GCoT: Chain-of-Thought Prompt Learning for Graphs

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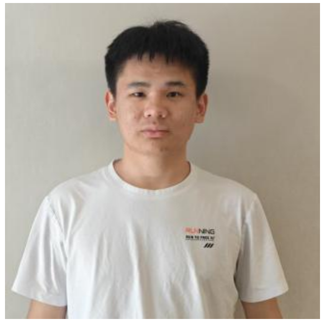

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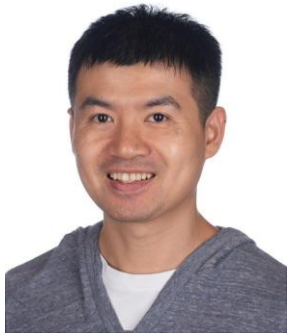

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Outline

- **Introduction**
- Proposed method: GCoT
- Experiments
- Conclusions

Chain-of-Thought Prompting

- Existing text-free graph learning methods produce a "final answer" **in a single inference step**.

- Would **introducing additional inference steps in a CoT style** enhance the ability of pre-trained graph models to refine their predictions?

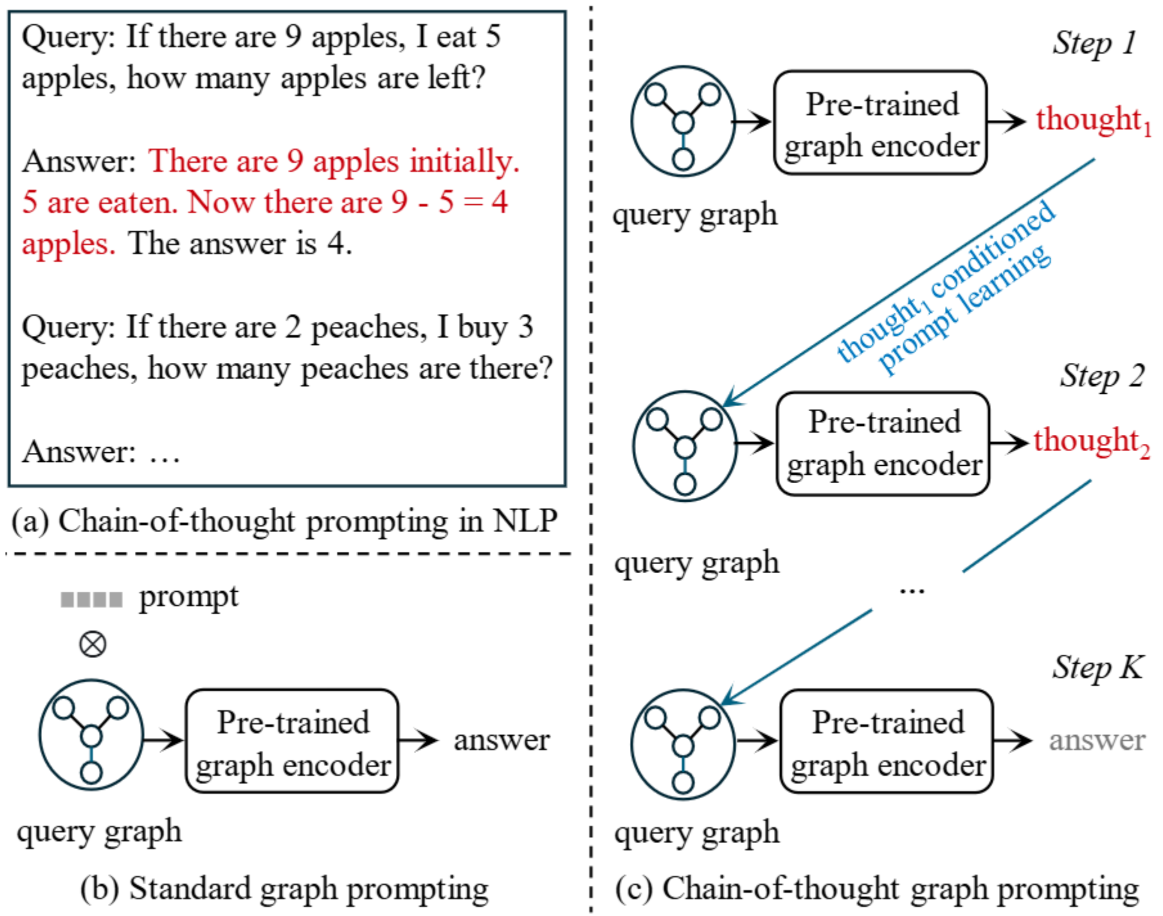


Figure 1: Illustration of chain-of-thought in NLP, standard graph prompts and graph chain-of-thought prompting.

Chain-of-Thought Prompting

- CoT prompt in NLP could be **handcrafted**.
- **⟨input, chain of thought, output⟩.**
- CoT prompt in NLP **serves as an example** to guide the model in generating intermediate thoughts that lead to the final answer.

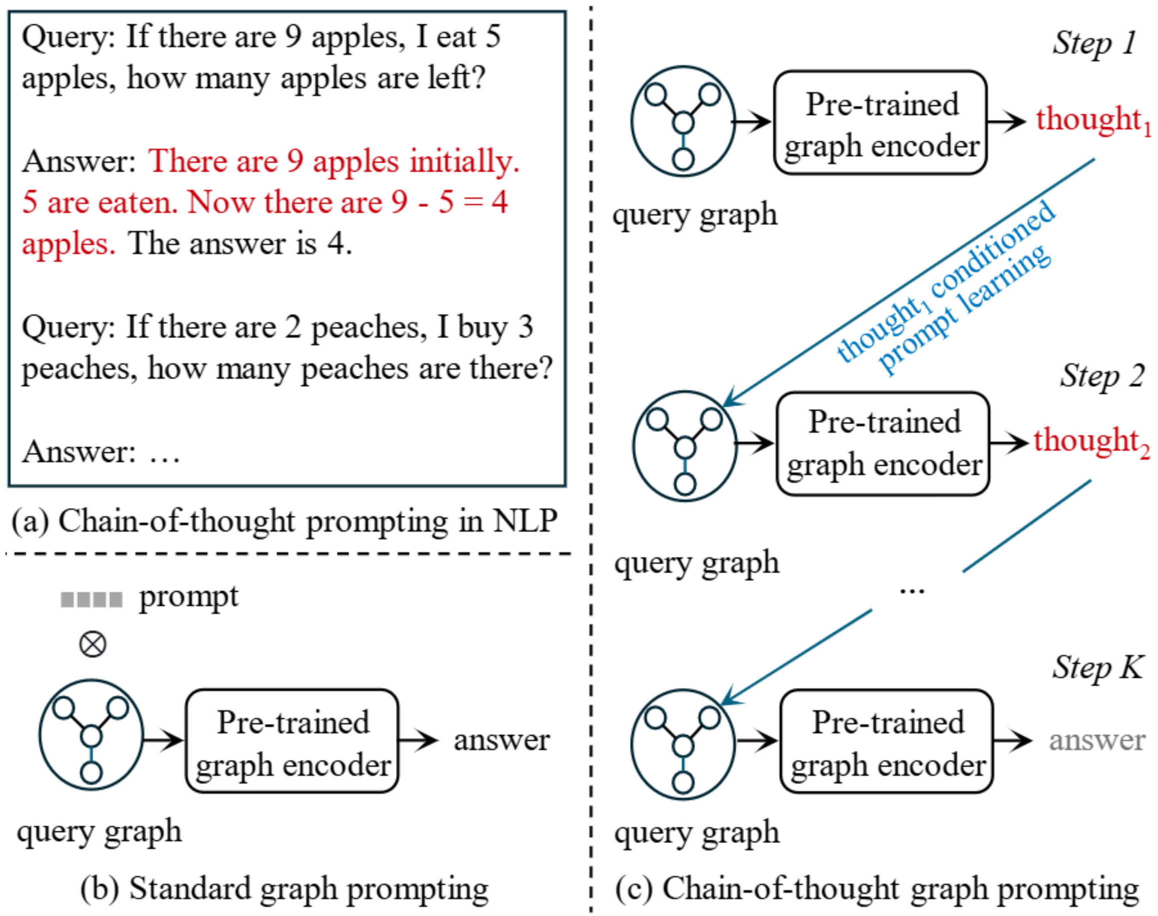
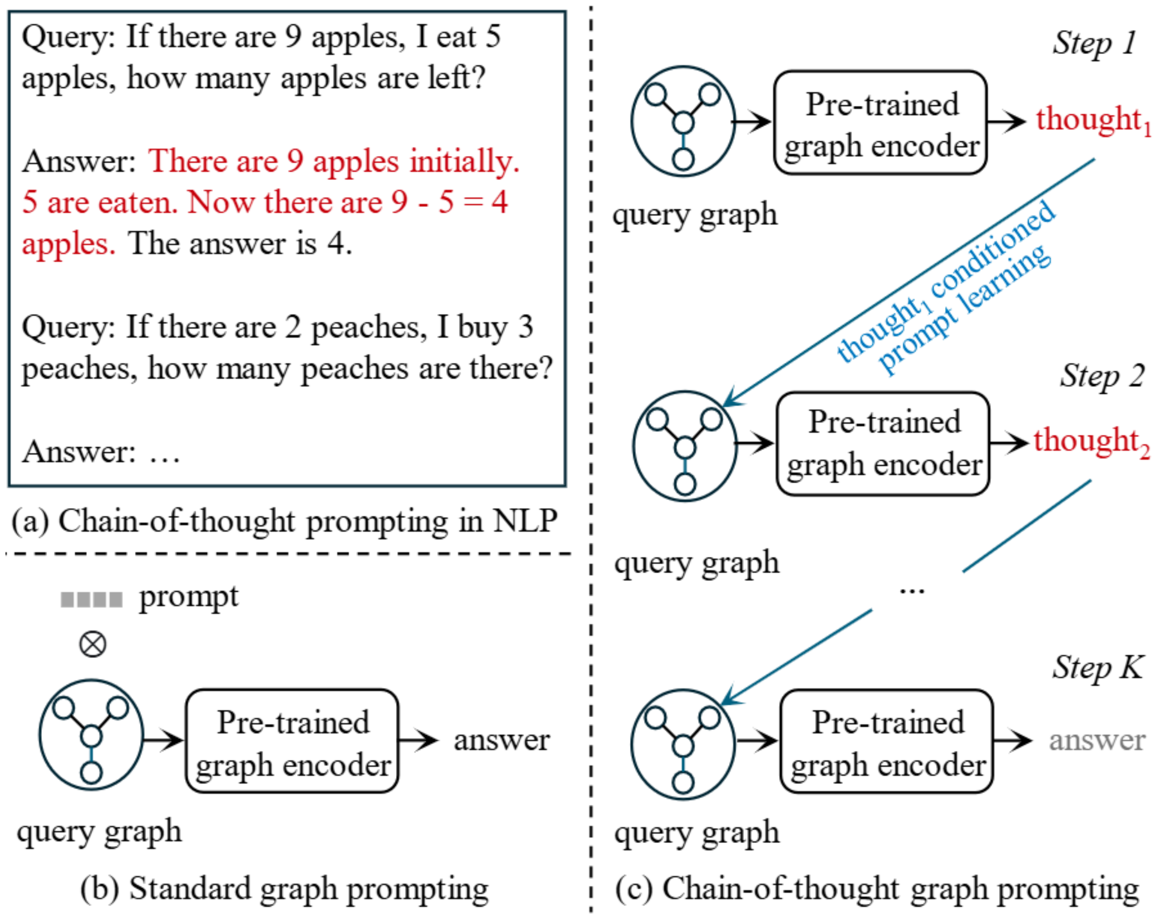


Figure 1: Illustration of chain-of-thought in NLP, standard graph prompts and graph chain-of-thought prompting.

Chain-of-Thought Prompting

- What should be the **inference steps** and **thoughts** for a graph task?

- How can we leverage a “thought” to **learn prompts** and **guide the next-step inference**?



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GCoT

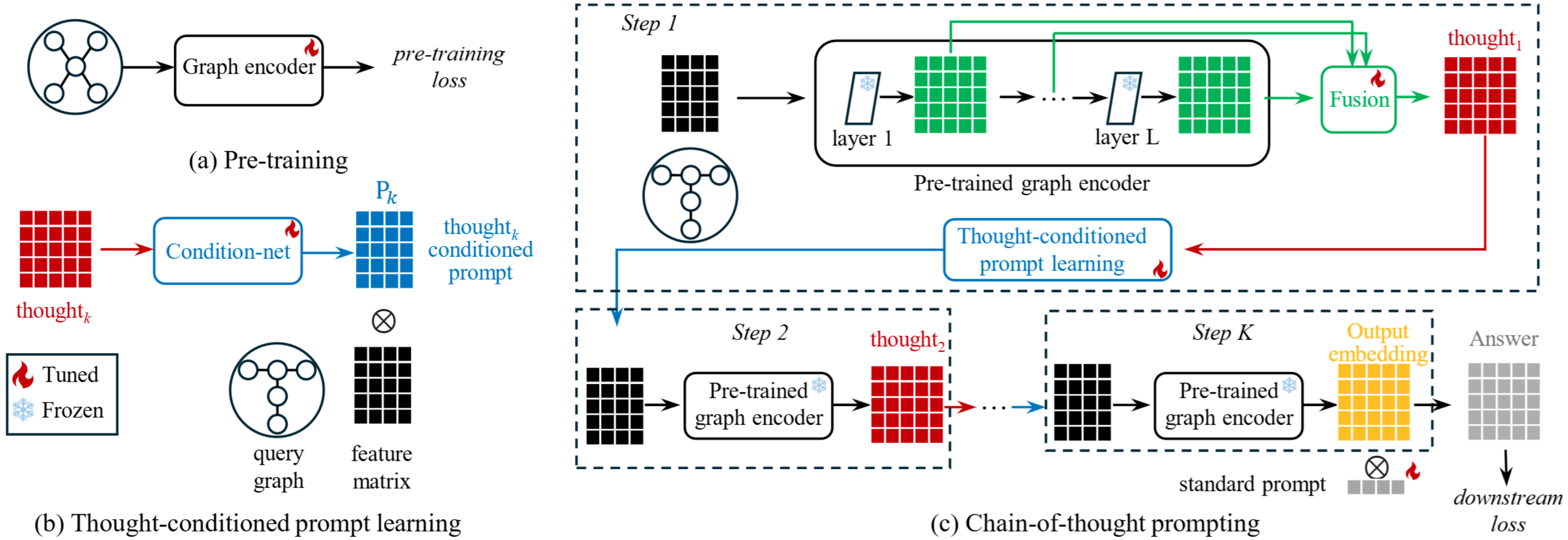
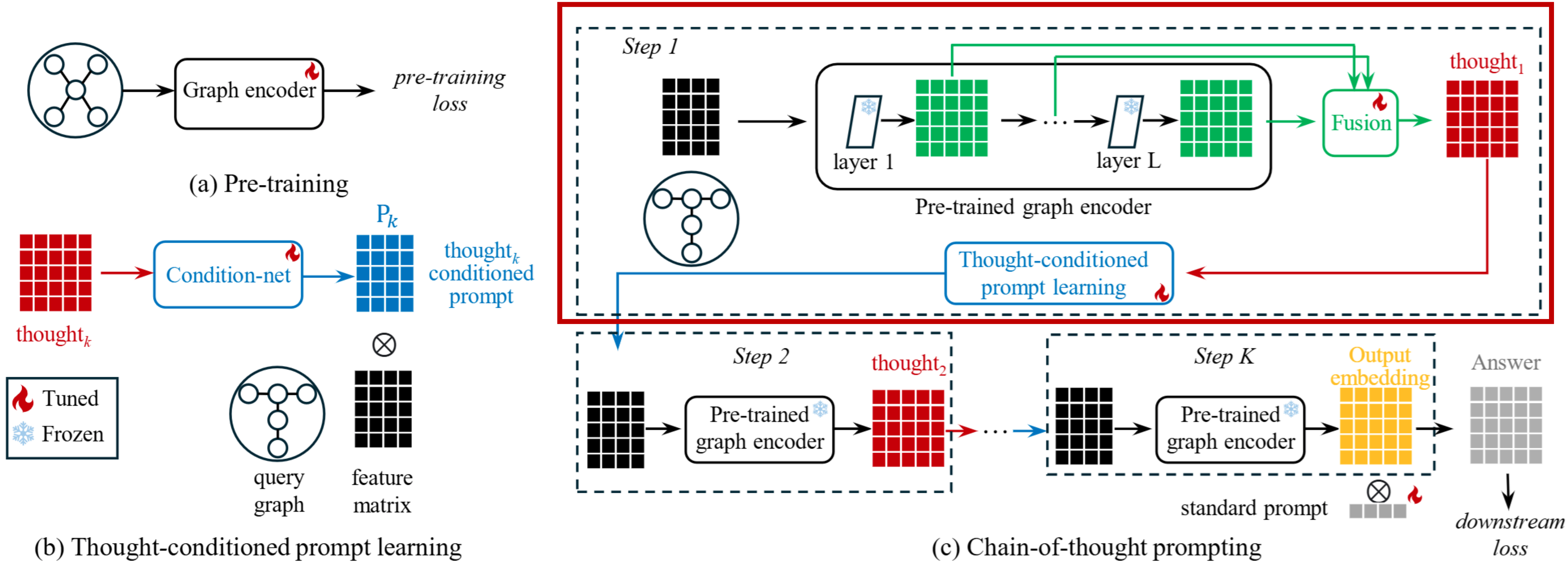


Figure 2: Overall framework of GCoT.

Yu, et al. "GCoT: Chain-of-Thought Prompt Learning for Graphs." SIGKDD'25.

GCoT



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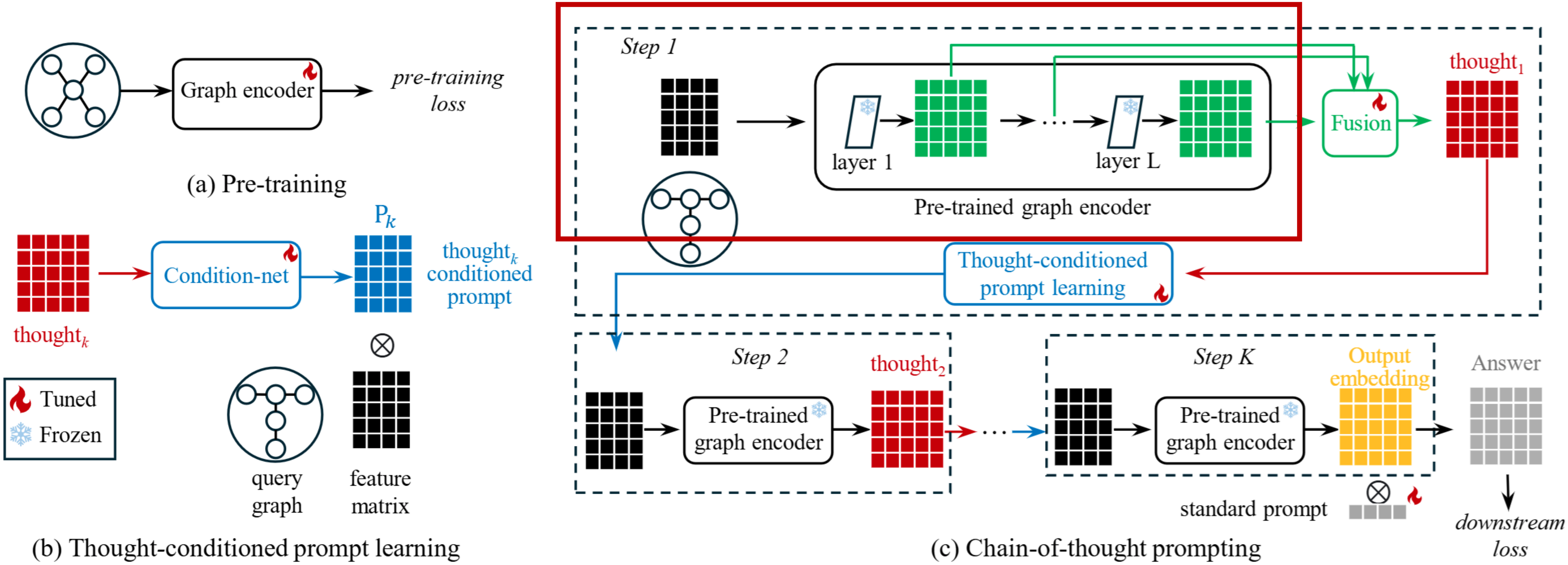
GCoT

Prompt-based inference $\{\mathbf{H}_k^1, \mathbf{H}_k^2, \cdots, \mathbf{H}_k^L\} = \textsc{GraphEncoder}(\mathbf{X}_k, G; \Theta_0)$



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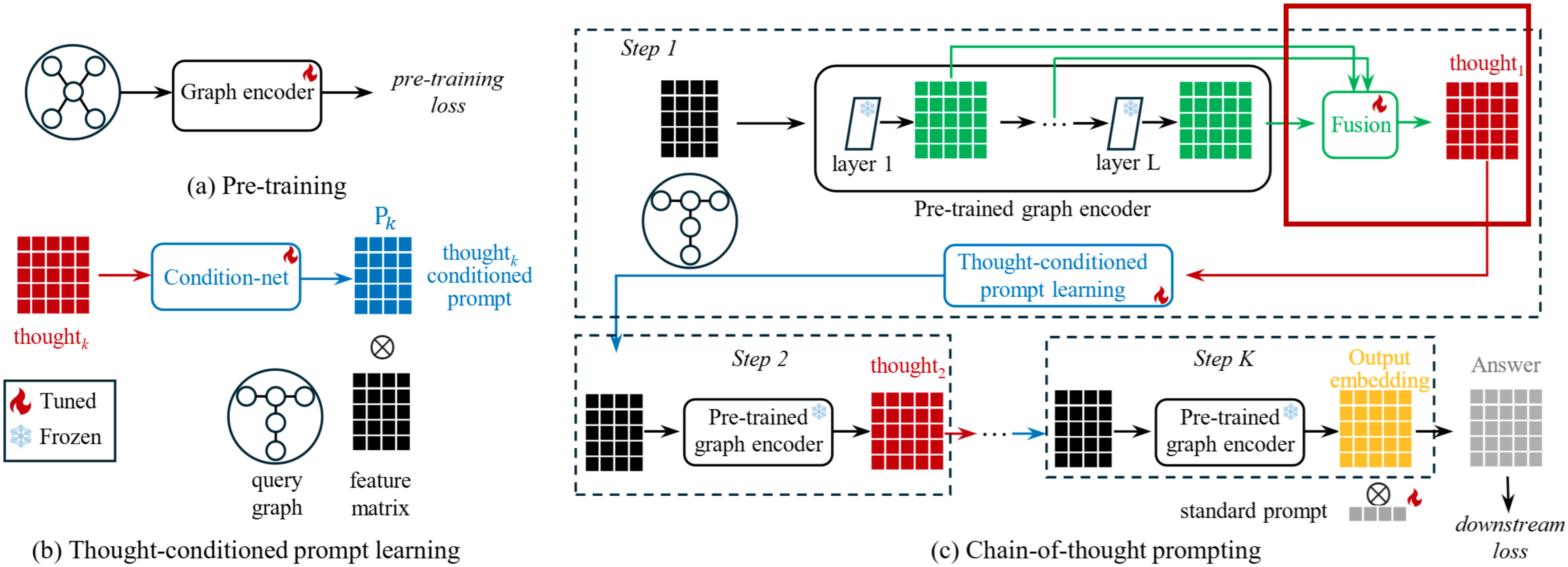
GCoT

$$\mathbf{T}_k = \textsc{Fuse}(\mathbf{H}_k^1, \mathbf{H}_k^2, \cdots, \mathbf{H}_k^L)$$

Thought construction



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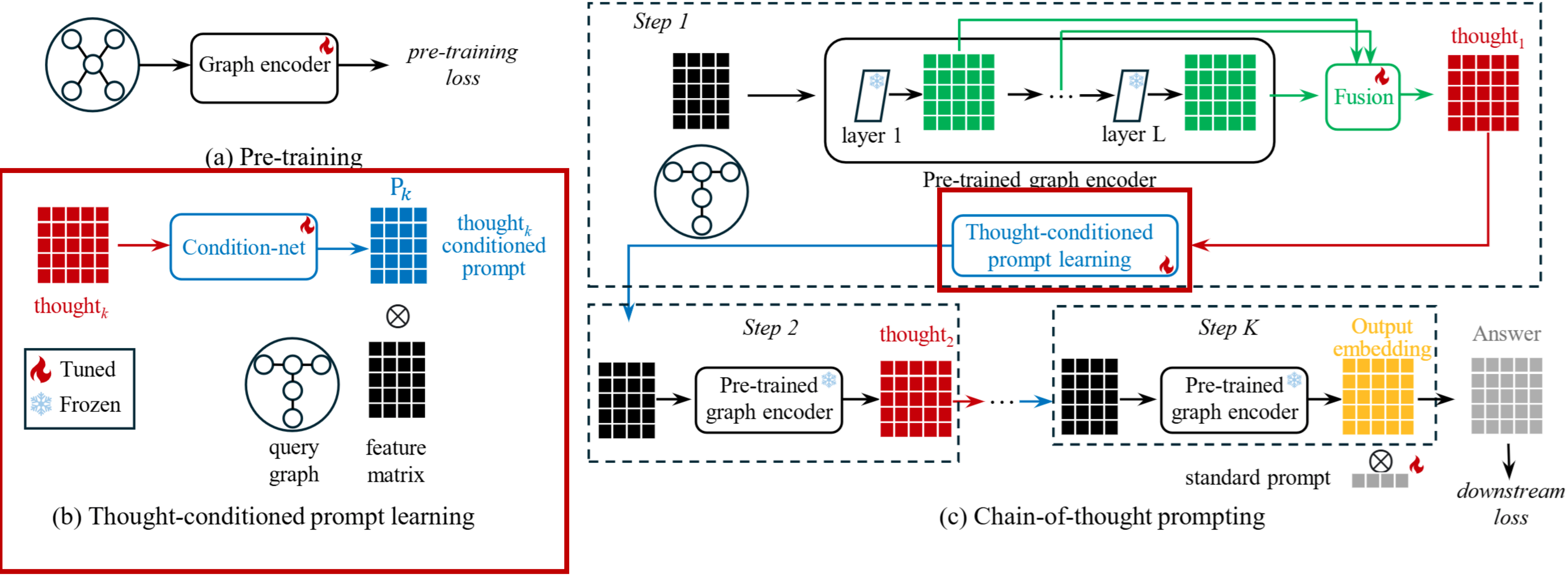
GCoT



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Thought-conditioned prompt learning

$$\mathbf{P}_k = \textsc{CondNet}(\mathbf{T}_k; \phi) \quad \mathbf{X}_{k+1} = \mathbf{P}_k \odot \mathbf{X}$$

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Experiment

Table 2: Accuracy (%) evaluation of node and graph classification.

Methods	Node classification				Graph classification			
	Cora	Citeseer	Pubmed	Photo	MUTAG	COX2	BZR	PROTEINS
GCN	32.50 ± 14.21	26.36 ± 9.03	52.18 ± 8.70	60.18 ± 12.04	43.44 ± 15.14	50.95 ± 23.48	47.25 ± 16.59	40.28 ± 0.03
GAT	31.00 ± 16.22	27.71 ± 8.74	50.02 ± 8.88	51.79 ± 12.85	37.33 ± 10.81	50.58 ± 26.16	46.55 ± 16.57	40.39 ± 0.04
DGI/InfoGraph	54.11 ± 9.60	45.00 ± 9.19	47.46 ± 12.19	58.89 ± 10.97	53.17 ± 17.29	53.82 ± 14.19	49.33 ± 15.11	52.51 ± 10.29
GraphCL	51.96 ± 9.43	43.12 ± 9.61	46.80 ± 9.04	57.78 ± 11.31	54.92 ± 17.09	53.81 ± 14.21	49.73 ± 14.66	53.81 ± 8.97
ProG	50.59 ± 14.64	43.17 ± 8.49	63.07 ± 11.96	66.50 ± 9.46	51.99 ± 4.50	53.45 ± 15.01	53.52 ± 11.97	52.73 ± 6.57
GPF	<u>57.60</u> ± 13.88	43.11 ± 8.80	55.63 ± 10.96	65.29 ± 10.07	56.55 ± 13.95	54.16 ± 14.07	48.65 ± 13.96	53.05 ± 7.62
GPF+	57.42 ± 13.87	43.28 ± 8.82	57.16 ± 10.99	65.07 ± 10.01	<u>56.81</u> ± 12.93	<u>55.24</u> ± 13.29	50.83 ± 19.74	<u>54.58</u> ± 8.70
GraphPrompt	54.25 ± 9.38	<u>45.34</u> ± 10.53	<u>63.11</u> ± 10.01	<u>66.62</u> ± 9.90	55.44 ± 12.56	54.34 ± 14.77	<u>54.59</u> ± 10.52	53.80 ± 7.93
GCoT	**59.67** ± 15.51	**46.21** ± 8.78	**64.43** ± 9.96	**67.16** ± 10.46	**58.75** ± 15.42	**56.26** ± 15.52	**58.03** ± 23.44	**56.24** ± 8.60

Best results are **bolded** and runner-up results are <u>underlined</u>.

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Experiment

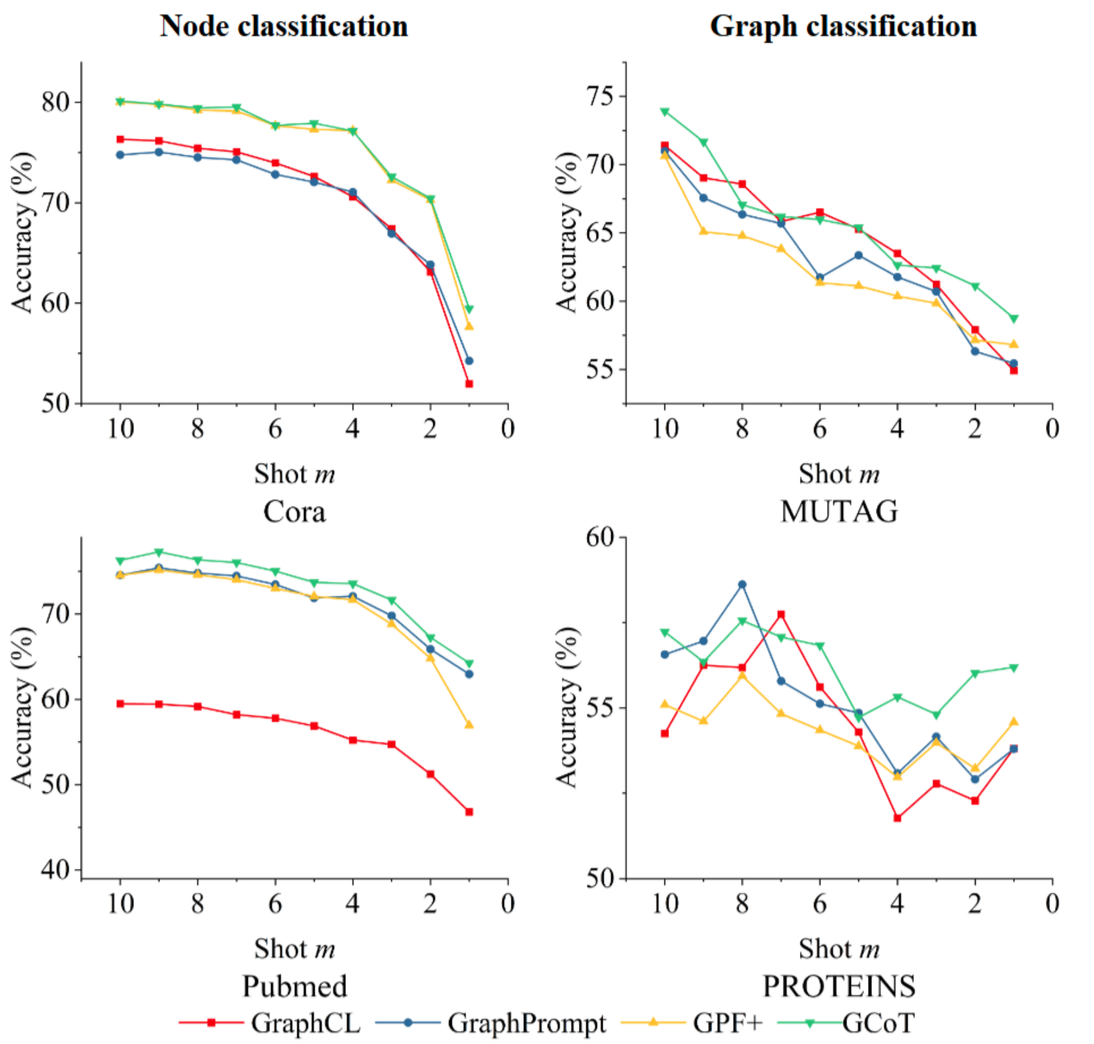

Figure 3: Impact of labeled data size (number of shots) on node and graph classification.

Table 3: Ablation study on the effects of key components.

Methods	Node classification		Graph classification	
	Cora	Pubmed	MUTAG	PROTEINS
GCoT\CoT	56.65±13.97	62.80±10.08	56.49±16.61	53.40±6.66
GCoT-L1	57.18±14.34	63.31±10.05	56.54±14.12	54.71±8.57
GCoT-L2	57.00±14.48	63.20±10.08	57.68±13.84	54.77±8.81
GCoT-L3	57.01±14.66	63.33±10.05	57.85±16.10	56.22±8.45
GCoT	**59.67**±15.51	**64.43**± 9.96	**58.75**±15.42	**56.24**±8.60

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Conclusions

- We hypothesized that multi-step inference could be useful to graph prompt learning

- We proposed GCoT, a CoT-style prompt learning framework that mimics CoT in NLP.

- Experiments showed promising results compared to traditional single-step prompt methods on graphs.

Thank you! Questions?

- GCoT paper & github repo:

GCoT: Chain-of-Thought Prompt Learning for Graphs

Xingtong Yu, Chang Zhou, Zhongwei Kuai, Xinming Zhang, Yuan Fang

https:// arxiv.org/pdf/2502.08092

Introduction

We provide the code (in pytorch) and datasets for our paper "GCoT: Chain-of-Thought Prompt Learning for Graphs" accepted by *SIGKDD* 2025.

https://github.com/Eric-Kuai/GCoT/tree/python