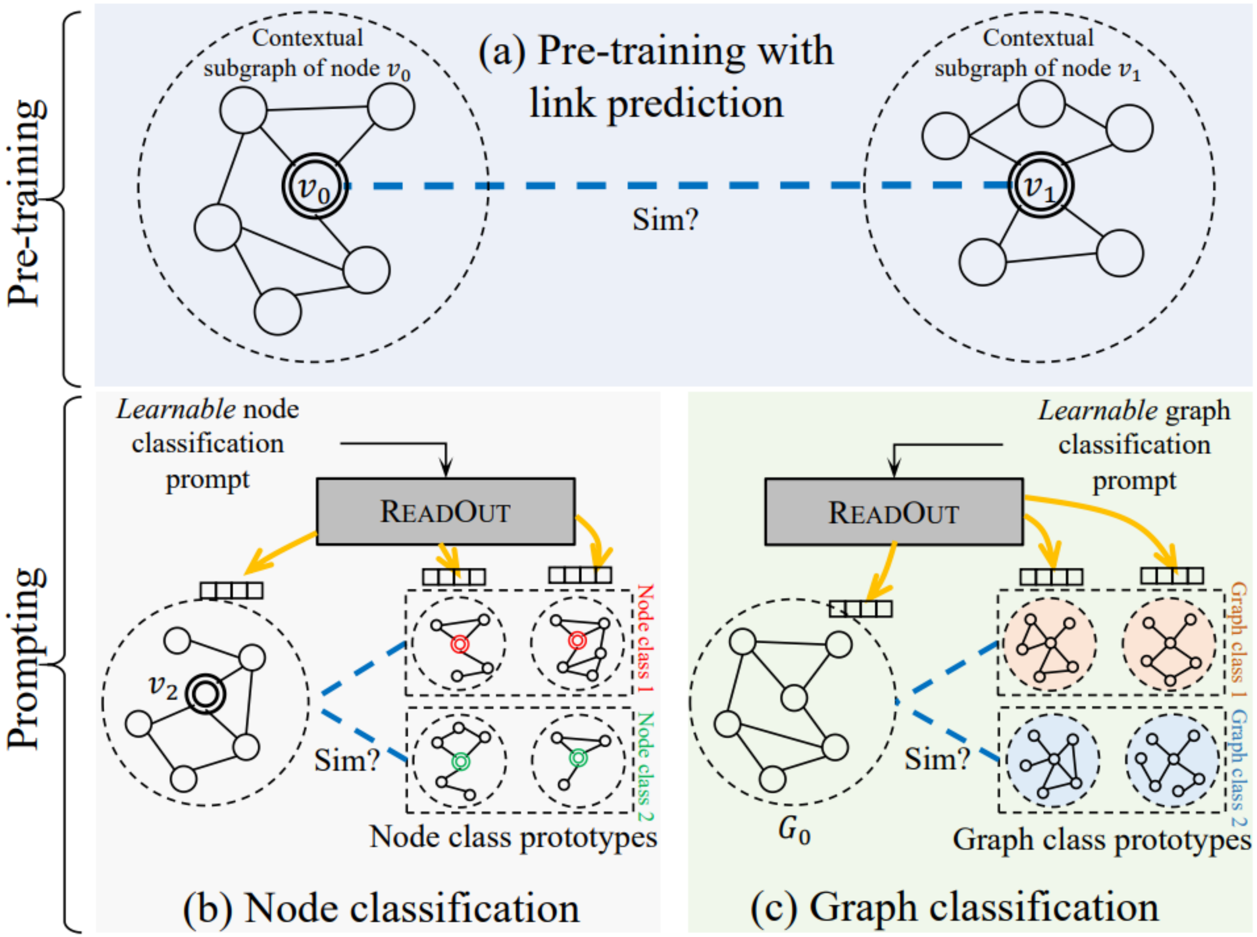
GraphPrompt: Pre-train, prompt on **graph only**

- Two challenges
  - How to unify various pre-training and downstream tasks on graph?
  - How to design prompts on graph?
- Insights
  - A **unified task template** based on subgraph similarity computation
  - Use a **learnable prompt** to guide graph readout for different tasks



[WWW23] Z. Liu, X. Yu, Y. Fang and X. Zhang. *GraphPrompt: Unifying Pre-Training and Downstream Tasks for Graph Neural Networks.*

GraphPrompt: Pre-train, prompt on **graph only**

Unified task template

Link prediction

Triplet (v, a, b), s.t. v is linked to a, but not b:

$$\mathrm{sim}(\mathbf{s}_v, \mathbf{s}_a) > \mathrm{sim}(\mathbf{s}_v, \mathbf{s}_b)$$

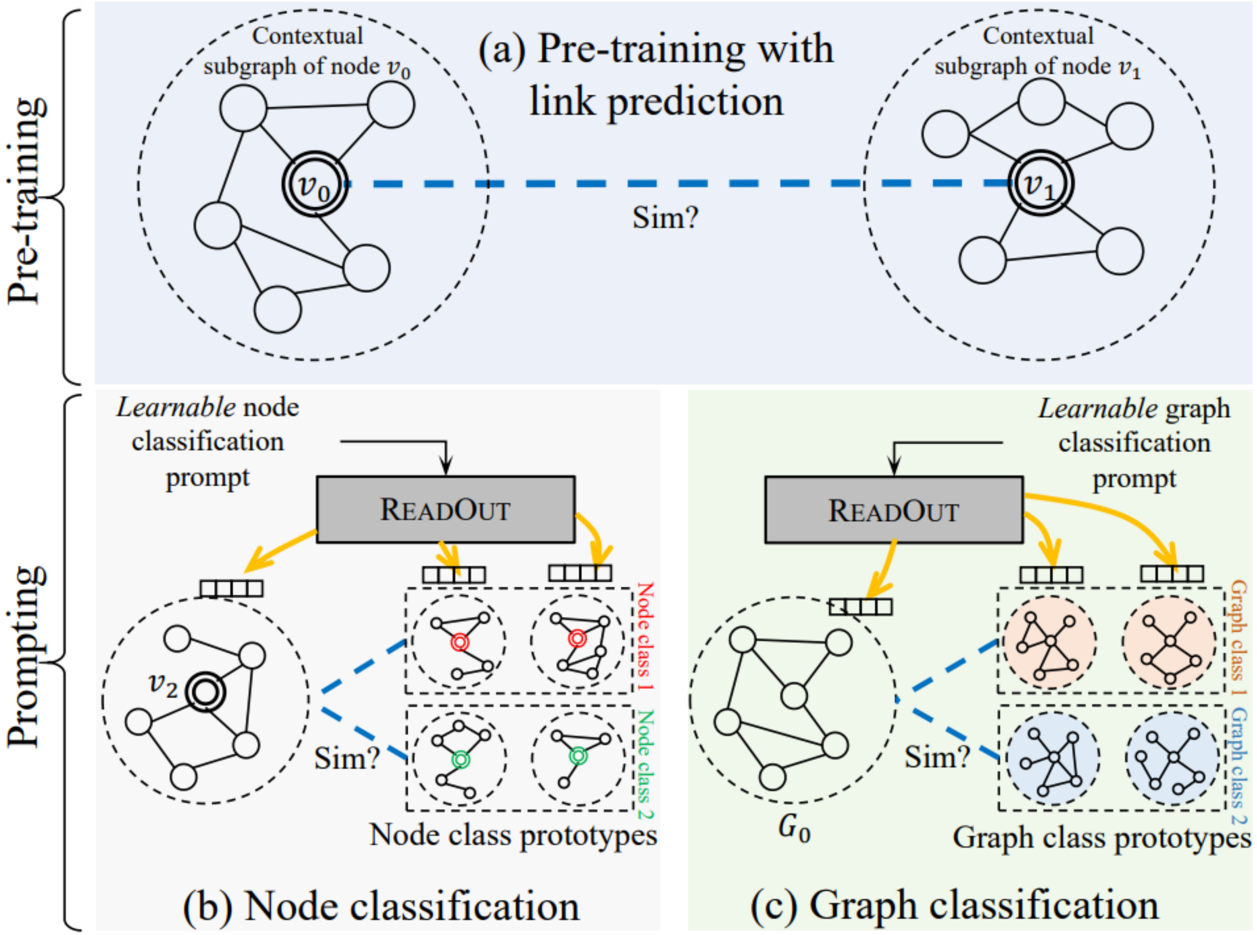
Node classification

$$\ell_j = \arg\max_{c \in C} \mathrm{sim}(\mathbf{s}_{v_j}, \tilde{\mathbf{s}}_c)$$

Graph classification

$$L_j = \arg\max_{c \in C} \mathrm{sim}(\mathbf{s}_{G_j}, \tilde{\mathbf{s}}_c)$$

All tasks converted to subgraph similarity computation!



$\mathbf{s}_x$: (sub)graph embedding of x (x is a node or graph)

$\tilde{\mathbf{s}}_c$: class c's prototype (a virtual subgraph, by aggregates all subgraph embeddings in the class)

GraphPrompt: Pre-train, prompt on **graph only**

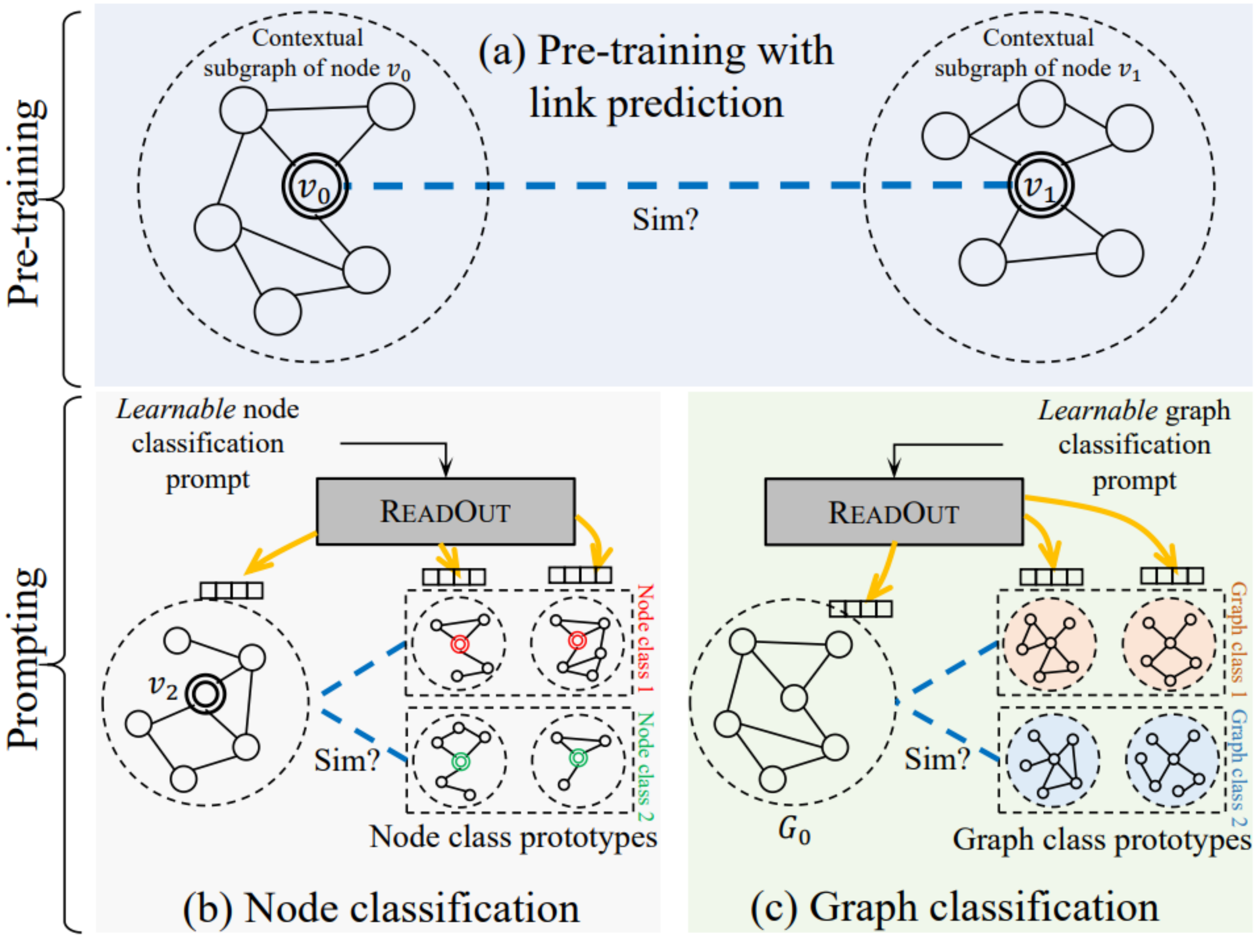
Prompt design

Different downstream tasks require different subgraph readout
→ Use task-specific learnable prompts

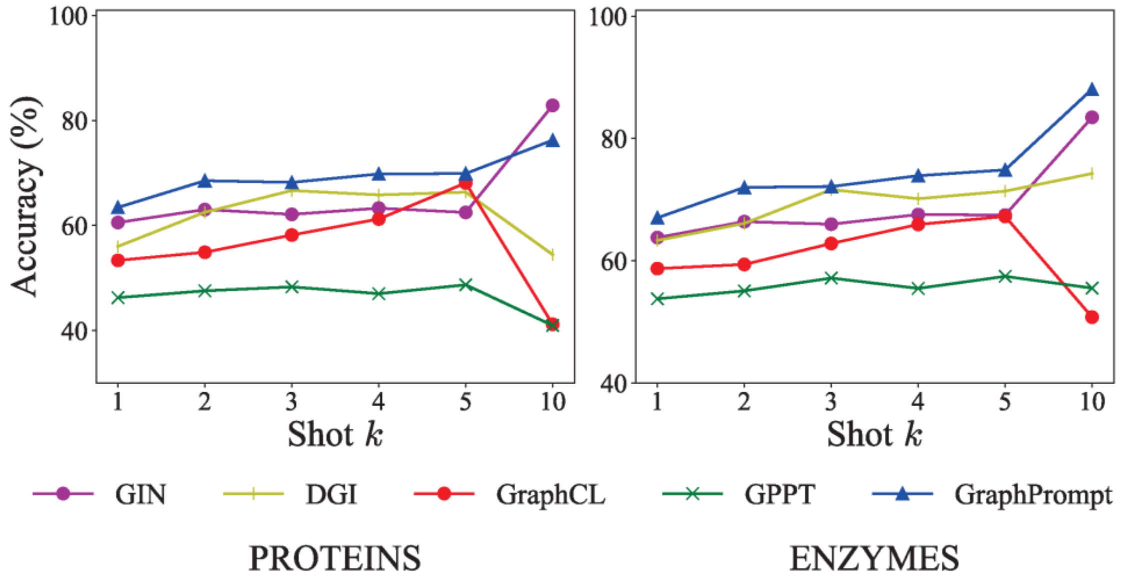
Prompt vector added to the readout layer of the pre-trained GNN

$$\mathbf{s}_{t,x} = \textsc{ReadOut}(\{\mathbf{p}_t \odot \mathbf{h}_v : v \in V(S_x)\})$$

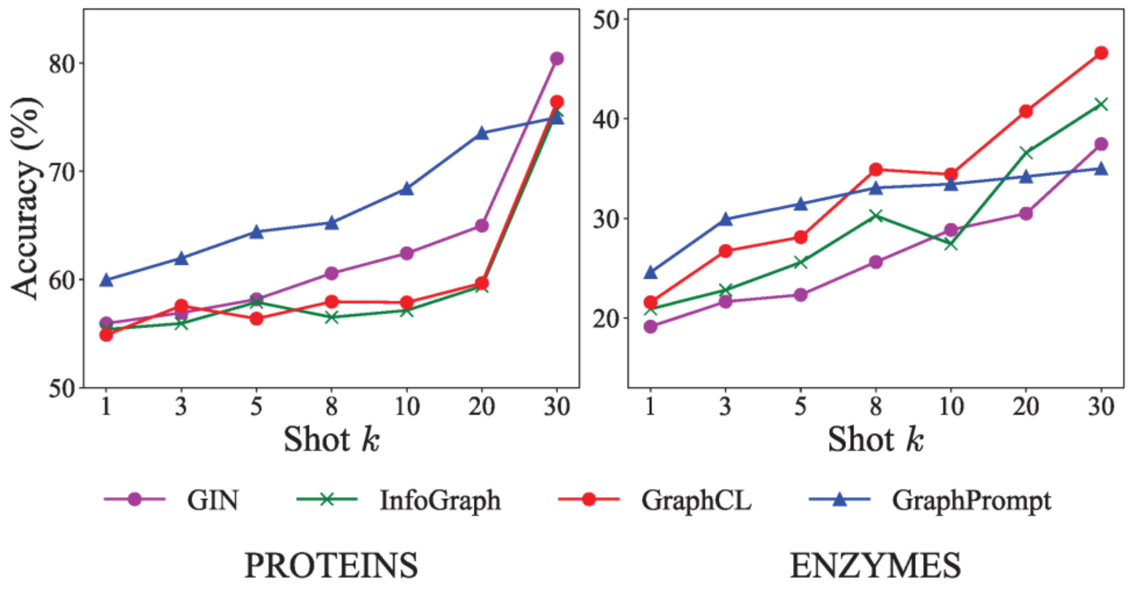
$\mathbf{s}_{t,x}$: (sub)graph embedding of x for a task t
$\mathbf{h}_v$: node v's embedding vector
$\mathbf{p}_t$ or $\mathbf{P}_t$: learnable prompt vector or matrix for task t



GraphPrompt: Pre-train, prompt on **graph only**



Impact of shots on few-shot node classification.



Impact of shots on few-shot graph classification.

<u>Few-shot:</u> Significantly better

<u>10-shot:</u> Still competitive
(as graphs are small – 10 shots are a lot)

<u>Few-shot:</u> Significantly better

<u>On ENZYMES:</u> worse performance on ≥20 shots
(only 600 graphs – 20 shots/class ~ 20% labels)

GraphPrompt: Pre-train, prompt on **graph only**

Comparison of parameter efficiency

Significantly fewer parameters/FLOPs than:

- *Supervised model (GIN [XHL19]),*
- *"Pretrain, fine-tune" model (GraphPrompt-ft),*
- *Existing prompt model (GPPT [SZH22])*

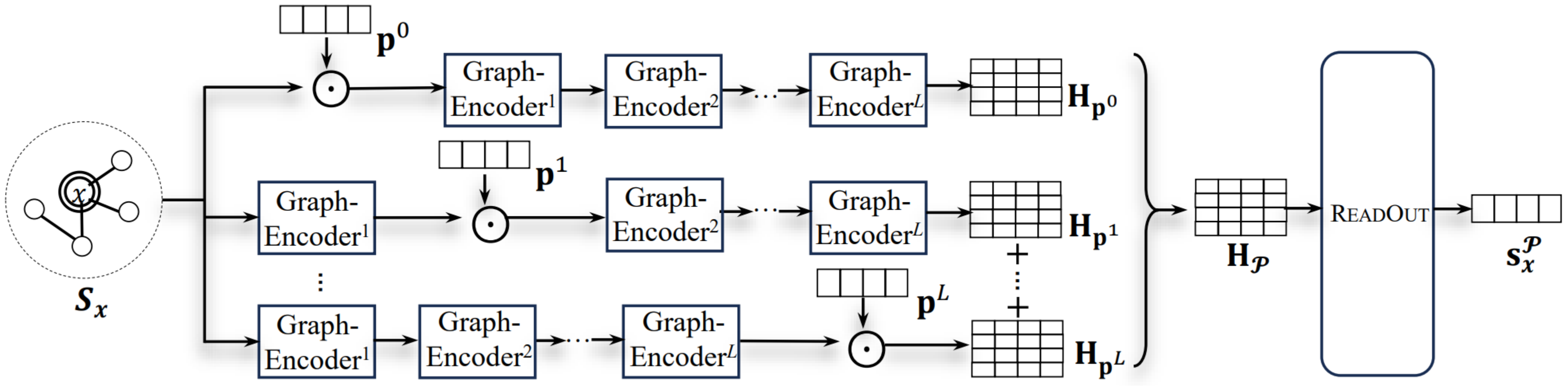
Methods	Flickr	
	Params	FLOPs
GIN	22,183	240,100
GPPT	4,096	4,582
GraphPrompt	96	96
GraphPrompt-ft	21,600	235,200

Methods	PROTEINS		ENZYMES	
	Params	FLOPs	Params	FLOPs
GIN	5,730	12,380	6,280	11,030
GPPT	1,536	1,659	1,536	1,659
GraphPrompt	96	96	96	96
GraphPrompt-ft	6,176	13,440	6,176	10,944

[XHL19] How Powerful are Graph Neural Networks? K. Xu *et al*. ICLR 2019
[SZH22] GPPT: Graph Pre-training and Prompt Tuning to Generalize Graph Neural Networks. M. Sun *et al*. KDD 2022

Generalized Graph Prompt

- Support more pre-training tasks beyond link prediction
  - DGI, InfoGraph, GraphCL, GCC, …
- Layer-wise prompts



Generalized Graph Prompt: Toward a Unification of Pre-Training and Downstream Tasks on Graphs. Xingtong Yu, Zhenghao Liu, Yuan Fang, Zemin Liu, Sihong Chen, Xinming Zhang. https://arxiv.org/pdf/2311.15317.pdf

HGPrompt: Extending to heterogeneous graphs

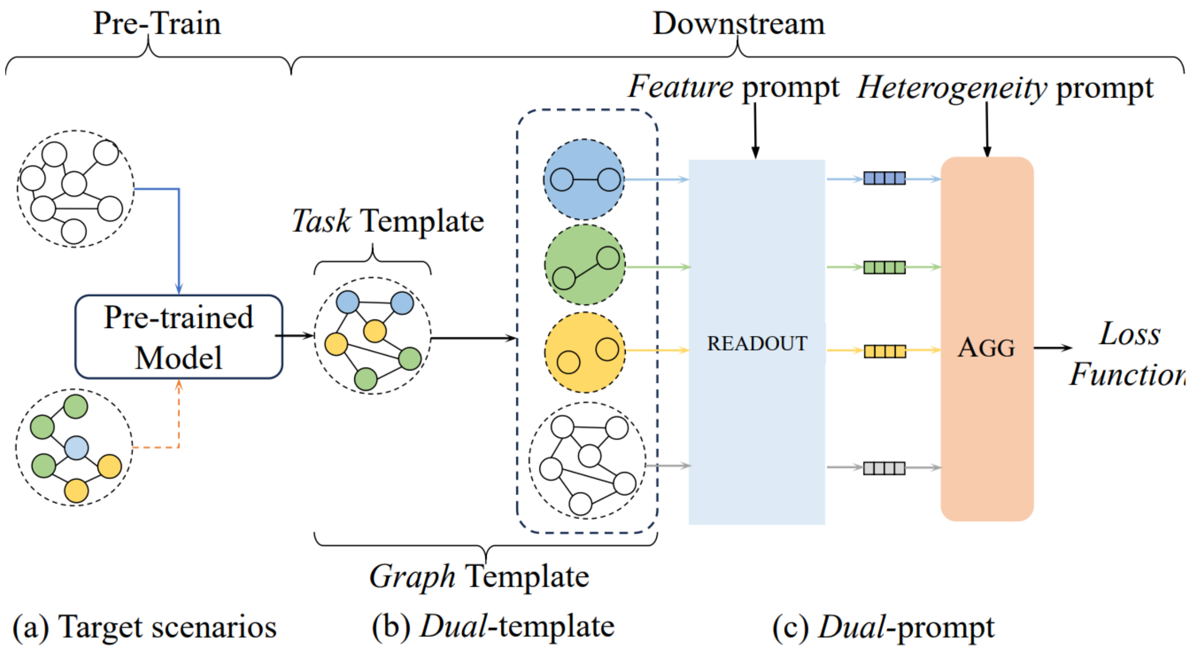
Two challenges

- Gap between homogeneous and heterogeneous graph
- Different downstream tasks focus on heterogeneous aspect

Insights

- Dual-template:
  Task + Graph template

- Dual-prompt:
  Feature + Heterogeneity prompt



[AAAI24] Xingtong Yu, Yuan Fang, Zemin Liu and Xinming Zhang. *HGPrompt: Bridging Homogeneous and Heterogeneous Graphs for Few-shot Prompt Learning.* https://arxiv.org/pdf/2312.01878.pdf

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Conclusion

- Few-shot learning on graphs: different kinds of graphs/tasks
- Learning and transferring/using prior is the key
- Prompt is a promising paradigm…

Jiawei Liu, Cheng Yang, Zhiyuan Lu, Junze Chen, Yibo Li, Mengmei Zhang, Ting Bai, Yuan Fang, Lichao Sun, Philip S. Yu, Chuan Shi. **Towards Graph Foundation Models: A Survey and Beyond.** https://arxiv.org/pdf/2310.11829.pdf

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Thank you

Questions?

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