How to Make LMs Strong Node Classifiers?

Anonymous ACL submission

Abstract

Language Models (LMs) are increasingly challenging the dominance of domain-specific models, such as Graph Neural Networks (GNNs) and Graph Transformers (GTs), in graph learning tasks. Following this trend, we propose a novel approach that empowers off-the-shelf LMs to achieve performance comparable to state-of-the-art (SOTA) GNNs on node classification tasks, without any architectural modification. By preserving the LM's original architecture, our approach retains a key benefit of LM instruction tuning: the ability to jointly train on diverse datasets, fostering greater flexibility and efficiency. To achieve this, we introduce two key augmentation strategies: (1) enriching LMs' input using topological and semantic retrieval methods, providing richer contextual information, and (2) guiding the LMs' classification process through a lightweight GNN classifier that effectively prunes class candidates. Experiments on real-world datasets show that backbone Flan-T5 LMs equipped with these augmentation strategies outperform SOTA text-output node classifiers and are comparable to top-performing vector-output node classifiers. By bridging the gap between specialized node classifiers and general LMs, this work paves the way for more versatile and widely applicable graph learning models. We will open-source the code upon publication.

1 Introduction

There is a growing trend of utilizing Language Models (LMs) for machine learning tasks across diverse domains. This approach has shown tremendous promise in areas such as vision (Desai and Johnson, 2021), audio (Mittal et al., 2021), and multimodal learning (Alayrac et al., 2022). In graph learning, recent efforts have begun to explore the capabilities of LMs in understanding and processing graph structures. (Wang et al., 2023) showed that LMs can detect node connectivity and identify cycles, while (Fatemi et al., 2024) explored LMs' ability to evaluate graph scale and identify connected components. Furthermore, InstructGLM (Ye et al., 2023) and LLaGA (Chen et al., 2024b) achieved state-of-the-art (SOTA) performance in text-output node classifiers on Text-Attributed Graphs (TAG) (Zhang et al., 2024a), whose nodes have textual features.

However, both InstructGLM and LLaGA suffer from a fundamental limitation that *compromises the generality of the backbone LM*. Specifically, InstructGLM expands the LM's vocabulary by creating *a unique token for each node*, whose token embeddings are topology-aware node embeddings. It comes at the cost of incompatibility with two important use cases: (1) multi-task learning on diverse datasets, a common strategy for training Foundational Models (Wei et al., 2022; Chung et al., 2024), and (2) certain personalized LM fine-tuning services (Li et al., 2024b) that restrict access to the backbone model architecture/code[1]. LLaGA uses a shared text encoder and a projector to overcome the first limitation but still bears inflexibility when *deploying different LMs* and cannot be applied to LMs without code/architecture access. The above discussion raises a crucial question: *How can off-the-shelf, **text-to-text** instruction-tuned LMs (Raffel et al., 2020) achieve competitive performance in node classification tasks without architectural modifications?*

In stark contrast to (Huang et al., 2023), which suggests that LMs may only interpret graph structures in prompts as contextual paragraphs, our work presents a more optimistic outlook. We aim to overcome this inherent limitation by augmenting the LMs' input while preserving their original architecture. Our proposed model, AUGLM (Aumented Graph Language Model), leverages two key aug-

[1] https://platform.openai.com/docs/guides/fine-tuning

mentation strategies to enhance the LM's ability to process graph data:

- **Relevant Node Retrieval**: In contrast to InstructGLM, which relies on multi-hop ego networks akin to message-passing GNNs for structure-aware contextualization, AUGLM draws inspiration from Graph Transformers (GTs) (Min et al., 2022) and Retrieval-Augmented Generation (RAG) (Lewis et al., 2020; Guu et al., 2020). This enables the LM to access long-range structural and semantic information about the target node. We propose two complementary approaches to achieve this: (1) topological retrieval, and (2) prototypical semantic retrieval.
- **Candidate Label Pruning**: To improve LMs' understanding of graph data while maintaining their text-to-text architecture, we convey the guidance from a specialist model, a pretrained lightweight GNN, to the input of LMs via narrowing down the candidate labels. This allows LMs to focus on discerning between closely related candidates, ultimately enhancing the performance.

We extensively evaluate our approach on four real-world TAGs, showing the effectiveness of AUGLM. The results indicate that (1) backbone LMs augmented with AUGLM consistently outperform SOTA text-output classifiers while also matching or surpassing the performance of SOTA vector-output classifiers, and (2) AUGLM can be jointly trained on multiple TAGs without performance degradation. These findings represent a crucial step towards bridging the gap between task-specific node classifiers and more general, fine-tuned LMs, highlighting the potential for a unified model excelling in multiple tasks.

2 Related Work

LMs for graphs. Recent studies have explored the ability of LMs to understand graph topology by investigating problems such as graph substructure recall (Wang et al., 2024), circle and connectivity detection (Wang et al., 2023; Perozzi et al., 2024), node/edge counting (Perozzi et al., 2024), spatial-temporal problems on dynamic graphs (Zhang et al., 2024b). Notably, (Fatemi et al., 2024) found that the text presentation of graph data impacts LMs' performance across various tasks, highlighting the importance of graph-to-text transformation. Building on these findings, several studies have explored tasks on TAGs, including node classification (Ye et al., 2023; Zhao et al., 2023b; Li et al., 2024a; Qin et al., 2023), link prediction (Brannon et al., 2023; Tan et al., 2024), transfer learning (Tang et al., 2024), and graph reasoning (Jin et al., 2024). (Chen et al., 2023) presents a systematic summary on existing solutions in two categories: LLMs-as-Enhancer and LLMs-as-Predictor. Furthermore, (Zhang, 2023) proposed Graph-ToolFormer, a framework that enhances LMs with graph reasoning API tools. GIANT (Chien et al., 2022) and GLEM (Zhao et al., 2023a) utilize the interaction between graph data and LMs for better graph representations. TAPE (He et al., 2024) leverages an LLM to augment the textual features and then fine-tunes two LMs for graph representation.

Retrieval-augmented generation (RAG) (Lewis et al., 2020; Karpukhin et al., 2020) enhances LMs by granting them access to external knowledge (Hashimoto et al., 2018). This technique involves retrieving relevant documents from a large corpus and conditioning the LM on the retrieved knowledge. Building on this, REALM (Guu et al., 2020) pretrains the retriever and generator end-to-end. Subsequently, RETRO (Borgeaud et al., 2022) scales RAG-enhanced autoregressive models to large datasets. A crucial component of RAG's success is the objective function proposed by (Shi et al., 2023), which enables the retriever to be trained even with black-box LMs. HyDE (Yu et al., 2023) uses hypothetical document generation to improve retrieval in RAG systems. Furthermore, RAG has extended to multimodal settings (Yasunaga et al., 2023). Recently, GraphRAG (Edge et al., 2024) has garnered significant attention; it constructs a Knowledge Graph (KG) and then generates responses based on the summaries of communities derived from KG. These advancements have significantly improved generated text's accuracy and contextual relevance, solidifying RAG as a promising technique for various applications.

3 Preliminaries

We use the following notation conventions: bold lower-case letters (e.g,. $\mathbf{x}$) denote column vectors, bold upper-case letters (e.g., $\mathbf{X}$) denote matrices, and calligraphic upper-case letters (e.g., $\mathcal{X}$) denote sets. We use $[\cdot]$ and $[\cdot, \cdot]$ to index vectors and matrices, respectively.

We study the node classification problem on TAGs where each node is associated with textual

attributes. A TAG with n nodes is represented as $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{T})$, where $\mathcal{V} = \{v_i\}_{i=1}^n$ denotes a set of nodes, and $\mathcal{E} = \{e_{ij}\}_{i,j=1}^n$ is a set of edges where $e_{ij} = 1$ indicates that nodes v_i and v_j are connected; otherwise, $e_{ij} = 0$. $\mathcal{T} = \{t_i\}_{i=1}^n$ indicates the set of node textual attributes. The edges can also be represented by an adjacency matrix $\mathbf{A} \in \{0,1\}^{n \times n}$, where $\mathbf{A}[i,j] = 1$ if and only if $e_{ij} = 1$. The training and test node labels are denoted by $\mathcal{Y} = \mathcal{Y}_{\text{train}} \cup \mathcal{Y}_{\text{test}} = \{y_i\}_{i=1}^n$, where each label y_i belongs to one of the C classes, i.e., $y_i \in \{1, \ldots, C\}, \forall i$. In the semi-supervised setting studied in this paper, the graph structure and training labels $\mathcal{V}, \mathcal{E}, \mathcal{T}, \mathcal{Y}_{\text{train}}$ are accessible, and the goal is to predict the labels of test nodes $\mathcal{Y}_{\text{test}}$.

Personalized PageRank (PPR) (Page, 1999; Jeh and Widom, 2003) ranks all the nodes according to their relevance to a given query node. Specifically, given the adjacency matrix $\mathbf{A}$, the PPR scores $\mathbf{r}_i \in \mathbb{R}^n$ for all nodes concerning the query node v_i are computed iteratively as:

$$\mathbf{r}_i \leftarrow (1-\alpha)\tilde{\mathbf{A}}\mathbf{r}_i + \alpha \mathbf{q}_i \tag{1}$$

where $\alpha \in (0,1)$ is the teleport probability, $\mathbf{q}_i \in \{0,1\}^n$ is a one-hot vector whose i-th entry is 1, $\tilde{\mathbf{A}} = \mathbf{A}\mathbf{D}^{-1}$ is the normalized adjacency matrix, and $\mathbf{D}$ is the degree matrix. Once $\mathbf{r}_i$ converges, the top-K relevant nodes concerning the query node v_i can be identified as follows:

$$\texttt{PPR}(v_i, K) = \{v_j : \mathbf{r}_i[j] \in \text{topK}(\mathbf{r}_i)\} \tag{2}$$

Language models (LMs). We employ autoregressive LMs that predict the next token z_i based on the input sequence t and the context of previously generated tokens $z_{1:i-1}$. The probability of generating a sequence z given the input t is:

$$p_{\text{LM}}(z|t) = \prod_{i=1}^{|z|} p_{\text{LM}}(z_i|t, z_{1:i-1}) \tag{3}$$

Retrieval-augmented generation (RAG) (Lewis et al., 2020; Guu et al., 2020) first retrieves a query t-relevant text d^* from an external corpus $\mathcal{D}$ via a similarity function s_ϕ:

$$d^* = \arg\max_{d \in \mathcal{D}} s_\phi(d, t) \tag{4}$$

s_ϕ is typically implemented as a dual-encoder architecture (Bromley et al., 1993):

$$s_\phi(d,t) = \langle \texttt{Encoder}_\phi(d), \texttt{Encoder}_\phi(t) \rangle \tag{5}$$

Once d^* is retrieved, it is fed into the LM together with the query t: $p_{\text{LM}}(z|d^*, t)$ for generation.

4 Method

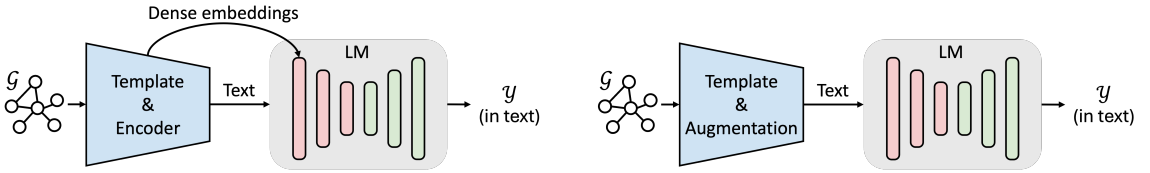
We explore the application of LMs to node classification by reformulating it as a text-to-text task (Raffel et al., 2020). Our method employs carefully designed prompt templates and augmentation techniques to transform graph and ground truth labels into text pairs, enabling LMs to process and be fine-tuned *without* modifying their underlying architecture.

As shown in Figure 1, AUGLM fundamentally differs from InstructGLM (Ye et al., 2023) and LLaGA (Chen et al., 2024b), the current SOTA LM node classifiers. While all three methods utilize prompt templates to transform input graphs into text, InstructGLM and LLaGA explicitly **encode node features into the LM's token embeddings** which can be categorized as **soft prompting** (Lester et al., 2021). In contrast, our approach provides a **data augmentation**-based framework without modifying LM's text-to-text architecture, enabling our model to retain the versatility of the original LM. The following section first details the augmentation techniques developed by this paper and then introduces the templates to incorporate all the augmented textual features.

4.1 Retrieval-based aggregation

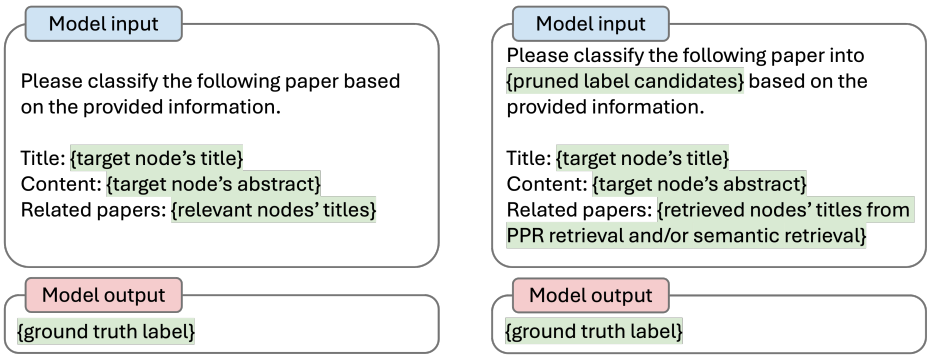
General LMs are not designed to process graph data directly. To overcome this, a common approach is to employ prompt templates to transform graphs and associated tasks into text that LMs can understand. For instance, for the Cora (Sen et al., 2008) literature citation graph, a typical template (Huang et al., 2023; Ye et al., 2023) for node classification, as shown in Figure 2a, consists of three main components: (1) a short task description, (2) the target node's textual features, e.g., its title and abstract, and (3) textual features from relevant nodes.

The success of the message-passing GNNs highlights the importance of the **aggregation** operation, whose typical example is the mean pooling of intermediate node embeddings. A similar spirit is followed for the LM-based classifiers, whose key design is the **selection of relevant nodes**. Existing works (Huang et al., 2023; Ye et al., 2023) select one/multi-hop neighbors as relevant nodes, but we posit that this approach is suboptimal for two reasons. Firstly, not all immediate or extended neighbors are relevant to the target node, which can introduce noise and degrade model performance. Secondly, incorporating multi-hop neigh-



(a) InstructGLM and LLaGA. (b) AUGLM (ours).

Figure 1: Comparison of pipelines between the existing LM-based node classifiers and our approach, AUGLM. Unlike InstructGLM and LLaGA, which explicitly encodes graph information into token embeddings as a form of soft prompting, AUGLM maintains the original text-to-text framework of the off-the-shelf LM, offering greater generality and flexibility.



(a) A typical graph-to-text template. (b) Our template with augmented text.

Figure 2: Comparison of a typical graph-to-text template (a) and our template with augmented text features (b).

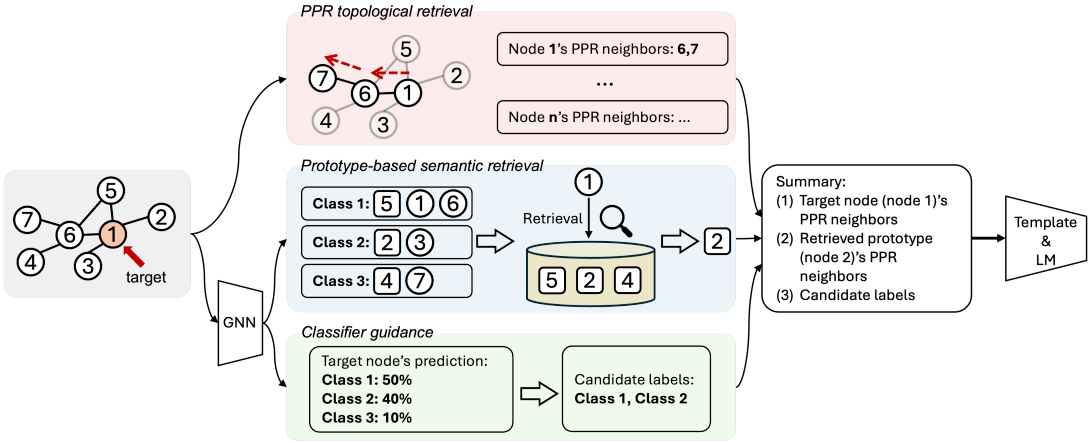


Figure 3: A detailed pipeline of AUGLM. In the semantic retrieval module, rectangles denote the class prototypes.

bors can lead to "neighbor explosion" (Hamilton et al., 2017; Chen et al., 2018; Fey et al., 2021), i.e., an exponentially-growing set of "relevant" nodes, resulting in increased computational costs and even leading to the out-of-memory issue. As a response, two novel solutions, *topological retrieval* and *prototypical semantic retrieval*, are proposed to efficiently identify the most informative nodes for the classification tasks.

Topological retrieval. PPR (Page, 1999; Jeh and Widom, 2003) is leveraged for topological retrieval, which has shown great effectiveness in conjunction with GNNs (Klicpera et al., 2019). The success of PPR suggests that its retrieved neighbors may provide more informative context than generic one/multi-hop neighbors. Specifically, for a target node v_i, we select its top-K neighbors $\text{PPR}(v_i, K)$ based on their PPR scores (Eqs. (1) and (2), Section 3). Then, the text features from the PPR neighbors are concatenated as the PPR-retrieved text $t_{\text{PPR}} = \oplus_{j;v_j \in \text{PPR}(v_i,K)} t_j$, where $\oplus$ denotes text concatenation.

It is worth noting that the classic PPR algorithm is computationally expensive for large graphs due to the matrix multiplication (Eq. (1)). However, efficient approximate solutions such as Ap-

proximatePR (Andersen et al., 2006), can be applied to mitigate this issue. Nevertheless, PPR is a topology-based heuristic that inherently cannot leverage textual features or supervision from downstream LMs. To enhance our framework's semantic awareness, we propose a complementary strategy called prototypical semantic retrieval as follows.

Prototypical semantic retrieval. Our semantic retrieval module draws inspiration from two popular techniques: (1) RAG (Lewis et al., 2020; Guu et al., 2020), which retrieves external corpora, and (2) Graph Transformers (Min et al., 2022), which aggregate messages from distant nodes via inner product-based attention weights. For node classification, we treat **the textual features of all nodes except the target node** as a surrogate "external corpus." However, unlike typical question-answering tasks, retrieving textual features from **a single node is often insufficient** for accurate node classification. To address this, we enhance the semantic retrieval by retrieving prototypes, which capture the essence of each class (Snell et al., 2017).

Prototypes (Biehl et al., 2016) are defined as representative examples in classification problems. To obtain prototypes, a lightweight GNN ψ is pretrained and generates a prediction vector for each node: $\tilde{\mathbf{y}}_i = \texttt{GNN}_\psi(v_i, \mathcal{G}) \in \mathbb{R}^C, \forall v_i$. The prediction confidence for each node v_i is defined as: $\texttt{Conf}(v_i) = \max_j \tilde{\mathbf{y}}_i[j]$. The predicted class-$c$ examples are $\tilde{\mathcal{Y}}_c = \{v_i : \arg\max_j \tilde{\mathbf{y}}_i[j] = c\}$ and their confidence is $\texttt{Conf}_c = \{\texttt{Conf}(v_i) : v_i \in \tilde{\mathcal{Y}}_c\}$. For each class c, the top-N confident examples are selected as prototypes:

$$\mathcal{P}_c = \left\{ v_i : v_i \in \tilde{\mathcal{Y}}_c \wedge \texttt{Conf}(v_i) \in \text{topN}\left(\texttt{Conf}_c\right) \right\} \tag{6}$$

For all the classes, there are $N \times C$ prototypes: $\mathcal{P} = \bigcup_{c\in\{1,\dots,C\}} \mathcal{P}_c$. To ensure every document in the corpus $\mathcal{D}$ includes text features from **multiple nodes**, $\mathcal{D}$ is constructed by concatenating the text of **each prototype's PPR neighbors**:

$$\mathcal{D} = \left\{ \bigoplus_{j;v_j\in\texttt{PPR}(v_i,K)} t_j : v_i \in \mathcal{P} \right\} \tag{7}$$

Next, for each target node with its associated text features t_{target}, we compute the prototypically retrieved text using Eq. (4): $t_{\text{proto}} = \arg\max_{d\in\mathcal{D}} s_\phi(d, t_{\text{target}})$. In our experiments, we may use t_{PPR} (from topological retrieval), or t_{proto}, or both by concatenation $t_{\text{PPR}} \oplus t_{\text{proto}}$. For simplicity, we denote the final retrieved text as t_{retri}.

4.2 Classifier guidance

Recent studies (Huang et al., 2023; Fatemi et al., 2024; Chen et al., 2024a) highlighted mainstream LMs' limited understanding of graph topology. While InstructGLM (Ye et al., 2023) and LLaGA (Chen et al., 2024b) address this limitation by incorporating topology-aware node embeddings (e.g., from a pretrained or parameter-free GNN) into the LM's token embeddings, this approach necessitates **modifications to the LM's architecture**. We propose an alternative method that conveys guidance from a pretrained GNN into the **input text of LMs**, thereby preserving the LM's original architecture. Concretely, such guidance is to **prune the classification candidates**.

We repurpose the pretrained $\texttt{GNN}_\psi$ from the prototypical semantic retrieval module. For each node v_i, we identify and save the top-I predicted labels:

$$\mathcal{L}_i = \{j : \tilde{\mathbf{y}}_i[j] \in \text{topI}\left(\tilde{\mathbf{y}}_i\right)\} \in \{1, \dots, C\}^I \tag{8}$$

where $I < C$. For datasets in the experiments, the `IndexToLabel` maps are available, which map numerical labels to their corresponding text. The pruned label candidates for node v_i can be presented as concatenated text: $t_{\text{candidates}} = \oplus_{i\in\mathcal{L}_i} \texttt{IndexToLabel}(i)$. The integration of pruned candidates into the template is detailed in Section 4.3.

By focusing on a more relevant set of candidate labels, valuable topology-aware inductive bias from the GNN is incorporated into the LM's input, thereby enhancing its node classification performance without altering its architecture.

4.3 Overall template

Our augmented training samples include three key elements: (1) the target node's text t_{target}, (2) the retrieved nodes' text t_{retri}, and (3) the pruned label candidates $t_{\text{candidates}}$. We collectively denote these elements as $t_{\text{in}} = (t_{\text{target}}, t_{\text{retri}}, t_{\text{candidates}})$. LM's prediction probability for the target sequence y_{target} is based on Eq. (3) whose input text t is t_{in} and the output sequence z is y_{target}. Figure 2b presents an exemplar template for the Cora dataset, showcasing the integration of t_{target}, t_{retri}, and $t_{\text{candidates}}$. The selection of the backbone LM will be detailed in Section 5. Appendix C contains a full list of templates. Note that we exclude the "abstracts" of the retrieved nodes to prevent exceeding the maximum input length of most LMs. We utilize only this template's "model input" part for evaluation.

4.4 Training

Our framework includes three parameterized modules that require training or fine-tuning: (1) GNNs for generating prototypes and candidate label pruning, as described in Sections 4.1 and 4.2, (2) the encoder ϕ from the semantic retriever, defined in Eq. 5, and (3) the backbone LM, utilized in Eq. 3. The GNNs from Sections 4.1 and 4.2 can be shared, and their training is independent of the other modules, which are supervised by ground truth labels. This process is detailed in Appendix A.

One of the standard LM's losses, the average token-wise negative log-likelihood (NLL), is used. For a target node, the loss is:

$$\mathcal{L}_{\text{NLL}}\left(p_{\text{LM}}(y_{\text{target}}|t_{\text{in}}), y_{\text{target}}\right) \tag{9}$$

To train the semantic retriever, we employ a distribution-matching loss. For a given target node's text t_{target}, its retrieval probability for a prototype text $t \in \mathcal{D}$ is:

$$p_\phi(t|t_{\text{target}}) = \frac{e^{s_\phi(t,t_{\text{target}})}}{\sum_{t'\in\mathcal{D}} e^{s_\phi(t',t_{\text{target}})}} \tag{10}$$

Next, an empirical distribution supervised by the LM is:

$$\tilde{p}_{\text{LM}}(t|t_{\text{target}}, y_{\text{target}}) = \frac{e^{p_{\text{LM}}(y_{\text{target}}|t_{\text{in}})}}{\sum_{t'\in\mathcal{D}} e^{p_{\text{LM}}\left(y_{\text{target}}|t'_{\text{in}}\right)}} \tag{11}$$

where $t_{\text{in}} = (t_{\text{target}}, t, t_{\text{candidates}})$ and $t'_{\text{in}} = (t_{\text{target}}, t', t_{\text{candidates}})$. This distribution represents the **normalized importance of each prototype text** $t \in \mathcal{D}$ based on the **LM's likelihood of generating the ground truth text** y_{target}. We use $\tilde{p}_{\text{LM}}$ to distinguish this distribution from the generation probability in Eq. (3).

The distribution matching loss is the Kullback-Leibler (KL) divergence between the retrieval and the LM-supervised distributions:

$$\text{KL}\left(\texttt{sg}\left(\tilde{p}_{\text{LM}}\left(\cdot|t_{\text{target}}, y_{\text{target}}\right)\right) \| p_\phi(\cdot|t_{\text{target}})\right) \tag{12}$$

This loss aims to align the retrieval probability of each prototype text $t \in \mathcal{D}$ with its importance in facilitating the LM's generation of the label text y_{target} for the target node. The stop gradient operator $\texttt{sg}$ ensures that the loss Eq. (12) only updates the semantic retriever ϕ but keeps the LM's parameters θ frozen. This objective has been used by previous works (Shi et al., 2023; Izacard et al., 2023) without thorough analysis. We provide an in-depth examination of its properties and implications in Appendix B.

Notably, Eq. (11) requires $|\mathcal{D}|$ inferences of the LM due to the denominator. However, the LM is fine-tuned via the NLL loss, Eq. (9), only for the most relevant prototype, $\arg\max_{d\in\mathcal{D}} s_\phi(d, t_{\text{target}})$. Consequently, each update step involves $|\mathcal{D}|$ forward passes but only one backpropagation. To reduce the computational overhead associated with $|\mathcal{D}|$ inferences, we can use a sampling strategy: selecting the top-M samples to form a retrieval mini-batch $\mathcal{D}_M = \{t : t \in \text{topM}_{t'\in\mathcal{D}} s_\phi(t', t_{\text{target}})\}$. By replacing $\mathcal{D}$ with $\mathcal{D}_M$ in Eqs. (10) and (11), the retrieval and the LM-supervised distributions can be computed "in-batch", reducing the inference times from $|\mathcal{D}|$ to M.

Algorithm 1 (Appendix D) outlines a step-by-step process for fine-tuning AUGLM, processing one training node per step. This procedure can be readily extended to mini-batch settings.

4.5 Model complexity

AUGLM consists of three parameterized modules: (1) a GNN ψ, (2) the semantic retriever ϕ, and (3) the backbone LM θ. Notably, ψ and ϕ are lightweight, whose number of parameters is only $1/30$ to $1/3$ of the number of LM θ parameters. Compared to the SOTA InstructGLM (Ye et al., 2023), AUGLM has an additional module ϕ, resulting in a slightly increased number of parameters. For training, the GNN ψ can be pretrained, and the PPR scores can be precomputed. The training of θ relies on the retrieved text from ϕ, while the training of ϕ requires $\tilde{p}_{\text{LM}}(\cdot|t_{\text{target}}, y_{\text{target}})$, which is obtained through forward inference of θ. Importantly, computational graphs (used for gradient computation) of θ and ϕ are **independent**. When training ϕ, the stop gradient operator $\texttt{sg}$ ensures θ has no gradient. As a result, the cost of backpropagation is close to the sum of the cost for updating the LM θ and the semantic encoder ϕ, separately.

4.6 Discussion on the flexibility of AUGLM

We noticed that LLaGA (Chen et al., 2024b) improves the generality of soft prompting-based solutions by a shared text encoder and a projector. Here, we compare the flexibility and generality of LLaGA and our proposed AUGLM to illustrate our unique contribution better.

- LlaGA **can achieve 0-shot transfer learning**, e.g., training on the Cora dataset and testing on the Amazon dataset. However, LLaGA **cannot switch the LM seamlessly** because it requires modifying the LM's code and architecture, e.g., including its graph encoder's output into the LM's token embeddings. The application of LLaGA is also limited if there is no access to the LM's architecture or code.
- Our AUGLM **cannot achieve 0-shot transfer learning** because we need a trained GNN to provide reliable label candidates for text input augmentation. However, thanks to such a data augmentation paradigm, AUGLM **can switch the LM seamlessly** as long as the LM works in a text-to-text manner.

5 Experiments

This section introduces the experimental setups, baseline methods, effectiveness studies, ablation studies, and multi-task training. Efficiency and hyperparameter studies are in the Appendix.

5.1 Setup

Following (He et al., 2024; Ye et al., 2023), we evaluate our approach on four benchmark datasets: Cora (Sen et al., 2008), Pubmed (Sen et al., 2008), ogbn-arxiv (Hu et al., 2020), and a subset of ogbn-products (Hu et al., 2020; He et al., 2024). The dataset statistics are in Table 5.

Our implementation employs two pretrained all-MiniLM-L6-v2 models (Wang et al., 2020) as the the semantic retriever ϕ (Eq. (5)) and the text encoder for GNN ψ (Eq. (13)). We set the PPR teleport probability $\alpha = 0.1$. We employ a 3-layer GraphSAGE (Hamilton et al., 2017) with a hidden dimension of 256 as ψ. Our hyperparameters include $K = 5$ PPR neighbors, $N = 10$ prototypes, and $M = 8$ samples for LM inference. The number of label candidates I is searched from $\{2, 3\}$. Flan-T5-small/base/large (Chung et al., 2022) are used as the backbone LM θ with templates detailed in Section C.

5.2 Comparison with state-of-the-arts

This section presents the comparison between AUGLM and SOTA baselines. We categorize models into two groups: (1) vector-output models which output a vector with dimension equal to the number of classes, and (2) text-output models, whose output is text. Specifically, results from GCN (Kipf and Welling, 2017), BernNet (He et al., 2021a), FAGCN (Bo et al., 2021), GCNII (Chen et al., 2020), ACM-GCN (Luan et al., 2022), GLEM (Zhao et al., 2023a)+RevGAT, InstructGLM (Ye et al., 2023) and LLaGA (Chen et al., 2024b) are reported according to the leaderboards (detailed in Appendix) and their papers. The results for TAPE+RevGAT, GIANT (Chien et al., 2022)+RevGAT (Li et al., 2021), GIANT+GCN, DeBERTa (He et al., 2021b), and ChatGPT3.5 are reported from (He et al., 2024). All models are (at least partially) fine-tuned on the training set except ChatGPT-3.5. Mean and standard deviation over 5 runs are reported. For text-output models, accuracy is evaluated by checking whether the model's generated text matches the ground truth text exactly.

Table 1 presents a comparison between AUGLM and SOTAs. AUGLM consistently outperforms InstructGLM and LLaGA, **achieving new SOTA performance** among text-output node classifiers. Notably, this superior performance is achieved without modifying any LMs' architecture, demonstrating the effectiveness of our approach. Furthermore, AUGLM exhibits **competitive performance compared to the best vector-output models**. Specifically, on Cora, Pubmed, and ogbn-arxiv datasets, AUGLM performs closely to that of the SOTA vector-output models. Furthermore, on the ogbn-products dataset, AUGLM surpasses the performance of the best vector-output model, TAPE.

5.3 Ablation study

To evaluate the contribution of each key component in AUGLM, we conducted an ablation study on three crucial modules: (1) topological retrieval, (2) semantic retrieval, and (3) candidate label pruning. In this subsection, Flan-T5-small is used. The results in Table 2 demonstrate that each module consistently improves performance across all datasets. Notably, our analysis reveals that the relative importance of each component varies across different datasets. For instance, candidate label pruning greatly impacts performance for the Cora dataset, whereas its effect is less pronounced for the ogbn-products dataset. This variation in component importance underscores the adaptability of our approach, which can effectively accommodate diverse datasets with different characteristics.

5.4 Multi-task training

One of the key advantages of pure text-to-text instruction tuning is that a single model can be trained

Table 1: Accuracy (%) comparison between AUGLM and existing SOTA models. The best-performing **vector-output** and **text-output** models on each dataset are highlighted in **blue** and **red**, respectively.

	Method	Cora	Pubmed	ogbn-arxiv	ogbn-products
Vector-output	GCN	87.78±0.96	88.90±0.32	73.60±0.18	75.64±0.21
	GraphSAGE	86.51±2.36	89.08±0.28	73.88±0.33	76.04±0.25
	BernNet	88.52±0.95	88.48±0.41	–	–
	FAGCN	88.85±1.36	89.98±0.52	–	–
	GCNII	88.98±1.33	89.80±0.52	72.74±0.16	–
	ACM-GCN	89.75±1.16	91.44±0.59	–	–
	GLEM + RevGAT	88.56±0.60	94.71±0.20	76.97±0.19	–
	GIANT + RevGAT	83.53±0.38	85.02±0.48	75.90±0.19	71.89±0.30
	GIANT + GCN	84.23±0.53	84.19±0.50	73.29±0.10	69.77±0.42
	DeBERTa	76.06±3.78	94.94±0.46	73.61±0.04	72.97±0.23
	TAPE + RevGAT	**92.90±3.07**	**96.18±0.53**	**77.50±0.12**	**82.34±0.36**
Text-output	ChatGPT-3.5	67.90	93.42	73.40	74.40
	InstructGLM	90.77±0.52	94.62±0.13	75.70±0.12	–
	LLaGA	89.85	95.06	76.66	–
	AUGLM (T5-small)	91.14±0.55	94.80±0.15	75.39±0.21	81.73±0.08
	AUGLM (T5-base)	91.24±0.46	95.03±0.35	**76.80±0.14**	81.91±0.11
	AUGLM (T5-large)	**91.51±0.26**	**95.16±0.18**	76.00±0.23	**82.90±0.10**

Table 2: Ablation study results (accuracy %). T, S, and L denote topological retrieval, semantic retrieval, and label pruning, respectively. ↓ indicates accuracy drop compared to the full model (T+S+L).

Model	Cora	Pubmed	ogbn-arxiv	ogbn-products
T+S	85.52 (↓5.62)	94.40 (↓0.40)	72.91 (↓2.48)	79.83 (↓1.90)
T+L	87.27 (↓3.87)	94.32 (↓0.48)	73.79 (↓1.60)	81.05 (↓0.68)
S+L	90.25 (↓0.89)	94.26 (↓0.54)	73.46 (↓1.93)	79.06 (↓2.67)
T+S+L	**91.14**	**94.80**	**75.39**	**81.73**

Table 3: Joint vs. separate training (accuracy %).

Training	Cora	Pubmed	ogbn-arxiv	ogbn-products
Joint	91.52	94.52	74.87	82.29
Separate	91.14	94.80	75.39	81.73

on multiple tasks with the same input-output format. To verify this, AUGLM with Flan-T5-small is jointly trained on diverse datasets: Cora, Pubmed, ogbn-arxiv, and ogbn-products. The results in Table 3 show that the jointly trained model achieves performance comparable to models trained separately on each individual dataset. We observe that on some datasets, such as Cora and ogbn-products, the jointly trained model even outperforms its dataset-specific counterparts.

These findings suggest that our approach can effectively **handle multiple graph datasets using a single model**, without incurring great performance losses compared to models trained individually. This capability is crucial for efficient model deployment when dealing with diverse graphs. In contrast, other approaches, such as InstructGLM, require the addition of a large token dictionary to accommodate all nodes in the joint dataset, which hinders their ability to achieve similar generality. Moreover, most vector-output models, including TAPE, are limited by their predefined input-output dimensions, making them inflexible and unable to handle multiple datasets.

6 Conclusion

We introduce a novel framework AUGLM for node classification on TAGs via text-to-text instruction-tuning. Our approach is built upon two key innovations: (1) topological and semantic retrieval of relevant nodes and (2) a lightweight GNN textual guidance. Extensive experimental results demonstrated (1) the effectiveness of our framework, which consistently outperformed the best text-output node classifiers while achieving performance comparable to SOTA vector-output node classifiers, and (2) the flexibility of AUGLM , which can be jointly trained over multiple datasets without performance drop. These findings suggest a promising direction for harnessing the power of LMs in graph learning tasks.

7 Limitations

One limitation of this work is the need for manual definition of prompt templates in Table 4. A promising direction for future research is to develop methods for automatically searching for optimal templates in a data-driven manner. Another limitation is the requirement for pretraining a GNN ψ on each dataset, which stems from the inherent challenges of language models in understanding graph data and limits our model to be adapted to zero-shot learning scenarios. Addressing this limitation by developing more powerful language models capable of handling graph data is a challenging yet impactful area of future work, which can lead to instruction-tuning only, highly generalizable graph foundation models.

8 Broader Impact

This paper presents work that aims to advance the fields of language models (LMs) and graph machine learning (GML). Thus, the broader societal impact of this research aligns with prior work in both LMs and GML.

While our proposed approach does not target any specific high-stakes application domain, it may be adopted in settings such as recommendation systems and social network analysis. As such, downstream uses could inherit ethical considerations, including privacy, fairness, and potential misuse. Mitigating such issues is an open challenge shared by the broader community, and we encourage future work to evaluate fairness, robustness, and interpretability as these models are adopted for critical tasks.

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Appendix

This appendix is organized as follows

- Section A: introduction of the architecture and training of GNNs used in this paper.
- Section B: interpretation of the distribution matching loss.
- Section C: templates used in this paper for node classification.
- Section D: the training algorithm of AUGLM.
- Section E: detailed dataset statistics and their leaderboards.
- Section F: hyperparameters and pretrained backbone models.
- Section G: additional experiments.
  - Section G.1: additional efficiency studies.
  - Section G.2: additional experiments on the backbone GNN selections, topological and semantic retrievers, and the PPR steps.
  - Section G.3 additional experiments on the link prediction tasks.
- Section 7: limitations and future work.

A Architecture and Training of the Graph Neural Network ψ

In our setting, semi-supervised node classification problem, $\mathcal{V}, \mathcal{E}, \mathcal{T}, \mathcal{Y}_{\text{train}}$ are accessible during training. Since Graph Neural Networks (GNNs) are not inherently capable of processing textual features, a pretrained text encoder is used to generate d-dimensional dense embeddings for each node

$$\texttt{Encoder}_{\psi_1}(t_i) = \mathbf{h}_i^{(0)} \in \mathbb{R}^d, \forall i \in 1, \ldots, n \quad (13)$$

In our implementation, the text encoder is all-MiniLM-L6-v2, a member of the sentence transformers. Subsequently, we apply a standard graph neural network, GraphSAGE (Hamilton et al., 2017), whose iterative architecture is

$$\mathbf{h}_i^{(l)} = \sigma^{(l)}\left(\texttt{MEAN}\left(\texttt{Message}_i\right) \cdot \mathbf{W}^{(l)}\right) \quad (14)$$

$$\texttt{Message}_i = \{\mathbf{h}_i^{(l-1)}\} \cup \{\mathbf{h}_j^{(l-1)} : (v_i, v_j) \in \mathcal{E}\} \quad (15)$$

where $\sigma^{(l)}$ is the activation function and $\mathbf{W}^{(l)} \in \mathbb{R}^{d \times d}$ is the learnable parameter of each layer. For an L-layer network, in the last layer, $\sigma^{(L)}$ is $\texttt{Softmax}$ and $\mathbf{W}^{(L)} \in \mathbb{R}^{d \times c}$ so that $\mathbf{h}_i^{(L)} \in \mathbb{R}^c$ is the prediction vector. The typical loss used for training the GNN is negative log-likelihood $\mathcal{L}_{\text{NLL}}(\mathbf{h}_i^{(L)}, y_i)$ for all the nodes in the training set $\mathcal{Y}_{\text{train}}$. The complete set of trainable parameters is denoted as $\psi = \{\psi_1\} \cup \{\mathbf{W}^{(l)}\}_{l=1}^{L}$.

B Interpretation of the distribution matching loss

We recap the objective function. For notation brevity, we use t_i to denote the input target node with its pruned candidates: $(t_{\text{target}}, t_{\text{candidates}})$:

$$\text{KL}(\tilde{p}_{\text{LM}}(\cdot|t_i, y_i) \| p_\phi(\cdot|t_i)) \quad (16)$$

where the stop gradient operator is removed if we only compute gradient with respect to ϕ and

$$p_\phi(t_j|t_i) = \frac{e^{s_\phi(t_i,t_j)}}{\sum_{t_k \in \mathcal{D}} e^{s_\phi(t_i,t_k)}} \quad (17)$$

$$\tilde{p}_{\text{LM}}(t_j|t_i, y_i) = \frac{e^{p_{\text{LM}}(y_i|t_i,t_j)}}{\sum_{k \in \mathcal{N}_i} e^{p_{\text{LM}}(y_i|t_i,t_k)}} \quad (18)$$

For notation brevity, we replace $\sum_{t_k \in \mathcal{D}}$ with $\sum_z$ if there is no ambiguity. Then

$$\min_\phi \ \text{KL}\big(\tilde{p}_{\texttt{LM}}(\cdot|t_i, y_i) \| p_\phi(\cdot|t_i)\big) \quad (19)$$

$$\Leftrightarrow \min_\phi -\sum_z \tilde{p}_{\texttt{LM}}(z|t_i, y_i) \log[p_\phi(z|t_i)] \quad (20)$$

$$= -\sum_z \tilde{p}_{\texttt{LM}}(z|t_i, y_i) \log\left(\frac{e^{s_\phi(z,t_i)}}{\sum_{z'} e^{s_\phi(z',t_i)}}\right) \quad (21)$$

$$= \sum_z \tilde{p}_{\texttt{LM}}(z|t_i, y_i) \log\left(\sum_{z'} e^{s_\phi(z',t_i)}\right) - \sum_z \tilde{p}_{\texttt{LM}}(z|t_i, y_i) s_\phi(z, t_i) \quad (22)$$

$$= \log\left(\sum_z e^{s_\phi(z,t_i)}\right) - \sum_z \tilde{p}_{\texttt{LM}}(z|t_i, y_i) s_\phi(z, t_i) \quad (23)$$

Hence,

$$\nabla \mathrm{KL} = \frac{\sum_z e^{s_\phi(z,t_i)} \nabla s_\phi(z,t_i)}{\sum_{z'} e^{s_\phi(z',t_i)}}) - \sum_z \tilde{p}_{\mathtt{LM}}(z|t_i,y_i) \nabla s_\phi(z,t_i) \quad (24)$$

$$= \sum_z \left(p_\phi(z|t_i) - \tilde{p}_{\mathtt{LM}}(z|t_i,y_i)\right) \cdot \nabla s_\phi(z,t_i) \quad (25)$$

$$= \sum_z \left(1 - \frac{\tilde{p}_{\mathtt{LM}}(z|t_i,y_i)}{p_\phi(z|t_i)}\right) \cdot p_\phi(z|t_i) \nabla s_\phi(z,t_i) \quad (26)$$

After changing the notation back from $\sum_z$ to $\sum_{t_k \in \mathcal{D}}$, we have

$$\nabla \mathrm{KL} = \sum_{t_k \in \mathcal{D}} \left(1 - \frac{\tilde{p}_{\mathtt{LM}}(t_j|t_i,y_i)}{p_\phi(t_j|t_i)}\right) \cdot p_\phi(t_j|t_i) \nabla s_\phi(t_j,t_i) \quad (27)$$

whose rationale is that **if the LM's feedback greatly prefers the neighbor v_j (and its associated text t_j), larger than its probability to be retrieved by the retriever (i.e., $\frac{\tilde{p}_{\mathtt{LM}}(t_j|t_i,y_i)}{p_\phi(t_j|t_i)} > 1$), then the similarity score between t_i and t_j will increase**, i.e., improve the probability of t_j to be retrieved.

C Templates

Table 4 presents templates used in this paper. We design the "Citation" template for the Cora, Pubmed, and ogbn-arxiv datasets and the "Amazon" template for the ogbn-products dataset.

Drawing inspiration from the findings of (He et al., 2024), who demonstrated the efficacy of positioning the title after the main content for certain datasets, we have also introduced two additional template variations: "Citation, Title Last" and "Amazon, Title Last."

D Algorithm

A step-by-step process for fine-tuning AUGLM, processing one training node per step, is presented in Algorithm 1. This procedure can be readily extended to mini-batch settings.

E Dataset Statistics

We present the detailed statistics of datasets used in this paper in Table 5.

Algorithm 1 Training procedure for AUGLM

Input:
(1) A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{T})$ and training labels $\mathcal{Y}_{\text{train}}$;
(2) initialized backbone LM θ;
(3) initialized semantic encoder ϕ;
(4) initialized GNN ψ.
Preprocessing:
(1) Pretrain GNN ψ on $(\mathcal{G}, \mathcal{Y}_{\text{train}})$.
(2) Generate prototypes and their text via Eqs. (6) and (7).
(3) Generate pruned label candidates for each node via Eq. (8).
while θ and ϕ not converged **do**
  Sample node $v_i \sim \mathcal{V}$ with text t_i.
  Retrieve relevant nodes' text $t_{\text{retri},i}$ via: topological retrieval (Eq. (2)) and/or semantic retrieval (Eq. (4)).
  Construct prompt with t_i, $t_{\text{retri},i}$, and $t_{\text{candidates},i}$ (from Preprocessing step (3)), based on the template (e.g., Figure 2b).
  Update θ based on Eq. (9).
  Compute $p_\phi(\cdot|t_i)$ via Eq. (10).
  Perform LM inference $|\mathcal{D}|$ times for: $\{p_{\text{LM}}(y_i|t_i,t)\}_{t\in\mathcal{D}}$ and $\tilde{p}_{\text{LM}}(\cdot|t_i,y_i)$.
  Update ϕ based on Eq. (12).
end while

All the baseline methods' performance on the Cora, Pubmed, and ogbn-arxiv is reported from the public leaderboards [2][3][4] and their published papers.

The ogbn-products dataset used in this paper is a subset of the original ogbn-products dataset (Hu et al., 2020) from TAPE (He et al., 2024). We follow the settings in TAPE and report baseline methods' performance from the TAPE (He et al., 2024) paper.

F Selected Hyperparameters

We report the hyperparameter used for every dataset in Table 6. As mentioned in the main content, we use two pretrained all-MiniLM-L6-v2 models as the dual encoder and the Flan-T5-small/base/large models as the backbone; they are

[2] https://paperswithcode.com/sota/node-classification-on-cora-60-20-20-random
[3] https://paperswithcode.com/sota/node-classification-on-pubmed-60-20-20-random
[4] https://ogb.stanford.edu/docs/leader_nodeprop/

Table 4: Templates used for all datasets.

Template Name	Prompt Text
Citation (Cora, Pubmed, ogbn-arxiv)	`Please classify the following paper into {pruned label candidates} based on the provided information\nTitle: {target node's title}\nContent: {target node's abstract}\nRelated papers: {retrieved nodes' titles}`
Citation, Title Last (Cora, Pubmed, ogbn-arxiv)	`Please classify the following paper into {pruned label candidates} based on the provided information\nContent: {target node's abstract}\nRelated papers: {retrieved nodes' titles}\nTitle: {target node's title}`
Amazon (ogbn-products)	`Please classify the following Amazon product into {pruned label candidates} based on the provided information\nProduct name: {target node's title}\nDescription: {target node's description}\nRelated products: {retrieved nodes' titles}`
Amazon, Title Last (ogbn-products)	`Please classify the following Amazon product into {pruned label candidates} based on the provided information\nDescription: {target node's description}\nRelated products: {retrieved nodes' titles}\nProduct name: {target node's title}`

Table 5: Dataset statistics.

Name	# Nodes	# Edges	# Classes	Split Strategy	Evaluation Metric
Cora	2 708	10 556	7	Random 60/20/20%	Accuracy
Pubmed	19 717	88 648	3	Random 60/20/20%	Accuracy
ogbn-arxiv	169 343	1 166 243	40	Given split	Accuracy
ogbn-products	54 025	198 663	47	Given split	Accuracy

all publicly available[5][6]. More detailed hyperparameters will be released with the code upon publication.

G Additional Experiments

G.1 Additional efficiency study

Memory usage. Memory usage is linear concerning batch size. We report the memory usage of AUGLM with different backbone LMs in Table 7, where we set the batch size to 1 and we found the experimental results reasonable because more powerful backbone LMs require more GPU memory.

Convergence curve. We train AUGLM with different backbone LMs: FLAN-T5-small/base/large on the Cora dataset and plot their loss curves regarding updating steps in Figure 4. In this experiment, the batch size is 16. It shows that our proposed AUGLM converges smoothly and quickly when equipped with various LMs of different scales.

FLOPs. The floating point operations (FLOPs) of AUGLM are studied. Specifically, the computation of our AUGLM includes (1) precomputing PPR neighbors for every node, (2) training and inference of the semantic retriever ϕ, and (3) training and inference of the LM θ. Hence, the extra on-the-fly computation cost is from the semantic retriever ϕ (all-MiniLM-L6-v2 in our experiments). We report the FLOPs of the retriever and different LM backbones in Table 8. The results show that (1) the retriever only adds a tiny amount of FLOPs to the backbone LMs and (2) our proposed AUGLM is efficient.

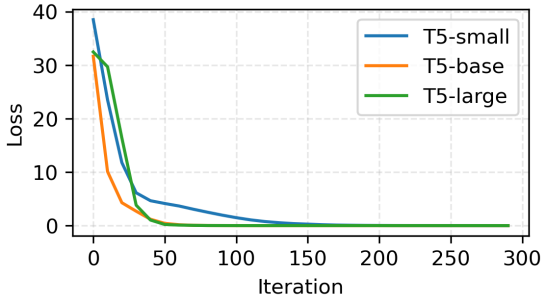

Figure 4: Convergence curve of AUGLM.

Running time. The running time (both forward and backpropagation) of the semantic retriever and the backbone LMs on the Cora dataset is recorded.

[5] https://huggingface.co/sentence-transformers/all-MiniLM-L6-v2

[6] https://huggingface.co/docs/transformers/en/model_doc/flan-t5

Table 6: Selected hyperparameters for AUGLM across different datasets.

Hyperparameter	Cora	Pubmed	ogbn-arxiv	ogbn-products
# PPR neighbors	5	2	5	5
# Semantic neighbors	5	2	5	5
Prompt template	Citation	Citation	Citation, Title Last	Amazon
# Candidate labels	3	2	3	3
LM learning rate	1×10^{-4}	1×10^{-4}	1×10^{-4}	1×10^{-4}
Retriever learning rate	1×10^{-5}	1×10^{-5}	1×10^{-5}	1×10^{-5}
Weight decay	0	0	0	0

Table 7: GPU Memory usage (MB) with different LMs.

Model	Memory
AUGLM (T5-small)	3 098
AUGLM (T5-base)	6 572
AUGLM (T5-large)	20 308

Table 8: FLOPs comparison between different modules.

Module	FLOPs (10^9)
Retriever	2.3
T5-small	71.7
T5-base	257.2
T5-large	845.4

Table 9: Running time (ms) of different modules.

Module	Forward	Backprop
Retriever	14.7	6.1
T5-small	90.0	32.0
T5-base	104.4	66.6
T5-large	277.2	197.0

The batch size is 1. This experiment is tested on an NVIDIA A100-SXM4-80GB. Table 9 shows that the semantic retriever only adds very limited on-the-fly computation overhead compared to the LM, showing the efficiency of AUGLM.

G.2 Additional hyperparameter study

In this section, we study the model's performance with various hyperparameters.

Selection of the backbone GNN. Specifically, we study the performance of AUGLM equipped with different GNNs. we compared the performance of AUGLM equipped with GraphSAGE (used in the reported results) with the counterpart equipped with GCN (Kipf and Welling, 2017). The comparison is in Table 10.

We observed that the performance is nearly identical between GCN and GraphSAGE. This can be attributed to two factors: (1) the classification performances of GCN and GraphSAGE are similar, and (2) the GNN is used to generate prototypes and prune candidate labels, which **does not require a highly powerful GNN** for accurate classification.

Number of PPR retrieved nodes. Next, we examined the relationship between the model performance and the number of nodes retrieved. In this auxiliary experiment, we fixed the number of nodes retrieved by semantic retrieval at 5 and varied the number of nodes retrieved by PPR retrieval. The results are reported in Table 11

Interestingly, we found that the model's performance remains relatively stable when the number of PPR nodes is less than 15. However, the performance degrades when too many nodes are retrieved (more than 15). A possible explanation is that when the number of PPR nodes becomes too large, every target node's **retrieved nodes become similar** (e.g., some hub nodes are retrieved by most nodes), reducing the discriminativeness of each target node. This phenomenon is reminiscent of the "oversmoothing" problem (Li et al., 2018) in GNNs, where a GNN with too many layers and a large receptive field produces indistinguishable latent representations for all the nodes.

Other topological retrieval options. In this auxiliary experiment, we use the link predictor to retrieve relevant neighbors. Specifically, we trained a graph autoencoder (GAE) (Kipf and Welling, 2016), a basic graph neural network-based link predictor, on the given graph. Then, we retrieved the **top-5 most confident neighbors from the reconstructed graph** to replace those obtained through PPR retrieval. The results are presented in Table 12,

Table 10: Performance (accuracy %) comparison of AUGLM equipped with different GNNs.

Model	Cora	Pubmed	ogbn-arxiv	ogbn-products
GraphSAGE	91.14	94.80	75.39	81.73
GCN	90.98	94.85	75.21	81.82

Table 11: Accuracy (%) of AUGLM on ogbn-arxiv with different numbers of PPR-retrieved neighbors. The best result is **bolded**.

# Neighbors	Accuracy (%)
1	75.18
3	75.76
5	75.39
7	75.19
9	76.05
10	**76.45**
15	75.99
20	74.81
25	74.48

where Flan-T5-small is used as the backbone LM. For better reference, we also provide a version where PPR retrieval is replaced with retrieving from 1-hop neighbors.

We observe that both 1-hop neighbor retrieval and GAE perform worse than their PPR counterparts. A possible reason is that both 1-hop neighbor retrieval and GAE are **local** retrieval methods, whereas PPR can effectively capture the **global** structure. Additionally, we note that GAE is trained using a reconstruction loss, which means it tends to assign high confidence to **existing edges**. In other words, the neighbors retrieved by GAE would be similar to those obtained through 1-hop neighbor retrieval, except for some low-degree nodes.

Other semantic retrieval options. This additional experiment uses different semantic retrievers to replace the prototype-based semantic retriever used in the proposed AUGLM. In detail, the prototype-based semantic retrieval module is replaced with a simple semantic retriever that **selects the most textually similar nodes** via inner product. Concretely, we use two pretrained models, (1) the original all-MiniLM-L6-v2[7] and (2) a fine-tuned all-MiniLM-L6-v2 by SimTeG (Duan et al., 2023)[8]. The remaining modules, including topological retrieval and classifier guidance, were left intact, and FLAN-T5-small is used as the LM backbone. The results are reported in Table 13.

We observe that the proposed prototype-based retriever is better than both the original all-MiniLM-L6-v2-based retriever and the SimTeg-tuned simple retriever. This is because:

1. The training objective of the SimTeG-tuned retriever is to align the classification loss with a GNN model (Duan et al., 2023), similar to knowledge distillation (Hinton et al., 2015). In other words, **the SimTeG-tuned retriever is a mixture of topological and semantic retrieval**, as the GNN incorporates both topology and node features. This means that its role partially overlaps with that of the topological PPR retriever.

2. Our prototype-based retriever can retrieve textual features from **multiple nodes**, but the other two cannot achieve this.

G.3 Additional link prediction experiments

The main task of this paper is on the node classification task, but we conducted a *preliminary* experiment to adapt our proposed AUGLM to the link prediction task, further showcasing the generality of the proposed AUGLM. A systematic study to adapt AUGLM to link prediction tasks is interesting, and we leave it as future work.

Link prediction can be viewed as **a classification task for a pair of nodes**. For all modules, we made the following adaptations:

1. We retained the topological PPR retrieval for the input node pair.

2. We concatenated the text of the node pair as input for the semantic retriever. The prototypes used as the corpus of the semantic retriever were still generated by a pre-trained GNN, which is consistent with our approach for the node classification task.

[7] https://huggingface.co/sentence-transformers/all-MiniLM-L6-v2

[8] https://huggingface.co/datasets/vermouthdky/SimTeG/tree/main/ogbn-arxiv/all-MiniLM-L6-v2/main/cached_embs

Table 12: Accuracy (%) of AUGLM with different *topological* retrieval techniques across datasets. The best result for each dataset is **bolded**.

Retrieval Technique	Cora	Pubmed	ogbn-arxiv	ogbn-products
1-hop neighbors	90.59	94.33	73.97	79.53
GAE	90.83	94.42	74.01	79.85
PPR neighbors	**91.14**	**94.80**	**75.39**	**81.73**

Table 13: Accuracy (%) of AUGLM with different *semantic* retrieval techniques across datasets. The best result for each dataset is **bolded**.

Retrieval Technique	Cora	Pubmed	ogbn-arxiv	ogbn-products
Simple semantic retriever	90.68	94.37	74.46	81.21
SimTeG-tuned simple retriever	—	—	74.70	—
Prototype-based retriever (ours)	**91.14**	**94.80**	**75.39**	**81.73**

3. For classifier guidance, we utilized a pre-trained graph autoencoder (GAE), whose output is the connection probability for every node pair. We transformed the connection probability into plain language based on the following rules: (1) less than 0.2: "improbable", (2) 0.2 to 0.4: "unlikely", (3) 0.4 to 0.6: "maybe", (4) 0.6 to 0.8: "likely", and (5) more than 0.8: "highly likely". The GAE's prediction (in plain language) was then incorporated into the following template.

4. The template we used is in the following format:

Prompt Template for Link Prediction

```
Please determine if the following two
papers are related or not.

Paper 1's title: {Paper 1's title}
Paper 1's abstract: {Paper 1's abstract}
Paper 1's related works: {Paper 1's PPR
neighbors' titles}

Paper 2's title: {Paper 2's title}
Paper 2's abstract: {Paper 2's abstract}
Paper 2's related works: {Paper 2's PPR
neighbors' titles}

Other related works: {Semantic retrieved
nodes' titles}

An expert link prediction model predicted
that the possibility of these two papers
being related is: {GAE's prediction}

Do you think these two papers are related
or not?
Please answer Yes or No.
```

We conducted preliminary experiments on the Cora dataset, following the settings from the benchmark[9]. In this setup, 5% and 10% of edges were removed for validation and testing, respectively. Also, an equal number of non-connected node pairs were used as negative samples. The accuracy results are reported in the following table.

Table 14: Accuracy (%) on the preliminary link prediction task for the Cora dataset.

Method	Accuracy
GAE	89.29
AUGLM (T5-small)	93.59
AUGLM (T5-base)	**94.25**

Our key findings are as follows:

1. Our proposed AUGLM can indeed be effectively adapted to link prediction tasks.

2. By leveraging a classic link predictor (GAE), our AUGLM achieves a significant performance boost over the backbone predictor GAE, which aligns with our observations in node classification tasks.

[9] https://paperswithcode.com/paper/variational-graph-auto-encoders