SAMGPT: Text-free Graph Foundation Model for Multi-domain Pre-training and Cross-domain Adaptation

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Outline

1 .Motivation

2 .Challenges

3 .Proposed Model: SAMGPT

4 .Experiment

Motivation

- Building foundation models paves a plausible path toward **artificial general intelligence**.
- World Wide Web is a **vast knowledge repository**
- *Can we build a universal graph model based on multi-domain graphs, to address various downstream graph-centric application?*

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Challenges

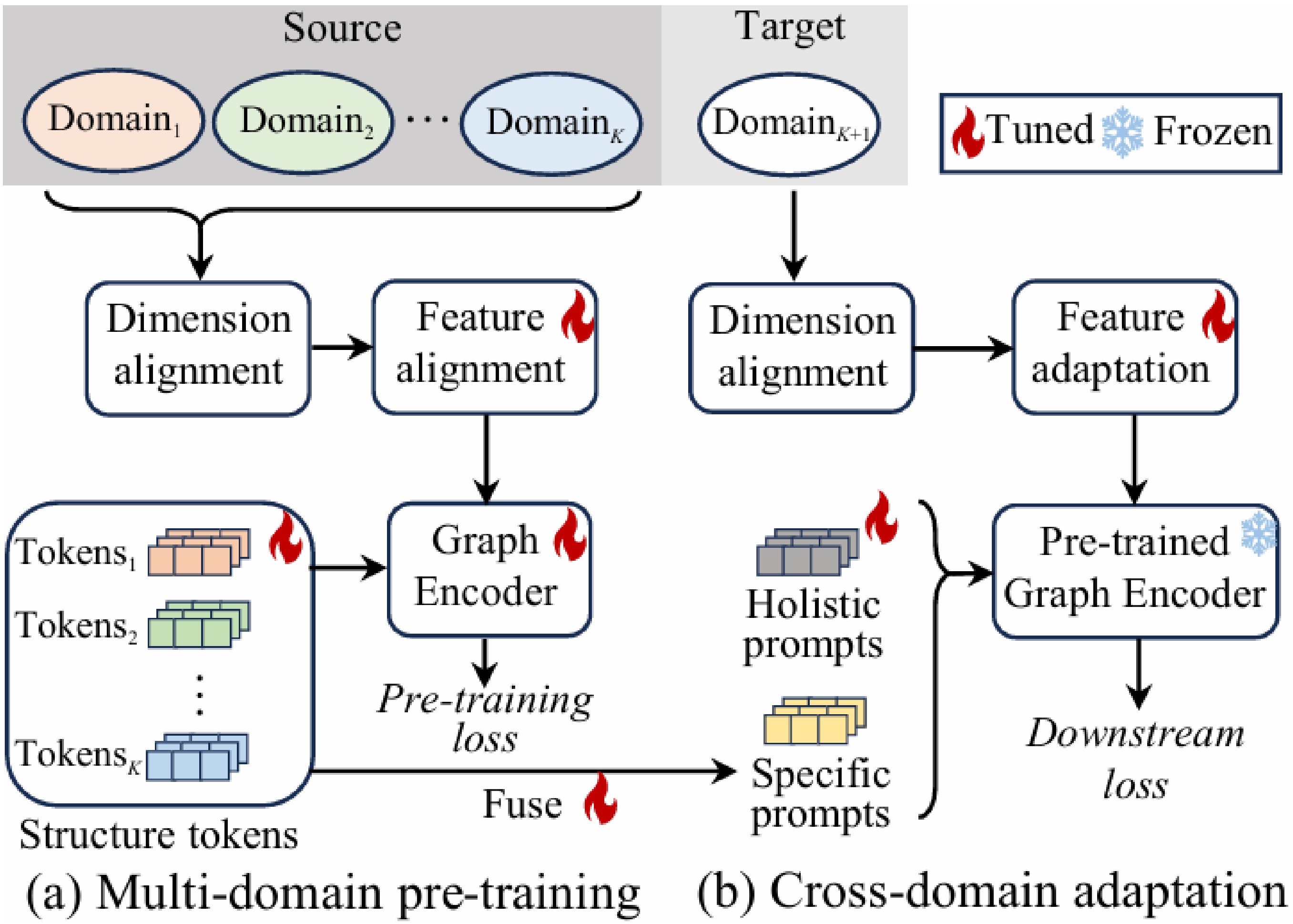

Figure 1: Motivation of SAMGPT.

Challenges:

- How do we harmonize structural variance across multiple domains during pre-training?
- How do we adapt multi-domain structural prior knowledge to cross-domain downstream tasks?

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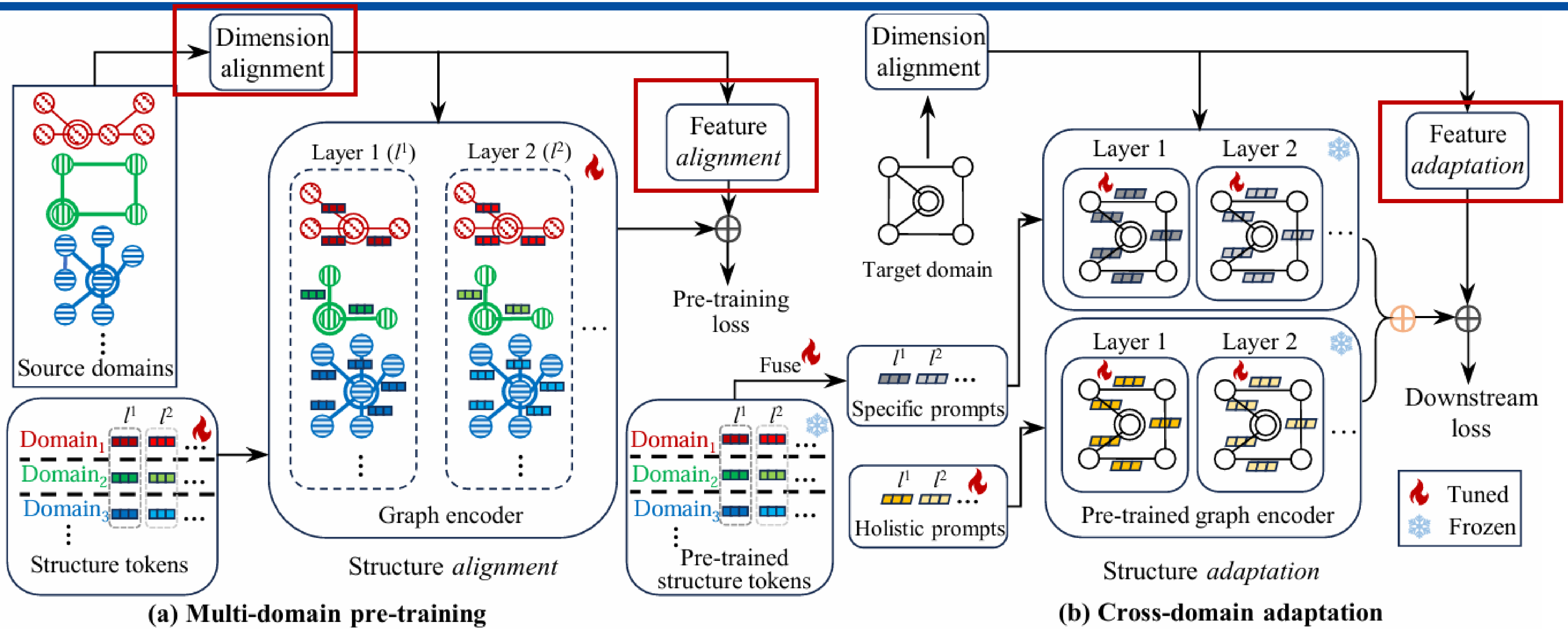


Figure 2: Overall framework of SAMGPT.

Multi-domain pre-training

Downstream adaptation

Structural alignment

$$\mathbf{h}_v^l = \mathrm{Aggr}(\mathbf{h}_v^{l-1}, \{\mathbf{t}_{S_i}^l \odot \mathbf{h}_u^{l-1} : u \in \mathcal{N}_v\}; \theta^l), \ \forall v \in V_i$$

Holistic prompt

$$\mathbf{h}_v^l = \mathrm{Aggr}(\mathbf{h}_v^{l-1}, \{\mathbf{p}_{\text{hol}}^l \odot \mathbf{h}_u^{l-1} : u \in \mathcal{N}_v\}; \theta_{\text{pre}}^l)$$

Specific prompt

$$\mathbf{p}_{\text{spe}}^l = \sum_{i=1}^K \lambda_i^l \mathbf{t}_{S_i}^l$$

Dimension alignment

$$\tilde{\mathbf{X}}_i = \mathsf{DAL}_{S_i}(\mathbf{X}_i),$$

Feature alignment

$$\mathbf{H}^{\mathsf{FAL}} = \mathsf{GE}(\mathsf{FAL}(\mathcal{G}_S, \tilde{\mathcal{X}}_S; \Psi); \Theta),$$

$$\tilde{\mathcal{X}}_S = \{\tilde{\mathbf{X}}_i : G_i \in \mathcal{G}_S\}$$

Structure alignment

Pretext tokens

$$\mathcal{T}_{S_i} = \{\mathbf{t}^l_{S_i} : l \in \{1, \ldots, L\}\}$$

Add token to each layer of graph encoder,
guiding structure-based aggregation

$$\mathbf{h}^l_v = \mathsf{Aggr}(\mathbf{h}^{l-1}_v, \{\mathbf{t}^l_{S_i} \odot \mathbf{h}^{l-1}_u : u \in \mathcal{N}_v\}; \theta^l), \ \forall v \in V_i,$$

Structure-aligned embedding matrix

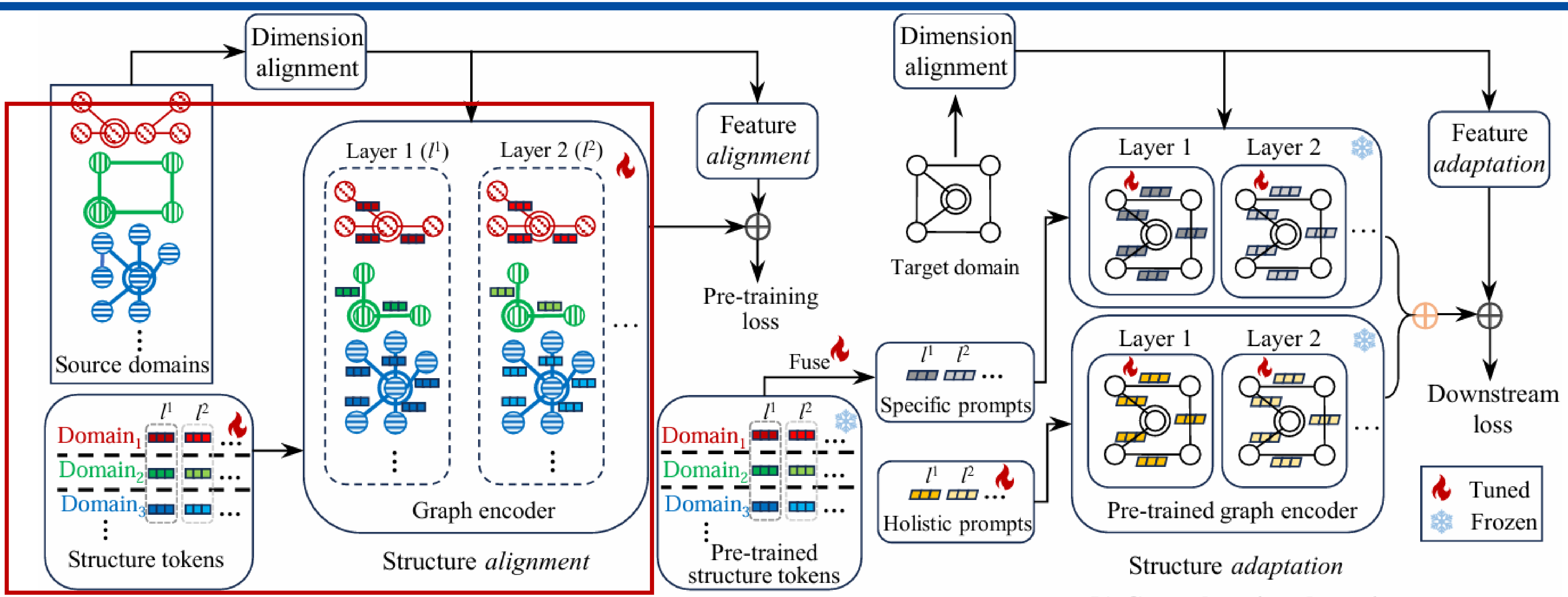
$$\mathbf{H}^{\mathsf{SAL}} = \mathtt{Stack}(\mathbf{H}^{\mathsf{SAL}}_1, \ldots, \mathbf{H}^{\mathsf{SAL}}_K)$$

Overall embedding

$$\mathbf{H}^{\mathsf{AL}} = \mathbf{H}^{\mathsf{FAL}} + \alpha \mathbf{H}^{\mathsf{SAL}}$$

Pre-training loss

$$\mathcal{L}_{\text{pre}}(\mathcal{O}; \Theta, \mathcal{T}, \Psi) = -\sum_{o \in \mathcal{O}} \ln \frac{\sum_{a \in \text{Pos}_o} \exp(\mathtt{sim}(\mathbf{h}_a, \mathbf{h}_o)/\tau)}{\sum_{b \in \text{Neg}_o} \exp(\mathtt{sim}(\mathbf{h}_b, \mathbf{h}_o)/\tau)}$$



(a) Multi-domain pre-training **(b) Cross-domain adaptation**

Figure 2: Overall framework of SAMGPT.

Multi-domain pre-training

Downstream adaptation

Structural alignment

$$\mathbf{h}_v^l = \mathrm{Aggr}(\mathbf{h}_v^{l-1}, \{\mathbf{t}_{S_i}^l \odot \mathbf{h}_u^{l-1} : u \in \mathcal{N}_v\}; \theta^l),\ \forall v \in V_i$$

Holistic prompt

$$\mathbf{h}_v^l = \mathrm{Aggr}(\mathbf{h}_v^{l-1}, \{\mathbf{p}_{\text{hol}}^l \odot \mathbf{h}_u^{l-1} : u \in \mathcal{N}_v\}; \theta_{\text{pre}}^l)$$

Specific prompt

$$\mathbf{p}_{\text{spe}}^l = \sum_{i=1}^{K} \lambda_i^l \mathbf{t}_{S_i}^l$$

Feature alignment [1]

$$\tilde{\mathbf{X}}_i = \mathsf{DAL}_{S_i}(\mathbf{X}_i), \qquad \mathbf{H}^{\mathsf{FAL}} = \mathsf{GE}(\mathsf{FAL}(\mathcal{G}_S, \tilde{\mathcal{X}}_S; \Psi); \Theta), \qquad \tilde{\mathcal{X}}_S = \{\tilde{\mathbf{X}}_i : G_i \in \mathcal{G}_S\}$$

Structure alignment

Pretext tokens

$$\mathcal{T}_{S_i} = \{\mathbf{t}^l_{S_i} : l \in \{1, \dots, L\}\}$$

Add token to each layer of graph encoder, guiding structure-based aggregation

$$\mathbf{h}^l_v = \mathsf{Aggr}(\mathbf{h}^{l-1}_v, \{\mathbf{t}^l_{S_i} \odot \mathbf{h}^{l-1}_u : u \in \mathcal{N}_v\}; \theta^l), \ \forall v \in V_i,$$

Structure-aligned embedding matrix

$$\mathbf{H}^{\mathsf{SAL}} = \mathsf{Stack}(\mathbf{H}^{\mathsf{SAL}}_1, \dots, \mathbf{H}^{\mathsf{SAL}}_K)$$

Overall embedding

$$\mathbf{H}^{\mathsf{AL}} = \mathbf{H}^{\mathsf{FAL}} + \alpha \mathbf{H}^{\mathsf{SAL}}$$

Pre-training loss

$$\mathcal{L}_{\text{pre}}(\mathcal{O}; \Theta, \mathcal{T}, \Psi) = -\sum_{o \in \mathcal{O}} \ln \frac{\sum_{a \in \text{Pos}_o} \exp(\mathsf{sim}(\mathbf{h}_a, \mathbf{h}_o)/\tau)}{\sum_{b \in \text{Neg}_o} \exp(\mathsf{sim}(\mathbf{h}_b, \mathbf{h}_o)/\tau)}$$

[1] Yu, et al. Text-free multi-domain graph pre-training: Toward graph foundation models. arXiv preprint.

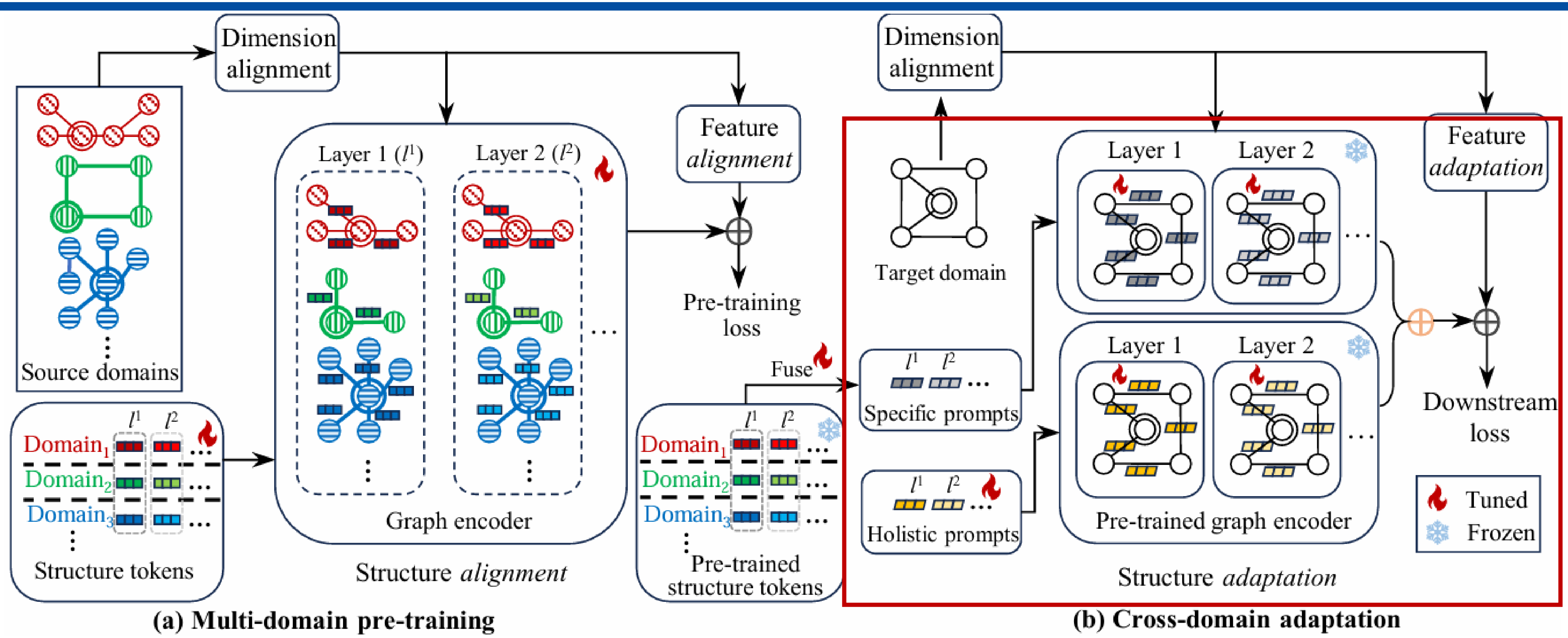


Figure 2: Overall framework of SAMGPT.

Multi-domain pre-training

Downstream adaptation

Structural alignment

$$\mathbf{h}_v^l = \mathtt{Aggr}(\mathbf{h}_v^{l-1}, \{\mathbf{t}_{S_i}^l \odot \mathbf{h}_u^{l-1} : u \in \mathcal{N}_v\}; \theta^l), \ \forall v \in V_i,$$

Holistic prompt

$$\mathbf{h}_v^l = \mathtt{Aggr}(\mathbf{h}_v^{l-1}, \{\mathbf{p}_{\text{hol}}^l \odot \mathbf{h}_u^{l-1} : u \in \mathcal{N}_v\}; \theta_{\text{pre}}^l),$$

Specific prompt

$$\mathbf{p}_{\text{spe}}^l = \sum_{i=1}^K \lambda_i^l \mathbf{t}_{S_i}^l,$$

Feature adaptation [1]

$$\mathbf{H}^{\mathsf{FAD}} = \mathsf{GE}(\mathsf{FAD}(G, \tilde{\mathbf{X}}; \Gamma); \Theta_{\text{pre}})$$

Structure adaptation

Holistic prompts

$$\mathcal{P}_{\text{hol}} = \{\mathbf{p}^1_{\text{hol}}, \dots, \mathbf{p}^L_{\text{hol}}\}$$

Prompt modification

$$\mathbf{h}^l_v = \mathsf{Aggr}(\mathbf{h}^{l-1}_v, \{\mathbf{p}^l_{\text{hol}} \odot \mathbf{h}^{l-1}_u : u \in \mathcal{N}_v\}; \theta^l_{\text{pre}}), \quad \forall v \in V$$

Specific prompts

$$\mathcal{P}_{\text{spe}} = \{\mathbf{p}^1_{\text{spe}}, \dots, \mathbf{p}^L_{\text{spe}}\}$$

$$\mathbf{p}^l_{\text{spe}} = \textstyle\sum_{i=1}^{K} \lambda^l_i \mathbf{t}^l_{S_i}$$

Fuse embeddings

$$\mathbf{H}^{\mathsf{SAD}} = \mathbf{H}^{\text{hol}} + \beta\mathbf{H}^{\text{spe}}$$

Overall embedding

$$\mathbf{H}^{\mathsf{AD}} = \mathbf{H}^{\mathsf{FAD}} + \alpha\mathbf{H}^{\mathsf{SAD}}$$

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Table 1: Accuracy (%) of one-shot *node classification* with standard deviations. Each column represents a target domain, using other columns as source domains. The best method in each column is bolded, and the runner-up is underlined.

Method\Target domain	Cora	Citeseer	Pubmed	Photo	Computers	Facebook	LastFM
GCN	29.53 ± 7.56	26.29 ± 6.50	23.32 ± 11.56	26.96 ± 12.94	24.40 ± 5.62	20.45 ± 5.62	9.21 ± 3.11
GAT	24.27 ± 9.26	21.56 ± 8.09	22.28 ± 9.76	17.85 ± 10.22	23.03 ± 12.12	29.27 ± 6.47	9.01 ± 2.61
DGI	33.40 ± 10.48	25.80 ± 8.27	47.22 ± 9.50	30.89 ± 10.54	25.75 ± 12.45	34.36 ± 9.57	14.14 ± 6.31
GraphCL	27.72 ± 9.37	35.02 ± 8.46	<u>48.89</u> ± 9.03	34.78 ± 11.56	23.79 ± 12.28	34.85 ± 7.07	18.93 ± 7.32
GPPT	27.18 ± 4.88	25.90 ± 4.68	39.82 ± 8.79	31.58 ± 10.27	19.94 ± 9.61	34.73 ± 3.99	20.98 ± 3.98
GraphPrompt	28.26 ± 12.68	32.51 ± 8.73	47.47 ± 9.15	48.11 ± 9.89	42.82 ± 11.67	40.44 ± 9.68	19.84 ± 7.23
GPF	32.17 ± 6.56	<u>36.79</u> ± 7.70	41.28 ± 8.14	47.47 ± 8.19	35.75 ± 7.12	40.45 ± 6.34	27.26 ± 5.50
Hassani	33.35 ± 6.93	33.66 ± 7.24	39.87 ± 8.16	48.48 ± 7.07	39.99 ± 7.91	37.70 ± 5.79	27.16 ± 4.94
GCOPE	<u>35.62</u> ± 11.93	**38.33** ± 9.28	45.38 ± 9.87	<u>52.87</u> ± 9.19	<u>45.65</u> ± 10.69	<u>40.63</u> ± 8.50	<u>28.84</u> ± 7.59
SAMGPT	**47.80** ± 11.88	36.38 ± 9.10	**50.25** ± 10.43	**58.71** ± 8.69	**48.22** ± 8.17	**42.70** ± 8.73	**33.36** ± 8.11

Table 2: Accuracy (%) of one-shot *graph classification* with standard deviations. Each column represents a target domain, using other columns as source domains. The best method in each column is bolded, and the runner-up is underlined.

Method\Target domain	Cora	Citeseer	Pubmed	Photo	Computers	Facebook	LastFM
GCN	30.64 ± 10.31	26.90 ± 7.15	38.84 ± 11.82	15.60 ± 8.77	21.94 ± 14.51	31.33 ± 9.47	28.83 ± 9.60
GAT	27.80 ± 7.85	27.50 ± 7.13	21.66 ± 8.70	15.74 ± 7.62	16.02 ± 13.46	21.20 ± 7.31	27.80 ± 7.85
InfoGraph	34.98 ± 10.15	35.87 ± 9.84	48.67 ± 12.29	25.70 ± 11.73	19.02 ± 14.09	31.26 ± 9.65	23.29 ± 7.99
GraphCL	<u>42.70</u> ± 10.64	36.66 ± 8.67	47.53 ± 11.52	33.07 ± 12.31	16.02 ± 13.47	21.99 ± 13.00	21.30 ± 10.45
GraphPrompt	37.38 ± 14.03	36.66 ± 9.19	**49.55** ± 10.25	50.79 ± 12.31	43.09 ± 11.45	<u>41.71</u> ± 10.61	32.62 ± 8.54
GPF	39.62 ± 8.52	36.73 ± 7.66	45.08 ± 10.36	47.57 ± 10.16	35.70 ± 8.71	34.84 ± 5.14	34.31 ± 7.05
Hassani	36.86 ± 10.74	35.78 ± 8.80	43.97 ± 13.27	41.55 ± 13.08	29.49 ± 13.86	35.57 ± 9.00	25.39 ± 8.14
GCOPE	38.85 ± 10.99	**39.93** ± 9.82	47.05 ± 11.74	<u>53.93</u> ± 9.74	<u>45.60</u> ± 10.96	40.26 ± 9.53	<u>34.68</u> ± 7.70
SAMGPT	**55.35** ± 13.62	<u>38.75</u> ± 9.40	<u>48.69</u> ± 10.16	**58.75** ± 11.67	**48.72** ± 11.18	**43.71** ± 9.54	**48.28** ± 9.72

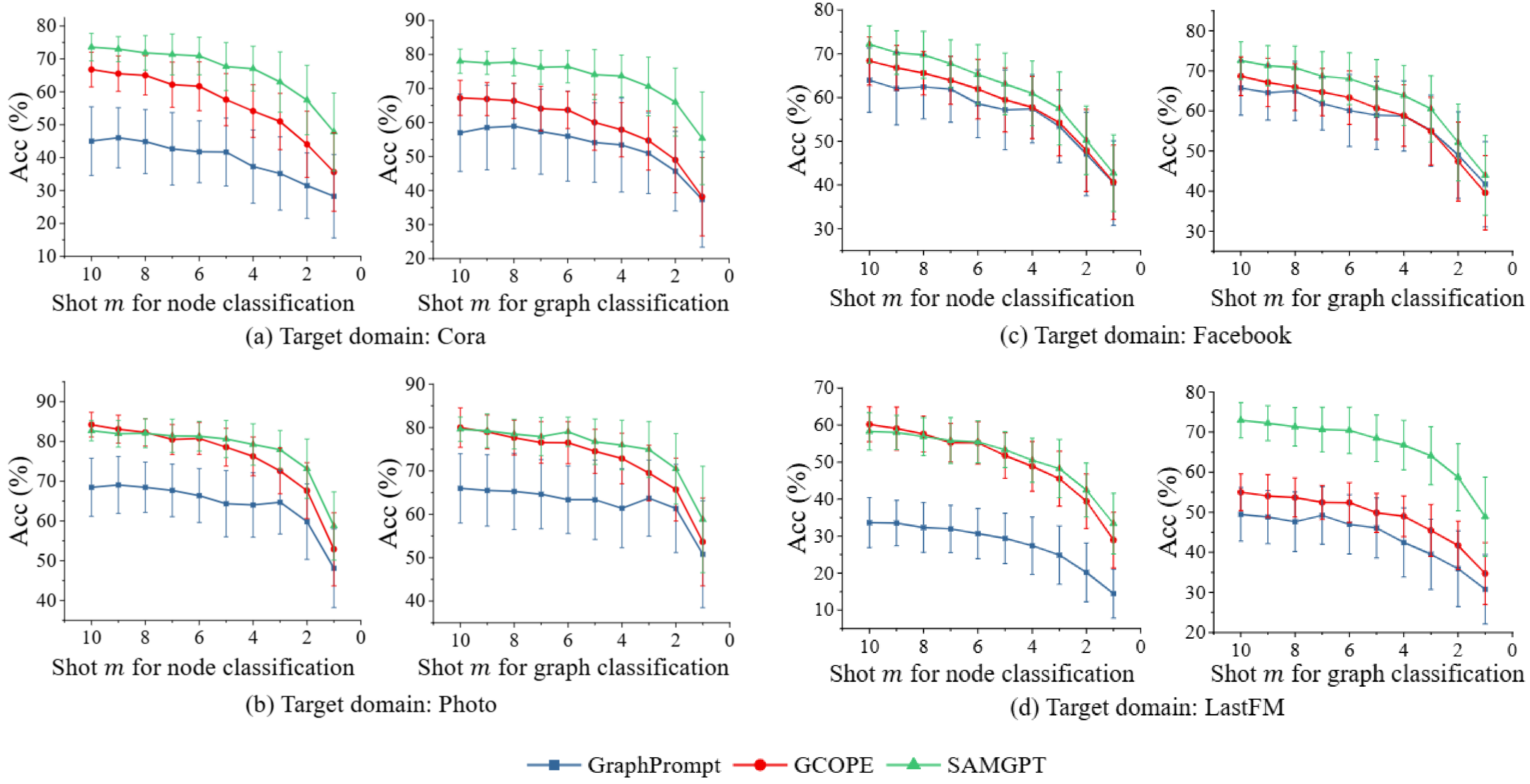

Figure 3: Impact of number of shots on node and graph classification on four target domains.

Table 3: Data ablation study with an increasing number of source domains.

Method	Number of source domains 1	2	3	4
GraphPrompt	35.53±12.06	37.13±11.79	36.90±11.23	38.54±11.84
GCOPE	39.47±12.14	36.63± 9.46	35.28±11.99	38.61±12.74
SAMGPT	**40.43**±11.00	**41.97**±11.01	**42.30**±11.56	**45.95**±12.96

Table 4: Model ablation study on key components of SAMGPT.

Methods	Structure tokens	Holistic prompts	Specific prompts	Target domain for node classification: Cora	Photo	Facebook	Target domain for graph classification: Cora	Photo	Facebook
Variant 1	×	×	×	36.36 ± 12.71	49.10 ± 9.94	35.36 ± 9.06	45.44 ± 13.47	52.45 ± 12.37	38.74 ± 10.26
Variant 2	×	×	✓	40.62 ± 11.79	56.23 ± 9.04	39.80 ± 10.39	45.63 ± 13.52	57.78 ± 11.64	42.22 ± 10.95
Variant 3	✓	×	×	44.26 ± 10.92	56.61 ± 10.14	41.11 ± 8.34	52.88 ± 12.25	58.14 ± 12.01	43.12 ± 9.76
Variant 4	✓	✓	×	46.10 ± 12.02	57.76 ± 10.00	40.46 ± 8.89	54.52 ± 14.32	58.12 ± 12.30	43.15 ± 10.12
SAMGPT	✓	✓	✓	47.80 ± 11.88	58.71 ± 8.69	42.70 ± 8.73	55.35 ± 13.62	**58.75** ± 11.67	43.71 ± 9.54

Thanks!

SAMGPT https://arxiv.org/abs/2502.05424