GOFA: A GENERATIVE ONE-FOR-ALL MODEL FOR JOINT GRAPH LANGUAGE MODELING

Anonymous authors

Paper under double-blind review

ABSTRACT

Foundation models, such as Large Language Models (LLMs) or Large Vision Models (LVMs), have emerged as one of the most powerful tools in the respective fields. However, unlike text and image data, graph data do not have a definitive structure, posing great challenges to developing a Graph Foundation Model (GFM). For example, current attempts at designing general graph models either transform graph data into a language format for LLM-based prediction or still train a GNN model with LLM as an assistant. The former can handle unlimited tasks, while the latter captures graph structure much better-yet, no existing work can achieve both simultaneously. In this paper, we first identify three key desirable properties of a GFM: self-supervised pretraining, fluidity in tasks, and graph awareness. To account for these properties, we extend the conventional language modeling to the graph domain and propose a novel generative graph language model GOFA. The model interleaves randomly initialized GNN layers into a frozen pre-trained LLM so that the semantic and structural modeling abilities are organically combined. GOFA is pre-trained on newly proposed graph-level next-word prediction, questionanswering, structural understanding, and information retrieval tasks to obtain the above GFM properties. The pre-trained model is further instruction fine-tuned to obtain the task-solving ability. Our GOFA model is evaluated on various downstream tasks unseen during the pre-training and fine-tuning phases, demonstrating a strong ability to solve structural and contextual problems in *zero-shot* scenarios.

029 030 031

032

004

010 011

012

013

014

015

016

017

018

019

021

024

025

026

027

028

1 INTRODUCTION

With the emergence of Large Language Models (LLMs), the field of artificial intelligence is undergoing a profound transformation, shifting from specialized, fragmented models to universal foundation models. A foundation model is pre-trained on large-scale datasets and can be further adapted to diverse downstream tasks using fine-tuning (Hu et al., 2022) or in-context learning (Bommasani et al., 2021; Touvron et al., 2023). Foundation models have been developed in different domains to handle text (Brown et al., 2020; Touvron et al., 2023), image (Kirillov et al., 2023; Bai et al., 2023), and even multi-modal data (Zhang et al., 2023c; Li et al., 2023; Alayrac et al., 2022). Because of their versatility and generalizability, foundation models have become prevalent in these domains.

041 However, despite preliminary efforts, a foundation model in the graph domain has arguably yet to be 042 proposed. In the graph domain, data are highly flexible and dynamic. For example, social networks 043 receive millions of new connections daily (Hardiman & Katzir, 2013), and novel molecules and 044 protein structures are frequently discovered (Abramson et al., 2024; Gilmer et al., 2017). While past researchers have proposed specialized models to learn graph data (Ying et al., 2021; Kipf & Welling, 2017), the models require retraining to accommodate new graphs (Dai et al., 2022; Mo et al., 046 2022). Moreover, trained models are usually tied to specific applications and cannot be generalized 047 to new domains and tasks. It becomes increasingly difficult for models to adjust to the ever-evolving 048 nature of graph data. Hence, a graph foundation model (GFM) applicable to new domains/tasks with minimal or no adaptation costs is urgently needed, spurring recent endeavors to study general graph models. In particular, a strong zero-shot ability is both challenging and fascinating for GFM 051 researchers. 052

The success of LLMs inspired a series of preliminary attempts which use LLMs to develop general graph models. They can be roughly divided into two categories: LLM as a predictor and LLM



Figure 1: Examples of our pre-training tasks.

071 as an enhancer (Chen et al., 2023). The LLM as a predictor approach transforms graph data into representations that LLMs can understand and use LLMs to generate predictions (Tang et al., 073 2023). However, as suggested by a recent study (Wang et al., 2023), such an approach falls short of 074 understanding graph structures. This inspired the LLM as an enhancer approach, which adopts 075 LLM to process and unify diverse graph data and feeds them to a GNN to train general graph models (Liu et al., 2023a; Huang et al., 2023a). Nevertheless, because GNN outputs fixed-sized 076 representations/predictions, they can only handle specific tasks such as classification, and cannot 077 generalize to arbitrary, new tasks due to the lack of generation ability. In summary, the current two approaches cannot fully utilize structural information and be generative simultaneously. We discuss 079 the pros and cons of existing approaches in detail in Section 2.

081 In this paper, we first identify three desirable properties of a graph foundation model (GFM), namely large-scale self-supervised pre-training, fluidity in tasks, and graph understanding. To achieve the first property, we propose a generic graph self-supervised learning problem similar to the next-083 token prediction problem in LLMs, allowing label-agnostic and continual training on highly diverse 084 graph data. We then propose a generative model termed Generative One-For-All (GOFA) that 085 interleaves GNN layers into an LLM to achieve the second and third properties. Such a novel design systematically integrates GNN into an LLM, granting the LLM graph structural learning ability 087 while keeping LLM's original free-form text generation ability. Meanwhile, this design allows the 088 pipeline of the original LLM to remain intact, giving GOFA a close-to-LLM level of task fluidity. We 089 pre-train the model with large-scale real-world graph data, Question-Answer (QA) chain data adopted 090 from the NLP domain, and graph structural data to empower the model with the aforementioned 091 foundational abilities in the graph domain (Examples in Figure 1). After pre-training, we further 092 instruction fine-tune the model on a small amount of data (relative to the pre-training data) to make it understand task formats. The fine-tuned model is finally evaluated on various downstream datasets unseen during pre-training and fine-tuning. GOFA achieved impressive results on the zero-shot 094 scenario, which demonstrates the strong potential of GOFA to serve as a graph foundation model. 095

096

098

068

069

2 A DESIRED FOUNDATION MODEL FOR GRAPH

In this section, we elaborate on three crucial properties a true graph foundation model should possess to motivate our GOFA model design. We note that many contemporary works (partly) propose similar ideas to ours and thus we do not claim the credit. We kindly refer readers to the latest surveys (Liu et al., 2023b; Jin et al., 2023; Zhang et al., 2023d) for more discussions on GFMs.

Large-Scale Self-Supervised Pre-training: One fundamental design of LLM is that it unifies all
 NLP tasks into a single next-token-prediction paradigm, which enables self-supervised pre-training
 on a large corpus collected from different sources. For pre-training graph models, while numerous
 efforts have been made from both the LLM as a predictor and LLM as an enhancer approaches,
 these attempts usually require the learning target to be labeled (Liu et al., 2023a; Chen et al., 2023).

However, a graph foundation model should have no constraint on the input graph (has labels or not) and can learn cross-domain knowledge from large-scale graph data in a self-supervised fashion.

Fluidity in Tasks: A graph foundation model should also possess the same level of versatility and 111 fluidity in handling different tasks as an LLM. Specifically, such ability can be broken down into 112 three levels: (a) The graph foundation model can naturally respond appropriately to different graph 113 tasks based on user instructions without requiring task-specific adjustment (e.g., the same model 114 performs classification and question-answering tasks without any modification.) (b) With appropriate 115 instruction-tuning, the model should have in-context learning ability on unseen tasks (e.g., a model 116 tuned on citation network also performs well on knowledge graphs with proper instructions). (c) Users 117 should be able to define new, previously unseen tasks by modifying the graph structure and features 118 in a way that aligns with the universal input representation of the model. They can continuously train the model on new data without special adaptation. Existing approaches that use GNN models as the 119 predictors are usually either restricted in the output format (Liu et al., 2023a; Xia et al., 2024; He 120 et al., 2024a) or need additional fine-tuning on the task head (Sun et al., 2023; Wang et al., 2022). 121 Consequently, despite having better structural modeling ability, such models cannot accommodate 122 task changes or deal with novel tasks, e.g., shifting from a classification task to a question-answering 123 task that requires outputting all shortest paths between two nodes. 124

Graph Understanding: Since the LLM as a predictor approach uses a generative LLM to take 125 text input and produce text output, it naturally has the fluidity to accept varied prompts to tackle 126 different tasks. However, such an approach processes the structural information poorly (Wang et al., 127 2023), making the utility of these models limited on many graph tasks. More importantly, even 128 though some recent variants can use auxiliary graph models (such as GNNs) to incorporate structural 129 information (Tang et al., 2023; He & Hooi, 2024; Zhang et al., 2024), the graph models are frozen 130 and not responsive to different prompts, and the output from the graph models may not be the most 131 relevant to the input prompt. On the contrary, a graph foundation model should account for the 132 unique structural information of graphs such as node degrees, shortest paths, common neighbors, 133 etc., and generate graph representations dependent on the input prompt. It should not only have 134 LLM's prompt learning capability but also learn graph structure and semantic information jointly.

135 136

137

3 Method

In this section, we first propose a generative modeling framework for graphs, serving as the graph counterpart of traditional language modeling. Next, we introduce a novel GNN-LLM architecture for the proposed graph generative modeling problem. Finally, we describe the unified pre-training tasks to train GOFA towards the proposed GFM properties.

142 143 144

3.1 GENERATIVE MODELING FOR GRAPH

145 **Unifed task formats.** A generative model usually takes existing contexts, such as user prompts 146 and passages, as input to generate conditional output related to the contexts, such as answers and 147 completed sentences. Defining unified input and output formats for tasks in language applications 148 is easy, as they are purely text-based. Further, because both the pre-training and downstream tasks 149 are constructed in the same format (i.e., next-token-prediction), the downstream tasks conveniently 150 adapt the knowledge from pre-training tasks, resulting in surprising capabilities, such as zero-shot 151 learning. However, graph data from different domains vary significantly by input feature (e.g., nodes 152 in a citation network have completely different vector representations as nodes in a knowledge graph) and output target, preventing direct knowledge transfer between tasks. Hence, the first challenge is 153 to define a unified format for graph tasks, such that the model can do large-scale self-supervised 154 pre-training on arbitrary graphs and transfer to downstream tasks seamlessly. 155

To **unify graph task input**, we follow the previous work OFA (Liu et al., 2023a) and extend the definition of Text-Attribute Graph (TAG) beyond graphs with text features such as citation and product networks. In fact, any node and edge features can be represented by texts. For example, textual attributes of metabolites and metabolic reactions replace the node and edge features in metabolic networks. Similarly, in airline networks, airport and flight route details can be converted into textual descriptions for nodes and edges. Non-textural features, like numerical data, can also be transformed into text strings, as in LLMs. Even for graphs without any features, we can still attach sentences like 162 *"The degree of this node is 3"* to nodes. Formally, a TAG is a graph $G = \{V, E, X_V, X_E\}$ where 163 V and E are the sets of nodes and edges. Each node $v \in V$ (edge $e \in E$) corresponds to a text 164 description $x(v) \in X_V$ ($x(e) \in X_E$). Such a format encodes almost all existing graph data and 165 serves well as a general input representation.

166 For self-supervised language modeling, the generated output essentially completes the input sentence. 167 Such a task requires the model to have a deep semantic and logical understanding of the provided 168 contexts, which is crucial for downstream applications. Similarly, in graph modeling, we aim to 169 achieve the same level of understanding through graph completion tasks. Given a TAG, the output 170 should complete the graph conditioned on its semantic and structural information. We choose to 171 use natural language as the most tangible output format to complete a TAG. Succinctly, all natural 172 language tasks can be modeled as sentence completion, and similarly, we aim to model all graph tasks with graph completion. 173

174 Generative Graph Modeling. We then formally define the generative graph modeling framework 175 for graph completion. This framework supports various graph-related tasks, including classification 176 and free-form question answering. An LLM starts generating only from the end of the input sentence. 177 However, in a TAG, every end of a sentence on a node is a potential generation starting point, but 178 users might only be interested in generating output for specific nodes. To accommodate this, we 179 introduce Nodes of Generation (NOG), allowing users to specify starting points for generation. The modeling task is to take a TAG as input and complete the TAG logically and sensibly by completing 180 the sentences on the potentially user-specified nodes. 181

We define graph generative modeling as the likelihood of the text y associated with the NOG v: 183

 $p(y|v,G) = \prod_{l=1}^{L} p(y_l|y_{< l}, v, G),$ (1)

where y_l is the *l*-th token of y, and $y_{< l}$ is its preceding 187 tokens. The NOG v is a completion target node with initial 188 corresponding text x(v), and x(v) can be empty. G con-189 tains structural and textual information of neighbor nodes 190 to help the model generate y. Under this framework, we 191 can design a range of self-supervised learning tasks. For 192 example, the graph completion task is shown on Figure 2, 193 where the text on the NOG v is incomplete, and the goal is to complete the sentence on it using the existing text 194 and the neighbor information. This task is covered by 195 Equation (1), which encourages the model to have a strong 196 graph structure and feature comprehension ability. Thus, 197 the importance of the framework is that a model properly solves such modeling problems can possess the three prop-199 erties of GFM discussed in Section 2, thus can benefit 200 diverse downstream tasks, even in the zero-shot fashion. 201 Section F.2 discusses how the proposed framework applies 202 to various tasks related to the three properties. 203

184

185 186

Sentence Completion



Figure 2: Task examples in TAG. Sentence completion/Next-word prediction. Orange node v represents NOG.

204 3.2 GOFA : GENERATIVE ONE-FOR-ALL MODEL 205 3.2 GOFA : GENERATIVE ONE-FOR-ALL MODEL

To solve the generative graph modeling problem proposed in Equation (1), we design the GOFA architecture shown in Figure 3. Overall, GOFA consists of a *graph language encoder* and an *LLM decoder*. The graph language encoder interleaves GNN layers with LLM compressor layers to learn node representations containing joint structural and semantic information. The LLM decoder is then used to generate texts from the NOG representation. The LLM compressor and decoders are all pre-trained decoder-only transformers. We describe each component in detail as follows.

LLM compressor: Because GNNs require node and edge representations to have the same input dimension, many previous works propose to pool all tokens' output embeddings from the LLM as the node and edge vector representations and feed them to a GNN (Liu et al., 2023a; Huang et al., 2023a; He & Hooi, 2024). While this approach shows effectiveness in tasks of fixed form, such as classification and regression, *it is insufficient in more complex tasks such as generation*, as 1) the

236

237

238 239

248 249 250

262 263



Figure 3: **GOFA Architecture**. Text tokens of TAG's node/edges are concatenated with memory tokens to be input to Graph Language Encoder. GNN layers are interleaved into LLM Compressor layers, where memory embeddings from LLM Compressor Layer are used as node/edge features for token-level GNN message passing. Memory embedding will be used for teacher-forcing training.

240 pooling process inevitably loses semantic information, 2) standard LLMs are not trained in a way 241 such that the pooled output embedding is a summarization of the input sentence, and 3) the pooled 242 representation space is no longer compatible with the space of the downstream LLM decoder. Hence, 243 we adopt a pre-trained sentence compressor (Ge et al., 2023) that preserves as much information as 244 possible from the original sentence in *fixed-size multi-token embeddings*. The core idea is to compress 245 a sentence into K embeddings instead of one embedding. Specifically, the sentence compressor has the same architecture as a decoder-only LLM, but the sentence to be compressed $\{q(x_i)\}_{i=1}^l$ is 246 appended by a sequence of K memory tokens $\{q(m_j)\}_{j=1}^K$, and the t-th layer of the LLM is: 247

$$\{Q_x^{t+1}, Q_{m,x}^{t+1}\} = \{q^{t+1}(x_1), ..., q^{t+1}(x_l), q^{t+1}(m_1), ..., q^{t+1}(m_K)\}$$

= $LLM^t(\{q^t(x_1), ..., q^t(x_l), h^t(m_1), ..., h^t(m_K)\}) = LLM^t(\{Q_x^t, H_x^t\}).$ (2)

We use Q_x^t and $Q_{m,x}^t$ to represent the *t*-th LLM layer outputs corresponding to actual text tokens in sentence *x* and the *K* memory tokens appended at the end of text tokens, respectively. We use H_x^t to represent the *t*-th GNN layer output, which will be explained later. In Equation (2), the text tokens (Q_x^t) and memory tokens (H_x^t) , processed by the previous GNN layer) are concatenated as a single sequence of embeddings, which are fed to the current LLM layer. *Because the last K tokens attend to all previous tokens, they can compress all information in the sentence into the output embeddings of the K tokens.* This compressor architecture is inspired by ICAE (Ge et al., 2023). The compression ability is obtained through auto-encoder-style fine-tuning, as discussed in Appendix A.1.

Token-level GNN: Conventional GNNs take one embedding vector for each node/edge. However, now each node/edge sentence is compressed into K memory token embeddings $Q_{m,x}$. Hence, we propose a simple extension of GNNs to the token level. For node $v \in V$, the t-th GNN layer is

$$H_{x(v)}^{t}[k] = GNN(Q_{m,x(v)}^{t}[k], \{(Q_{m,x(u)}^{t}[k], Q_{m,x(e_{uv})}^{t}[k]) | u \in \mathcal{N}(v)\}), \quad k = 1...K.$$
(3)

In the GNN layer, tokens at different indices do not communicate. If we directly stack these GNN layers, they degenerate into multiple isolated GNNs for each token. Nevertheless, because we interleave the GNN layers into the LLM layers, as shown in Figure 3, the isolated tokens exchange information in the subsequent self-attention layers of the LLM. This approach significantly reduces memory usage because we do not allow cross-token attention between different nodes. While edge memory tokens $Q_{m,x(e)}^t$ are passed into GNN to assist message passing, their representations are not updated in the GNN layer but directly passed to the next LLM layer, hence $H_{x(e)}^t = Q_{m,x(e)}^t$. In GOFA, we use a modified Transformer Convolutional GNN (Shi et al., 2021) to be consistent with the transformer architecture of LLM (see Appendix A.3 for details).

We insert one GNN layer between two transformer layers, while the first and the last layer are always 273 transformer layers. In GOFA, we only insert GNN between the last few transformer layers, but 274 this can be flexible depending on the computational resources. Following previous practice, we 275 incorporate feed-forward (FF) layers into the GNN to increase expressivity and residual connections 276 to stabilize training. Moreover, GOFA should maintain the functions of an LLM on plain texts, hence, 277 inspired by the gating mechanism in earlier works (Hochreiter & Schmidhuber, 1997; Alayrac et al., 278 2022), we apply a *tanh* gate, initialized at 0, to the GNN and FF layer outputs so that the *initial model* 279 ignores the information from GNN layers and is equivalent to the pre-trained LLM. We introduce 280 weight decay in the gating module to promote gate value staying in large non-zero values only when graph information helps generate more accurate final text outputs. 281

282 **LLM decoder:** After applying the model to the textual graph, the memory tokens $Q_{m,x}$ of every node 283 contain information about the text on the node, the surrounding node text, and the graph structure 284 due to the message-passing process in the GNN layers. Then, for the NOG v and its corresponding 285 target text y, we insert $Q_{m,x}$ at the front of the token embeddings of the target text to generate and 286 use teacher-forcing to maximize the standard log-likelihood of y using the next-token-prediction 287 objective. In this way, we have modeled the problem in Equation (1). The compressor, decoder, and GNN parameters can be jointly or separately optimized, potentially with PEFT methods like 288 LoRA (Hu et al., 2022). In this paper, we use ICAE (Ge et al., 2023) as our backbone LLM, but the 289 GOFA architecture is not tied to any specific LLM. More details are discussed in Appendix A.2. 290

Discussion. Our proposed graph language encoder has several advantages over existing methods. Suppose a graph has V nodes, E edges, and the average number of tokens for all nodes is k. The complexity of one GOFA layer is $O(Vk^2)$, as the self-attention only happens within each node. Note that we have omitted the extra computation complexity of message-passing because it only happens at individual indices with $O(E) \ll O(Vk^2)$ in practical graphs. Instead, if we concatenate texts in all nodes and input them to a regular LLM, the complexity of one layer is $O((Vk)^2)$, which is significantly larger than GOFA. Further, introducing GNN layers in LLMs is theoretically more powerful than pure LLMs for modeling graph structures, which is discussed in Appendix E.2.

298 299

300

3.3 UNIFIED TASK REPRESENTATION IN GOFA

301 The formulation in Equation (1) provides a natural way for users to query the graph by selecting a 302 NOG. Users can combine NOG with graph prompting techniques on subgraphs to solve tasks unique 303 to the graph domain, such as node-, link-, and graph-level tasks. Following OFA (Liu et al., 2023a), 304 we convert all tasks into tasks on k-hop rooted subgraphs extracted around the target nodes. For 305 node-level tasks, the target node is a single node in the graph. For link-level tasks, the target nodes 306 are the node pair. If the target node is not specified (e.g., the task is a graph task), we set the default 307 target nodes to all nodes in the graph. We connect a prompt node with the user query as NOG to all target nodes. GOFA completes the prompted input TAG by answering the query on the NOG, which 308 still aligns with the proposed generative modeling framework. This design has several advantages: (1) 309 All tasks are represented by a NOG, so the distribution of all tasks can be unified into a single space, 310 helping the model generalize to unseen tasks from learned task representations; (2) The text feature 311 for the prompt node describes the task details. Connecting the prompt node to target nodes enables 312 the prompt node to query the most important knowledge from the input graph through attention. This 313 ensures the output embedding for NOG is conditionally learned from the GNN process subject to the 314 different prompts. Conversely, most of the previous works (He & Hooi, 2024; Tang et al., 2023; 2024; 315 Zhang et al., 2024) only computed a fixed embedding for each node before any prompt is introduced.

316 317

3.4 LARGE-SCALE PRE-TRAINING

318

As discussed in Section 2 and Section 3.1, we design self-supervised pre-training tasks based on the three GFM properties to train GOFA. The training datasets include MAG240M (Hu et al., 2021a) to upscale the model's text understanding ability, Pubmed and Arxiv (Hu et al., 2021b) for academic knowledge, Wikikg90mv2 (Hu et al., 2021a) and WikiGraph (proposed by us) for semantic diversity, and Ultrachat200k (Ding et al., 2023) dataset for question-answering ability. Details about the datasets can be found in Appendix C. Each node is assigned a unique ID (e.g., [Node A]) to enable

node querying in the graph. We design four pre-training tasks as shown in Figure 1. We describe
 the rationale of each task below and leave some implementation details and additional discussion in
 Appendix F and Appendix E.3.

Sentence Completion Task. This task aims for large-scale pre-training (GFM property one) by training GOFA to predict the remaining text in a node based on both the existing node text and the surrounding graph information. Such a task can be applied to any TAG without labeling, thus facilitating large-scale pre-training for GOFA to acquire diverse knowledge.

Structural Understanding Task. This task aims to provide structural modeling ability for GOFA
 (GFM property three). The structural task connects NOG randomly selected node pairs to generate
 the actual shortest path or common neighbors between them. Through these two tasks, the model is
 expected to gain the ability to identify basic graph structures fundamental for graph-related problems.

Question Answering Task. This task aims to ensure fluidity in generation for GOFA (GFM property two). Unlike language corpus, which naturally contains many question-and-answer (QA) pairs, graph data usually only contain objective descriptions of entities. Hence, we convert natural language Question-Answer sequences into chain graphs and connect a NOG with a question to the chain graph for open-ended answer generation. This essential task enables GOFA to be responsive to arbitrary downstream applications expressed in free-form text questions.

Information Retrieval Task. In most downstream tasks, GOFA links a prompt node to target nodes
 in the graph to address related problems. To facilitate effective information extraction, we design
 an information retrieval task where a NOG queries a target node using its node ID. The model
 must retrieve and isolate information specific to the queried node from the remaining target nodes,
 encouraging a message-passing process conditioned on the input, as discussed in Section 3.2.

- 347
- 348 349

4 RELATED WORK

- 350 351 352
- 353

Here we mainly discuss the two tracks of general graph models, and leave discussion about graph prompt learning and graph neural networks to Appendix D.

356 LLMs as enhancers: One direction uses LLMs to convert the text features of graphs to unified 357 representations (Liu et al., 2023a; Chen et al., 2023; Li et al., 2024; He et al., 2024a; Plenz & Frank, 358 2024) for downstream graph models to distinguish and transfer knowledge between different domains. For example, OFA (Liu et al., 2023a) uses LLM to unify the input features in different datasets and 359 transforms multiple types of graph classification tasks into a unified binary classification format. 360 TAPE (He et al., 2024a) utilizes LLM to generate question answers and explanations as enhanced 361 node features. Such approaches have good structural modeling ability, but they usually cannot 362 generate free-form output to handle arbitrary tasks. 363

LLMs as predictors: Another line of research proposes using LLMs as predictors and aligning 364 graph representation with LLM inputs. Preliminary attempts flatten graphs into text representations and feed them into LLM (Chen et al., 2023; Zhao et al., 2023b; Guo et al., 2023; Zhao et al., 2023a; 366 Qian et al., 2023). These approaches can benefit from LLM for task fluidity but fail to model 367 structural information unique to graph data properly (Zhao et al., 2023b; Mao et al., 2024; Ye et al., 368 2023). Realizing this problem, follow-up work extends methods in vision-language domain (Alayrac 369 et al., 2022; Li et al., 2023) to the graph domain and train adapters to link graph model outputs 370 to LLM (Tang et al., 2023; 2024; Huang et al., 2024; Zhang et al., 2024; He & Hooi, 2024). For 371 example, GraphGPT (Tang et al., 2023) first implements a text-structure alignment between graph 372 representation and text embedding to pretrain a GNN. LLaGA (Chen et al., 2024) creatively uses 373 a template to represent a subgraph with pooled node embeddings for LLM input. Inspired by 374 Q-former (Li et al., 2023), GraphTranslator (Zhang et al., 2024) aligns node and text tokens from pre-375 trained GNN and LLM. UniGraph (He & Hooi, 2024) pretrains GNN using masked word prediction and then tuning a projector to map graph embedding to language space and enable zero-shot learning. 376 However, the GNN and LLM parts of these methods are usually detached, meaning the prompt 377 information can not attend to the message-passing process.

Table 2: Zero-shot experiment results with instruction tuning (Accuracy).

Task	Cora-	Node	Wik	tiCS		Products	8	ExplaGraphs	Cora-Link
Way	7	2	10	5	47	10	5	2	2
LLama2-7B Mistral-7B	47.92 60.54	73.45 88.39	40.10 63.63	58.77 71.90	27.65 43.99	58.71 70.16	64.33 74.94	57.76 68.77	48.15 49.43
OFA-Llama2 GraphGPT UniGraph ZeroG LLaGA	28.65 44.65 69.53 64.21 51.85	56.92 89.74 87.83 62.73	21.20 - 43.45 31.26 -	35.15 60.23 48.25	19.37 18.84 38.45 31.24 23.10	30.43 66.07 51.24 34.15	39.31 - 75.73 71.29 39.72	51.36 - - - -	52.22 50.74 - 88.09
GOFA-T GOFA-F	70.81 69.41	85.73 87.52	71.17 68.84	80.93 80.62	54.60 56.13	79.33 80.03	87.13 88.34	79.49 71.34	85.10 86.31

394

396

397

398

399 400

402

378

5 EXPERIMENT

This section evaluates the proposed methods by answering the following four questions: Q1: Are the pre-training tasks in GOFA effective for graph-language modeling and structure understanding? Q2: Does the pre-trained GOFA help with critical general graph model application, zero-shot learning? Q3: Is using GOFA more advantageous than LLMs in graph tasks? Q4: Does GOFA have the fluidity to handle open-ended graph-related tasks? Additionally, we also include supervised experiments in Appendix F.5.

401 5.1 GOFA PRE-TRAINING

403 To answer **O1**, we pre-train the GOFA model using ICAE models on Mistral-7B (Jiang et al., 2023), optimizing the ob-404 jective in Equation (1) using the proposed tasks. The training 405 details can be found in Appendix F.3. After training, we eval-406 uate the perplexity of both GOFA and base LLM on Cora, 407 Product, and Wikics datasets (all three are not included in the 408 pre-training). We report the perplexity in Table 1. Note that 409 during pre-training, we only update the weight of the GNN 410 layers, and GOFA 's lower perplexity shows that the structural 411

Table 1:	Evaluatio	on for pre-
trained GO	OFA . (RM	SE for SPD
and CN)		

	Perplexity \downarrow	$\text{SPD}\downarrow$	$\mathrm{CN}\downarrow$
Mistral-7B	30.12	1.254	1.035
GOFA-SN	26.20	-	-
GOFA	21.34	0.634	0.326

and semantic information in the node's neighbor can effectively help complete the sentence with 412 more relevance than the original LLM. Further, to validate that training of GOFA will not affect the 413 original LLMs' ability, we input GOFA with single node graphs without any connections (denoted as GOFA-SN) to evaluate the perplexity, as shown in Table 1. We can see that without connection 414 information around the center node, generation on a single node graph remains comparable to LLM 415 and even better due to the pre-training process, showing that GOFA training does not destroy the 416 desirable property of a pre-trained LLM. Besides sentence completion, another important GOFA 417 pre-training objective is the structure learning ability. We report shortest path distance and common 418 neighbor count prediction results in Table 1, compared with LLM models whose inputs are textualized 419 graphs, with descriptions of edge connections. The datasets we used are Cora and Product. We see a 420 significant performance improvement of GOFA over base LLM, showing that a difficult graph task 421 for LLM can be well solved by the GNN layers with better structure modeling ability.

422 423

424

5.2 ZERO-SHOT LEARNING WITH GOFA

To answer Q2, we performed zero-shot experiments on various graph tasks. Despite using QA-chain data in the pre-training stage, the graph data does not include knowledge about task formats like classification and does not output exact matches to the answers. Hence, we first instruction-tuned the pre-trained GOFA in Section 5.1 on a small amount of data. We report the zero-shot results of two GOFA instruction tuning settings named GOFA-T and GOFA-F, as shown in Table 2 and Table 3. GOFA-T includes node and link classification tasks from Arxiv and Pubmed and GOFA-F addtionally adds MAG240M and Wiki90mv2 datasets. The instruction-tuning details can be found in Appendix F.4. Note that the zero-shot datasets are unseen during both pre-training and instruction



Table 4: Comparison between GOFA and LLM with the same input.

Task	ExplaGraphs	Time	WikiCS	Time	Cora-Link	Time	FB15k237	Time
Metric	Acc ↑	sec/sample ↓	Acc↑	sec/sample ↓	Acc↑	sec/sample ↓	Acc ↑	sec/sample ↓
LLM-N	74.13	1.50	OOM	OOM	50.36	3.84	51.25	3.92
GOFA-F	79.49	0.48	71.17	2.43	85.10	1.67	73.49	3.37
Improvement	7.23%	68.00%	NA	NA	68.98%	56.51%	43.40%	14.03%

452 finetuning. The goal of instruction fine-tuning is not to let the model learn particular knowledge from 453 these datasets but to make the model understand the task format described in Appendix F.4.

454 While the instruction-tuning dataset only covers the relatively small spectrum of the graph datasets, 455 we observe that GOFA achieves very non-trivial performance on all node-level (Cora-Node, WikiCS, 456 Products), link-level (FB15K237, Cora-Link), and graph-level (ExplaGraphs, SceneGraphs) tasks. 457 GOFA also generalizes to different ways and even question-answering (SceneGraphs) tasks, showing 458 its desirable fluidity. GOFA outperforms LLM and graph foundation model baselines on most 459 datasets and exceeds best baselines by a large margin (> 10%) on WikiCS, Products, FB15K237 and 460 ExplaGraphs, showing GOFA's ability to combine the advantage of both LLM and graph models. GOFA not only achieves remarkable results on the knowledge graph and academic graph, which 461 are proximal to the trained data but also excels in Products and ExplaGraphs whose distribution 462 shifts significantly from training data, which further highlights GOFA 's substantial generalizability. 463 Meanwhile, we observe that GOFA is only achieving comparable performance to LLM on the 464 SceneGraph dataset. We suspect that the instruct-tuning data contains information-dense texts, 465 reducing the model's ability on common sense questions that this dataset requires. In the future, we 466 plan to diversify instruction-tuning datasets with common sense knowledge to enhance such ability. 467

We further conducted the same experiments on intermediate pre-training checkpoints, and show 468 results in Figure 4. We observe that as the model witnesses more pre-training samples/tokens, the 469 downstream task performance also increases significantly, confirming the importance of large-scale 470 pre-training on graph data. The performance continues to improve, meaning that the model can 471 potentially scale to higher capability with more samples; we leave this to future work. In Figure 5, 472 we plot the instruction-tuning performance when we remove the Wikipedia datasets and information 473 retrieval task (w/o R+W), only remove the retrieval task, (w/o R), and full tasks. We can see that 474 Wikipedia datasets improve the model performance of all the datasets for the diverse corpus it 475 introduced. The retrieval tasks particularly improve the knowledge graph performance due to the 476 improved ability to retrieve key correlations between target entities. These show the necessity and 477 effectiveness of the overall pre-training task selection and design.

478 479

443

5.3 COMPARING GOFA WITH LLMS

480

481 Answering Q3 is critical to understanding the necessity of the GNN layers and the effectiveness of 482 GOFA as a general graph model. We compare GOFA to LLM whose textual prompt contains the same information as the input graph to GOFA. Specifically, for a GOFA input graph, we concatenate 483 all node texts as the prompt and append the connection information to it, as in "Node A connects 484 to Node B". The text is then combined with task and question descriptions as input to an LLM for 485 classification tasks. Approaches similar to this are widely adopted and acknowledged (Chen et al.,



Figure 6: GOFA diverse responses to open-ended questions.

2023; Fatemi et al.). We present both the classification performance and per sample inference time in 507 Table 4 and denote the LLM method as LLM-N. We observe impressive performance improvement 508 of GOFA on all datasets, even when the LLM is prompted with the same information, showing that 509 GOFA, with the help of the GNN and interleaving design, utilizes the graph information much more 510 effectively. Moreover, we also observe a fundamental reduction in inference costs, confirming our 511 analysis in Section 3.2 that, with the same input, GOFA is more efficient than LLMs. Note that when 512 the input size is large, such as in WikiCS, LLM struggles with high memory consumption of the long 513 sequence, whereas the GOFA avoids that by leveraging the sparsity of graph data and using edge 514 information to compute the most important attention information.

515 516 517

504

505 506

5.4 GOFA RESPONSES ON DIVERSE TASKS

Finally, we answer Q4 by providing generation examples of GOFA in Figure 6, where we prompt 518 the same citation graph differently and achieved corresponding and high-quality responses. The top 519 and middle examples have the same connection for their NOGs (both connected to the same five 520 nodes), but when we change the prompt text on the NOGs, the generated texts also adjust accordingly, 521 utilizing the neighbor node information, validating that the message-passing is conditioned on the 522 prompt. As in the bottom example, we can also prompt the graph differently by connecting the NOG 523 to two target nodes and querying about the shortest path distance. In this case, the model successfully 524 generates actual paths between the two nodes, which is an ability not seen in traditional graph models 525 that can only output numerical predictions about the path length. These examples demonstrate 526 GOFA's outstanding ability to answer open-ended questions. More examples are provided in B.2.

527 528

529

6 CONCLUSION, LIMITATIONS, AND FUTURE WORKS

530 We introduce GOFA, a generative One-for-All graph foundation model. GOFA is pre-trained 531 under graph completion framework to enable large-scale self-supervised learning. By integrating 532 GNN layers with LLM layers, GOFA combines the generative capabilities of LLMs for free-form output with the structural learning strengths of GNNs for understanding complex graph connections. 534 Our experiments demonstrate that GOFA, when fine-tuned with a small number of data, achieves impressive zero-shot performance, highlighting its potential as a robust graph foundation model. One limitation of our work is the extensive training time required due to the use of abundant graph data. Additionally, we employ a frozen LLM compressor in our architecture; hence, the compression capability is not dynamically integrated with the graph data, potentially impacting the efficiency and 538 adaptability of the model. We believe finetuning a graph language compressor can further enhance the performance of GOFA and will explore it in the future.

540 REFERENCES

582

583

584

588

- Josh Abramson, Jonas Adler, Jack Dunger, Richard Evans, Tim Green, Alexander Pritzel, Olaf
 Ronneberger, Lindsay Willmore, Andrew J Ballard, Joshua Bambrick, et al. Accurate structure
 prediction of biomolecular interactions with alphafold 3. *Nature*, pp. 1–3, 2024.
- Jean-Baptiste Alayrac, Jeff Donahue, Pauline Luc, Antoine Miech, Iain Barr, Yana Hasson, Karel
 Lenc, Arthur Mensch, Katherine Millican, Malcolm Reynolds, et al. Flamingo: a visual language
 model for few-shot learning. *Advances in neural information processing systems*, 35:23716–23736,
 2022.
- 549
 550
 550
 551
 552
 Yutong Bai, Xinyang Geng, Karttikeya Mangalam, Amir Bar, Alan Yuille, Trevor Darrell, Jitendra Malik, and Alexei A Efros. Sequential modeling enables scalable learning for large vision models. *arXiv preprint arXiv:2312.00785*, 2023.

Rishi Bommasani, Drew A. Hudson, Ehsan Adeli, Russ Altman, Simran Arora, Sydney von Arx, 553 Michael S. Bernstein, Jeannette Bohg, Antoine Bosselut, Emma Brunskill, Erik Brynjolfsson, 554 S. Buch, Dallas Card, Rodrigo Castellon, Niladri S. Chatterji, Annie S. Chen, Kathleen A. Creel, 555 Jared Davis, Dora Demszky, Chris Donahue, Moussa Doumbouya, Esin Durmus, Stefano Ermon, John Etchemendy, Kawin Ethayarajh, Li Fei-Fei, Chelsea Finn, Trevor Gale, Lauren E. Gillespie, Karan Goel, Noah D. Goodman, Shelby Grossman, Neel Guha, Tatsunori Hashimoto, Peter 558 Henderson, John Hewitt, Daniel E. Ho, Jenny Hong, Kyle Hsu, Jing Huang, Thomas F. Icard, 559 Saahil Jain, Dan Jurafsky, Pratyusha Kalluri, Siddharth Karamcheti, Geoff Keeling, Fereshte Khani, O. Khattab, Pang Wei Koh, Mark S. Krass, Ranjay Krishna, Rohith Kuditipudi, Ananya 561 Kumar, Faisal Ladhak, Mina Lee, Tony Lee, Jure Leskovec, Isabelle Levent, Xiang Lisa Li, 562 Xuechen Li, Tengyu Ma, Ali Malik, Christopher D. Manning, Suvir Mirchandani, Eric Mitchell, 563 Zanele Munyikwa, Suraj Nair, Avanika Narayan, Deepak Narayanan, Benjamin Newman, Allen Nie, Juan Carlos Niebles, Hamed Nilforoshan, J. F. Nyarko, Giray Ogut, Laurel J. Orr, Isabel Papadimitriou, Joon Sung Park, Chris Piech, Eva Portelance, Christopher Potts, Aditi Raghunathan, 565 Robert Reich, Hongyu Ren, Frieda Rong, Yusuf H. Roohani, Camilo Ruiz, Jack Ryan, Christopher 566 R'e, Dorsa Sadigh, Shiori Sagawa, Keshav Santhanam, Andy Shih, Krishna Parasuram Srinivasan, 567 Alex Tamkin, Rohan Taori, Armin W. Thomas, Florian Tramèr, Rose E. Wang, William Wang, 568 Bohan Wu, Jiajun Wu, Yuhuai Wu, Sang Michael Xie, Michihiro Yasunaga, Jiaxuan You, Matei A. 569 Zaharia, Michael Zhang, Tianyi Zhang, Xikun Zhang, Yuhui Zhang, Lucia Zheng, Kaitlyn Zhou, 570 and Percy Liang. On the opportunities and risks of foundation models. ArXiv, abs/2108.07258, 571 2021. URL https://api.semanticscholar.org/CorpusID:237091588. 572

- Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhari-573 wal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agar-574 wal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, 575 Daniel Ziegler, Jeffrey Wu, Clemens Winter, Chris Hesse, Mark Chen, Eric Sigler, Ma-576 teusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCan-577 dlish, Alec Radford, Ilya Sutskever, and Dario Amodei. Language models are few-shot 578 learners. In H. Larochelle, M. Ranzato, R. Hadsell, M.F. Balcan, and H. Lin (eds.), Ad-579 vances in Neural Information Processing Systems, volume 33, pp. 1877–1901. Curran Asso-580 ciates, Inc., 2020. URL https://proceedings.neurips.cc/paper files/paper/ 581 2020/file/1457c0d6bfcb4967418bfb8ac142f64a-Paper.pdf.
 - Runjin Chen, Tong Zhao, Ajay Jaiswal, Neil Shah, and Zhangyang Wang. Llaga: Large language and graph assistant. *arXiv preprint arXiv:2402.08170*, 2024.
- Zhikai Chen, Haitao Mao, Hang Li, Wei Jin, Hongzhi Wen, Xiaochi Wei, Shuaiqiang Wang, Dawei
 Yin, Wenqi Fan, Hui Liu, and Jiliang Tang. Exploring the potential of large language models (llms)
 in learning on graphs, 2023.
 - Quanyu Dai, Xiao-Ming Wu, Jiaren Xiao, Xiao Shen, and Dan Wang. Graph transfer learning via adversarial domain adaptation with graph convolution. *IEEE Transactions on Knowledge and Data Engineering*, 35(5):4908–4922, 2022.
- Ning Ding, Yulin Chen, Bokai Xu, Yujia Qin, Zhi Zheng, Shengding Hu, Zhiyuan Liu, Maosong
 Sun, and Bowen Zhou. Enhancing chat language models by scaling high-quality instructional conversations, 2023.

594 595 596	Bahare Fatemi, Jonathan Halcrow, and Bryan Perozzi. Talk like a graph: Encoding graphs for large language models. In <i>The Twelfth International Conference on Learning Representations</i> .
597 598 599 600	Jiarui Feng, Yixin Chen, Fuhai Li, Anindya Sarkar, and Muhan Zhang. How powerful are k-hop message passing graph neural networks. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and Kyunghyun Cho (eds.), <i>Advances in Neural Information Processing Systems</i> , 2022. URL https://openreview.net/forum?id=nN3aVRQsxGd.
601 602 603 604 605 606	Jiarui Feng, Lecheng Kong, Hao Liu, Dacheng Tao, Fuhai Li, Muhan Zhang, and Yixin Chen. Extending the design space of graph neural networks by rethinking folklore weisfeiler-lehman. In A. Oh, T. Neumann, A. Globerson, K. Saenko, M. Hardt, and S. Levine (eds.), Advances in Neural Information Processing Systems, volume 36, pp. 9029–9064. Curran Associates, Inc., 2023. URL https://proceedings.neurips.cc/paper_files/paper/2023/file/lcac8326ce3fbe79171db9754211530c-Paper-Conference.pdf.
607 608	Matthias Fey and Jan Eric Lenssen. Fast graph representation learning with pytorch geometric, 2019.
609 610 611 612	Mikhail Galkin, Xinyu Yuan, Hesham Mostafa, Jian Tang, and Zhaocheng Zhu. Towards foundation models for knowledge graph reasoning. In <i>The Twelfth International Conference on Learning Representations</i> , 2023.
613 614 615	Tao Ge, Hu Jing, Lei Wang, Xun Wang, Si-Qing Chen, and Furu Wei. In-context autoencoder for context compression in a large language model. In <i>The Twelfth International Conference on Learning Representations</i> , 2023.
616 617 618	Justin Gilmer, Samuel S Schoenholz, Patrick F Riley, Oriol Vinyals, and George E Dahl. Neural message passing for quantum chemistry. In <i>International conference on machine learning</i> , pp. 1263–1272. PMLR, 2017.
619 620 621 622	Jiayan Guo, Lun Du, Hengyu Liu, Mengyu Zhou, Xinyi He, and Shi Han. Gpt4graph: Can large language models understand graph structured data ? an empirical evaluation and benchmarking, 2023.
623 624 625	Stephen J Hardiman and Liran Katzir. Estimating clustering coefficients and size of social networks via random walk. In <i>Proceedings of the 22nd international conference on World Wide Web</i> , pp. 539–550, 2013.
626 627 628 629	Xiaoxin He, Xavier Bresson, Thomas Laurent, Adam Perold, Yann LeCun, and Bryan Hooi. Har- nessing explanations: LLM-to-LM interpreter for enhanced text-attributed graph representation learning. In <i>The Twelfth International Conference on Learning Representations</i> , 2024a. URL https://openreview.net/forum?id=RXFVcynVel.
630 631 632 633	Xiaoxin He, Yijun Tian, Yifei Sun, Nitesh V. Chawla, Thomas Laurent, Yann LeCun, Xavier Bresson, and Bryan Hooi. G-retriever: Retrieval-augmented generation for textual graph understanding and question answering, 2024b.
634 635	Yufei He and Bryan Hooi. Unigraph: Learning a cross-domain graph foundation model from natural language. <i>arXiv preprint arXiv:2402.13630</i> , 2024.
636 637 638 639	Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. <i>Neural Comput.</i> , 9(8): 1735–1780, nov 1997. ISSN 0899-7667. doi: 10.1162/neco.1997.9.8.1735. URL https://doi.org/10.1162/neco.1997.9.8.1735.
640 641 642 643	Edward J Hu, yelong shen, Phillip Wallis, Zeyuan Allen-Zhu, Yuanzhi Li, Shean Wang, Lu Wang, and Weizhu Chen. LoRA: Low-rank adaptation of large language models. In <i>International Conference on Learning Representations</i> , 2022. URL https://openreview.net/forum?id=nZeVKeeFYf9.
644 645 646	Weihua Hu, Matthias Fey, Hongyu Ren, Maho Nakata, Yuxiao Dong, and Jure Leskovec. Ogb-lsc: A large-scale challenge for machine learning on graphs, 2021a.

647 Weihua Hu, Matthias Fey, Hongyu Ren, Maho Nakata, Yuxiao Dong, and Jure Leskovec. Ogb-lsc: A large-scale challenge for machine learning on graphs. *arXiv preprint arXiv:2103.09430*, 2021b.

648 Qian Huang, Hongyu Ren, Peng Chen, Gregor Kržmanc, Daniel Zeng, Percy Liang, and Jure 649 Leskovec. Prodigy: Enabling in-context learning over graphs. arXiv preprint arXiv:2305.12600, 650 2023a. 651 Xuanwen Huang, Kaiqiao Han, Yang Yang, Dezheng Bao, Quanjin Tao, Ziwei Chai, and Qi Zhu. 652 Can gnn be good adapter for llms? arXiv preprint arXiv:2402.12984, 2024. 653 654 Yinan Huang, Xingang Peng, Jianzhu Ma, and Muhan Zhang. Boosting the cycle counting power of 655 graph neural networks with i\$^2\$-GNNs. In The Eleventh International Conference on Learning 656 Representations, 2023b. URL https://openreview.net/forum?id=kDSmxOspsXQ. 657 Albert Q. Jiang, Alexandre Sablayrolles, Arthur Mensch, Chris Bamford, Devendra Singh Chaplot, 658 Diego de las Casas, Florian Bressand, Gianna Lengyel, Guillaume Lample, Lucile Saulnier, 659 Lélio Renard Lavaud, Marie-Anne Lachaux, Pierre Stock, Teven Le Scao, Thibaut Lavril, Thomas 660 Wang, Timothée Lacroix, and William El Sayed. Mistral 7b, 2023. 661 Bowen Jin, Gang Liu, Chi Han, Meng Jiang, Heng Ji, and Jiawei Han. Large language models on 662 graphs: A comprehensive survey. arXiv preprint arXiv:2312.02783, 2023. 663 664 Nicolas Keriven and Gabriel Peyré. Universal invariant and equivariant graph neural networks. 665 Advances in Neural Information Processing Systems, 32, 2019. 666 Thomas N. Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. 667 In International Conference on Learning Representations, 2017. URL https://openreview. 668 net/forum?id=SJU4ayYgl. 669 670 Alexander Kirillov, Eric Mintun, Nikhila Ravi, Hanzi Mao, Chloe Rolland, Laura Gustafson, Tete 671 Xiao, Spencer Whitehead, Alexander C Berg, Wan-Yen Lo, et al. Segment anything. In Proceedings of the IEEE/CVF International Conference on Computer Vision, pp. 4015–4026, 2023. 672 673 Lecheng Kong, Yixin Chen, and Muhan Zhang. Geodesic graph neural network for efficient 674 graph representation learning. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and 675 Kyunghyun Cho (eds.), Advances in Neural Information Processing Systems, 2022. URL 676 https://openreview.net/forum?id=6pC50tP7eBx. 677 Lecheng Kong, Jiarui Feng, Hao Liu, Dacheng Tao, Yixin Chen, and Muhan Zhang. 678 Mag-gnn: Reinforcement learning boosted graph neural network. In A. Oh, T. Neu-679 mann, A. Globerson, K. Saenko, M. Hardt, and S. Levine (eds.), Advances in Neural 680 Information Processing Systems, volume 36, pp. 12000-12021. Curran Associates, Inc., 681 URL https://proceedings.neurips.cc/paper_files/paper/2023/ 2023. 682 file/2788b4cdf421e03650868cc4184bfed8-Paper-Conference.pdf. 683 Junnan Li, Dongxu Li, Silvio Savarese, and Steven Hoi. Blip-2: Bootstrapping language-image 684 pre-training with frozen image encoders and large language models. In International conference 685 on machine learning, pp. 19730–19742. PMLR, 2023. 686 687 Yuhan Li, Peisong Wang, Zhixun Li, Jeffrey Xu Yu, and Jia Li. Zerog: Investigating cross-dataset 688 zero-shot transferability in graphs. arXiv preprint arXiv:2402.11235, 2024. 689 Hao Liu, Jiarui Feng, Lecheng Kong, Ningyue Liang, Dacheng Tao, Yixin Chen, and Muhan 690 Zhang. One for all: Towards training one graph model for all classification tasks. In The Twelfth 691 International Conference on Learning Representations, 2023a. 692 693 Jiawei Liu, Cheng Yang, Zhiyuan Lu, Junze Chen, Yibo Li, Mengmei Zhang, Ting Bai, Yuan Fang, 694 Lichao Sun, Philip S Yu, et al. Towards graph foundation models: A survey and beyond. arXiv *preprint arXiv:2310.11829*, 2023b. 696 Yixin Liu, Ming Jin, Shirui Pan, Chuan Zhou, Yu Zheng, Feng Xia, and S Yu Philip. Graph self-697 supervised learning: A survey. *IEEE transactions on knowledge and data engineering*, 35(6): 5879-5900, 2022. 699 Zemin Liu, Xingtong Yu, Yuan Fang, and Xinming Zhang. Graphprompt: Unifying pre-training and 700 downstream tasks for graph neural networks. In Proceedings of the ACM Web Conference 2023, 701 2023c.

702 703 704	Haitao Mao, Zhikai Chen, Wenzhuo Tang, Jianan Zhao, Yao Ma, Tong Zhao, Neil Shah, Michael Galkin, and Jiliang Tang. Graph foundation models. <i>arXiv preprint arXiv:2402.02216</i> , 2024.
705 706	Stephen Merity, Caiming Xiong, James Bradbury, and Richard Socher. Pointer sentinel mixture models. In <i>International Conference on Learning Representations</i> , 2022.
707 708 709	Péter Mernyei and Cătălina Cangea. Wiki-cs: A wikipedia-based benchmark for graph neural networks. <i>arXiv preprint arXiv:2007.02901</i> , 2020.
710 711 712	Yujie Mo, Liang Peng, Jie Xu, Xiaoshuang Shi, and Xiaofeng Zhu. Simple unsupervised graph repre- sentation learning. In <i>Proceedings of the AAAI Conference on Artificial Intelligence</i> , volume 36, pp. 7797–7805, 2022.
713 714 715	Christopher Morris, Martin Ritzert, Matthias Fey, William L Hamilton, Jan Eric Lenssen, Gaurav Rattan, and Martin Grohe. Weisfeiler and leman go neural: Higher-order graph neural networks. In <i>Proceedings of the AAAI conference on artificial intelligence</i> , pp. 4602–4609, 2019.
716 717 718	Moritz Plenz and Anette Frank. Graph language models, 2024. URL https://arxiv.org/ abs/2401.07105.
719 720 721	Chen Qian, Huayi Tang, Zhirui Yang, Hong Liang, and Yong Liu. Can large language models empower molecular property prediction?, 2023.
722 723 724	Samyam Rajbhandari, Jeff Rasley, Olatunji Ruwase, and Yuxiong He. Zero: Memory optimizations toward training trillion parameter models. In <i>SC20: International Conference for High Performance Computing, Networking, Storage and Analysis</i> , pp. 1–16. IEEE, 2020.
725 726 727	Yu Rong, Yatao Bian, Tingyang Xu, Weiyang Xie, Ying Wei, Wenbing Huang, and Junzhou Huang. Self-supervised graph transformer on large-scale molecular data. <i>Advances in Neural Information</i> <i>Processing Systems</i> , 33, 2020.
728 729 730	Yunsheng Shi, Zhengjie Huang, Shikun Feng, Hui Zhong, Wenjin Wang, and Yu Sun. Masked label prediction: Unified message passing model for semi-supervised classification, 2021.
731 732 733 734 735	Xiangguo Sun, Hong Cheng, Jia Li, Bo Liu, and Jihong Guan. All in one: Multi-task prompting for graph neural networks. In <i>Proceedings of the 29th ACM SIGKDD Conference on Knowledge</i> <i>Discovery and Data Mining</i> , KDD '23, pp. 2120–2131, New York, NY, USA, 2023. Association for Computing Machinery. ISBN 9798400701030. doi: 10.1145/3580305.3599256. URL https://doi.org/10.1145/3580305.3599256.
736 737 738	Jiabin Tang, Yuhao Yang, Wei Wei, Lei Shi, Lixin Su, Suqi Cheng, Dawei Yin, and Chao Huang. Graphgpt: Graph instruction tuning for large language models, 2023.
739 740	Jiabin Tang, Yuhao Yang, Wei Wei, Lei Shi, Long Xia, Dawei Yin, and Chao Huang. Higpt: Heterogeneous graph language model. <i>arXiv preprint arXiv:2402.16024</i> , 2024.
741 742 743 744	Shantanu Thakoor, Corentin Tallec, Mohammad Gheshlaghi Azar, Rémi Munos, Petar Veličković, and Michal Valko. Bootstrapped representation learning on graphs. In <i>ICLR 2021 Workshop on Geometrical and Topological Representation Learning</i> , 2021.
745 746 747 748 749 750 751 752 753 754 755	Hugo Touvron, Louis Martin, Kevin Stone, Peter Albert, Amjad Almahairi, Yasmine Babaei, Nikolay Bashlykov, Soumya Batra, Prajjwal Bhargava, Shruti Bhosale, Dan Bikel, Lukas Blecher, Cris- tian Canton Ferrer, Moya Chen, Guillem Cucurull, David Esiobu, Jude Fernandes, Jeremy Fu, Wenyin Fu, Brian Fuller, Cynthia Gao, Vedanuj Goswami, Naman Goyal, Anthony Hartshorn, Saghar Hosseini, Rui Hou, Hakan Inan, Marcin Kardas, Viktor Kerkez, Madian Khabsa, Isabel Kloumann, Artem Korenev, Punit Singh Koura, Marie-Anne Lachaux, Thibaut Lavril, Jenya Lee, Diana Liskovich, Yinghai Lu, Yuning Mao, Xavier Martinet, Todor Mihaylov, Pushkar Mishra, Igor Molybog, Yixin Nie, Andrew Poulton, Jeremy Reizenstein, Rashi Rungta, Kalyan Saladi, Alan Schelten, Ruan Silva, Eric Michael Smith, Ranjan Subramanian, Xiaoqing Ellen Tan, Binh Tang, Ross Taylor, Adina Williams, Jian Xiang Kuan, Puxin Xu, Zheng Yan, Iliyan Zarov, Yuchen Zhang, Angela Fan, Melanie Kambadur, Sharan Narang, Aurelien Rodriguez, Robert Stojnic, Sergey Edunov, and Thomas Scialom. Llama 2: Open foundation and fine-tuned chat models, 2023.

756 757 758	Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. <i>Advances in neural information processing systems</i> , 30, 2017.
760 761	Petar Veličković, William Fedus, William L Hamilton, Pietro Liò, Yoshua Bengio, and R Devon Hjelm. Deep graph infomax. <i>arXiv preprint arXiv:1809.10341</i> , 2018.
762 763 764 765	Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. Graph attention networks. In <i>International Conference on Learning Representations</i> , 2018. URL https://openreview.net/forum?id=rJXMpikCZ.
766 767	Heng Wang, Shangbin Feng, Tianxing He, Zhaoxuan Tan, Xiaochuang Han, and Yulia Tsvetkov. Can language models solve graph problems in natural language?, 2023.
768 769 770 771	Song Wang, Kaize Ding, Chuxu Zhang, Chen Chen, and Jundong Li. Task-adaptive few-shot node classification. In <i>Proceedings of the 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining</i> , pp. 1910–1919, 2022.
772 773 774	Xixi Wu, Yifei Shen, Caihua Shan, Kaitao Song, Siwei Wang, Bohang Zhang, Jiarui Feng, Hong Cheng, Wei Chen, Yun Xiong, et al. Can graph learning improve task planning? <i>arXiv preprint arXiv:2405.19119</i> , 2024.
775 776 777	Lianghao Xia, Ben Kao, and Chao Huang. Opengraph: Towards open graph foundation models. <i>arXiv preprint arXiv:2403.01121</i> , 2024.
778 779 780	Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In <i>International Conference on Learning Representations</i> , 2018.
781 782 783 784 785	Junhan Yang, Zheng Liu, Shitao Xiao, Chaozhuo Li, Defu Lian, Sanjay Agrawal, Amit S, Guangzhong Sun, and Xing Xie. Graphformers: GNN-nested transformers for representation learning on textual graph. In A. Beygelzimer, Y. Dauphin, P. Liang, and J. Wortman Vaughan (eds.), <i>Advances in Neural Information Processing Systems</i> , 2021. URL https://openreview.net/forum?id=yILzFBjR0Y.
786 787	Ruosong Ye, Caiqi Zhang, Runhui Wang, Shuyuan Xu, and Yongfeng Zhang. Natural language is all a graph needs, 2023.
788 789 790 791 792	Chengxuan Ying, Tianle Cai, Shengjie Luo, Shuxin Zheng, Guolin Ke, Di He, Yanming Shen, and Tie-Yan Liu. Do transformers really perform badly for graph representation? In A. Beygelzimer, Y. Dauphin, P. Liang, and J. Wortman Vaughan (eds.), <i>Advances in Neural Information Processing</i> <i>Systems</i> , 2021. URL https://openreview.net/forum?id=OeWooOxFwDa.
793 794	Xingtong Yu, Zhenghao Liu, Yuan Fang, Zemin Liu, Sihong Chen, and Xinming Zhang. Generalized graph prompt: Toward a unification of pre-training and downstream tasks on graphs, 2023.
795 796 797	Bohang Zhang, Guhao Feng, Yiheng Du, Di He, and Liwei Wang. A complete expressiveness hierarchy for subgraph gnns via subgraph weisfeiler-lehman tests, 2023a.
798 799 800 801	Bohang Zhang, Shengjie Luo, Liwei Wang, and Di He. Rethinking the expressive power of GNNs via graph biconnectivity. In <i>The Eleventh International Conference on Learning Representations</i> , 2023b. URL https://openreview.net/forum?id=r9hNv76KoT3.
802 803 804	Hang Zhang, Xin Li, and Lidong Bing. Video-Ilama: An instruction-tuned audio-visual language model for video understanding. arXiv preprint arXiv:2306.02858, 2023c. URL https:// arxiv.org/abs/2306.02858.
805 806 807 808	Mengmei Zhang, Mingwei Sun, Peng Wang, Shen Fan, Yanhu Mo, Xiaoxiao Xu, Hong Liu, Cheng Yang, and Chuan Shi. Graphtranslator: Aligning graph model to large language model for open-ended tasks. <i>arXiv preprint arXiv:2402.07197</i> , 2024.
809	Muhan Zhang and Pan Li. Nested graph neural networks. <i>Advances in Neural Information Processing</i> Systems, 34:15734–15747, 2021.

810 811 812 813	Muhan Zhang, Pan Li, Yinglong Xia, Kai Wang, and Long Jin. Labeling trick: A theory of using graph neural networks for multi-node representation learning. In A. Beygelzimer, Y. Dauphin, P. Liang, and J. Wortman Vaughan (eds.), <i>Advances in Neural Information Processing Systems</i> , 2021. URL https://openreview.net/forum?id=Hcr9mgBG6ds.
815 816 817	Ziwei Zhang, Haoyang Li, Zeyang Zhang, Yijian Qin, Xin Wang, and Wenwu Zhu. Graph meets llms: Towards large graph models. In <i>NeurIPS 2023 Workshop: New Frontiers in Graph Learning</i> , 2023d.
818 819 820	Haiteng Zhao, Shengchao Liu, Chang Ma, Hannan Xu, Jie Fu, Zhi-Hong Deng, Lingpeng Kong, and Qi Liu. Gimlet: A unified graph-text model for instruction-based molecule zero-shot learning, 2023a.
821 822 823	Jianan Zhao, Le Zhuo, Yikang Shen, Meng Qu, Kai Liu, Michael Bronstein, Zhaocheng Zhu, and Jian Tang. Graphtext: Graph reasoning in text space, 2023b.
824 825 826	
827 828 829	
830 831 832	
833 834 835	
836 837 838	
839 840 841	
842 843 844	
845 846 847	
848 849 850	
851 852 853	
854 855 856	
858 859	
860 861 862 863	

APPENDIX

865 866 867

868

877 878

879

883

IMPLEMENTATION DETAILS А

IN-CONTEXT AUTOENCODER (ICAE) A.1

870 This section briefly introduces ICAE and how it helps build the GOFA model; please refer to ICAE 871 paper (Ge et al., 2023) for the specifics of the model. ICAE contains two decoder-only LLMs. One 872 serves as a language compressor that compresses sentences into a fixed-length sequence of vectors, 873 and the other serves as a language decoder that decodes or queries into the compressed sentence representations. Specifically, during training, an input token sequence $x = \{x_1, ..., x_l\}$ is appended 874 by a K memory tokens $\{m_1, ..., m_k\}$ with trainable embeddings. The concatenated sequence is fed 875 to the LLM compressor with a LoRA adapter (Hu et al., 2022). 876

$$\{h(x_1), ..., h(x_l), h(m_1), ..., h(m_K)\} = LLM_{comp}(\{e(x_1), ..., e(x_l), e(m_1), ..., e(m_K)\}), \quad (4)$$

where $e(\cdot)$ and $h(\cdot)$ are the token embeddings and LLM outputs. Then, the decoder LLM only attends to the memory token outputs and tries to decode the original sentence from the memory tokens. 880

$$\{l(m_1), ..., l(m_K), l(x_1), ..., l(x_l)\} = LLM_{dec}(\{h(m_1), ..., h(m_K), e(x_1), ..., e(x_l)\}),$$

$$\min_{\Theta_{comp}} CrossEntropy(\{l(m_K), l(x_1), ..., l(x_{l-1})\}, \{x_1, ..., x_l\}).$$
(5)

884 The ICAE model is also trained on QA and Language modeling tasks to have more diverse embed-885 dings.

By training this auto-encoder objective on a large-scale, the compressor model learns to compress 887 all information about a sentence to the memory token outputs like in a conventional auto-encoder model. In Table 5, we provide a few examples of the comparison between the original text and the 889 text decoded from the compressed memory tokens by ICAE's decoder. Because the compressed 890 representation contains as much information as possible, GNN can pass messages between nodes 891 with minimal information loss.

892 Table 5: Comparison between original texts and decoded text from the compressed representation. 893

894 Original Text Decoded Text 895 896 Actress Halle Berry has been sharing a number Halle Berry has been sharing a number of stunof stunning photos from the time she has spent ning photos from the time she has spent in Mo-897 in Morocco and she just posted a new one to her rocco and just posted a new one on her Instagram 898 Instagram page that fans will not want to miss. page that fans won't want to miss. 899 900 Utah avoided the turnover bug on Saturday for the Utah avoided the turnover bug on Saturday for the 901 first time since its season opener. In addition, the first time since its season opener. In addition, the running game was clicking and the defense was running game was clicking and the defense was 902 dominant as the Utes snapped a two-game windominant as the Utes snapped a two-game win-903 ning streak on the road, beating Pittsburgh 26-14. ning streak on the road, beating Pittsburgh 26-14. 904 Five keys to Utah's victory: 1. Utah running back Five keys to Utah's victory: 1. 2. 3. 4. 5. Utah 905 John White IV: Running strong and with purpose running back John John White IV IV ran strong 906 from the beginning, White was a big reason why and with purpose from the beginning, being a big 907 the Utes were within striking distance at halftime. reason why the Utes were within striking distance 908 at halftime. He took a couple of shots that dis-White, who took a couple pops that dislodged his 909 helmet and caused a cut below his ear, seemed to lodged his helmet and caused a cut below his ear, 910 get stronger as the game wore on. He finished the but seemed to get stronger as the game went on. 911 afternoon with 171 yards on 36 carries. He finished the afternoon with 171 yards on 36 912 carries.

913 914

916

915 A.2 LLM CHOICES OF GOFA

Because ICAE preserves as much information in a sentence as possible, we can use it in the GOFA 917 model to comprehensively pass information between sentences, as shown in Section 3.2. However,

the GOFA model is not limited to ICAE. Users can first train an ICAE-like objective on any existing
LLM and apply the GOFA model to the trained LLM. Or, users can apply the GOFA directly to
a pre-trained LLM and train the GOFA without the auto-encoder training. Note that the ICAE
architecture has a function similar to an encoder-decoder LLM. We do not use an off-the-shelve
encoder-decoder LLM because its encoder output is still subject to the sentence length, which does
not fit GNN's need for fixed-sized input.

$$\{Q_x^{t+1}, Q_{m,x}^{t+1}, Q_y^{t+1}\} = LLM^t(\{Q_x^t, H_x^t, Q_y^t\}),\tag{6}$$

where the GNN is still applied on K memory tokens inserted between the node text x and target text y. This allows the target text to attend to the node text, which may improve the performance of GOFA. However, this formulation forces every node to have a target text, which is usually not what users desire and poses extra computation costs. We will explore this architecture in our future work.

A.3 TRANSFORMER CONVOLUTIONAL GNN

As mentioned in Section 3.2, we customize a Transformer Convolutional GNN(TransConv) (Shi et al., 2021) as the GNN used in Equation 3. Since GNN layers operate on token representations and tokens at different indices do not communicate, we describe the GNN at one index for simplicity. The *t*-th GNN layer on node *i* and its neighbors $\mathcal{N}(i)$ is:

$$h^{t+1}(i) = \boldsymbol{W}_{o}(\sum_{j \in \mathcal{N}(i)} \alpha_{i,j}(\boldsymbol{W}_{v,node}h^{t}(j) + \boldsymbol{W}_{v,edge}h(e_{i,j}))),$$

$$\alpha_{i,j} = \text{Softmax}(\frac{\boldsymbol{W}_{q}h^{t}(i) * (\boldsymbol{W}_{k,node}h^{t}(j) + \boldsymbol{W}_{k,edge}h(e_{i,j}))}{\sqrt{d}}),$$
(7)

 $h(\cdot)$ represents input node and edge features. W represents query (q), key (k), value (v), output (o) linear projection for nodes and edges. The formulation closely follows the transformer design (Vaswani et al., 2017) and its GNN adaptation (Shi et al., 2021). This formulation does not aggregate the last layer embedding $h^t(i)$ into the next layer, because we already add residual to maintain the same effect. We use pre-layer normalization following Llama (Touvron et al., 2023).

950

951

943

944

945

927

928

929

930

931 932

933

B ADDITIONAL EXPERIMENTS

B.1 SUPERVISED EXPERIMENT RESULTS

952 In this section, we conduct supervised learning experiment with the pre-trained GOFA. In the 953 supervised experiment, GOFA's prompt does not include class optional. We show the supervised 954 results in Table 6. Specifically, we compare the result of GOFA with the following baselines: 1. 955 basic GNNs, which are trained individually on each dataset, including GCN (Kipf & Welling, 2017) 956 and GAT (Veličković et al., 2018). 2. The contrastive learning methods, including DGI (Veličković et al., 2018) and BGRL (Thakoor et al., 2021). For these methods, we directly report the best 957 result from (He & Hooi, 2024). 3. Graph foundation model, including OFA (Liu et al., 2023a) 958 and UniGraph (He & Hooi, 2024). GOFA achieved competitive performance on most datasets. In 959 particular, GOFA achieved SOTA performance on the Pubmed dataset, demonstrating that GOFA can 960 transfer pre-trained knowledge to downstream tasks. We also notice that GOFA is not performing 961 as well on some datasets, possibly because in a supervised setting, we only train a small portion of 962 the data for one epoch (specific numbers in the experimental details section in Appendix F.5), and 963 in the supervised setting, it is important to see training samples multiple times to ensure detailed 964 understanding of the distribution. As we pre-train the model with more diverse datasets, GOFA can 965 potentially obtain world knowledge as an LLM, which makes transfer learning in the supervised 966 setting more accurate.

968 B.2 EXAMPLE OF GOFA'S FREE-FORM ANSWER

969

967

Figure 6 in the main body illustrates GOFA's capability to respond to various questions based on the
 same graph from ogbn-arXiv. In this section, we provide additional examples in Figure 7 to further
 show the ability of GOFA's free-form text answer.

Task type Metric	Cora Link Acc ↑	Cora Node Acc ↑	PubMed Link Acc ↑	PubMed Node Acc ↑	Arxiv Node Acc ↑	WikiCS Node Acc ↑	WN Link Acc ↑	FB Link Acc ↑	Products Node Acc ↑
GCN GAT	$\begin{array}{c} 78.9{\pm}0.6 \\ 80.1{\pm}0.3 \end{array}$	$\substack{\textbf{82.3} \pm 1.1 \\ 80.4 \pm 0.4}$	$77.5{\pm}0.4 \\ 80.5{\pm}0.2$	$\begin{array}{c} 77.8{\scriptstyle\pm0.7}\\ 76.6{\scriptstyle\pm0.5}\end{array}$	$\begin{array}{c} 73.9{\pm}0.6\\ \textbf{75.8}{\pm}0.3\end{array}$	$\begin{array}{c} 77.0{\pm}0.6\\ 79.8{\pm}0.5\end{array}$	$\substack{82.7 \pm 0.4 \\ 88.8 \pm 0.3}$	$90.1{\scriptstyle \pm 0.3} \\ 93.6{\scriptstyle \pm 0.1}$	80.0±0.7 81.4±0.2
DGI BGRL		${\begin{array}{c}{51.99 \pm 0.45}\\{56.73 \pm 0.23}\end{array}}$	-	$55.76{\scriptstyle\pm 0.56}\\63.77{\scriptstyle\pm 0.23}$	$55.21{\scriptstyle\pm 0.21}\atop_{\scriptstyle62.21{\scriptstyle\pm 0.21}}$	$\begin{array}{c} 67.11{\scriptstyle \pm 0.12} \\ 70.12{\scriptstyle \pm 0.15} \end{array}$	$52.04{\scriptstyle\pm0.22}\atop{\scriptstyle56.44{\scriptstyle\pm0.21}}$	$\begin{array}{c} 26.99 {\pm} 0.22 \\ 64.91 {\pm} 0.22 \end{array}$	64.21±0.2
OFA UniGraph	<u>87.97</u> -	$75.34 \\ \underline{81.43} \pm 0.55$	95.89 -	$\frac{77.89}{74.33\pm0.23}$	73.44 72.91±0.42	77.62 79.98 ±1.21	98.31 85.45±0.34	95.78 <u>94.81</u> ±1.32	- <u>80.11</u> ±0.2
GOFA	89.54	76.50	<u>93.97</u>	83.83	74.77	79.96	<u>92.16</u>	88.21	79.98

Table 6: Experiment results in supervised learning. **Bold** and <u>underlined</u> shows best and runner-up results.



Figure 7: Demonstration of GOFA's ability to respond to any question to the given graph. Above is an example of the products dataset, where the model need to output the majority category of its connected nodes. Below is another example on wikics dataset, GOFA is asked to generate Wikipedia page named based on the graph information.

C DATASETS

Cora. The Cora dataset is a co-citation network, where nodes are papers related to artificial intelli-gence. Edges mean the connected two papers are co-cited by other papers. The Cora dataset contains 2708 nodes and 10556 edges. We collect the Cora dataset and its raw text from OFA (Liu et al., 2023a). We evaluate the performance of the baseline and our proposed model on Cora for both node-level and link-level tasks. For the node-level task, the aim is to classify the node into the correct paper category from 7 different categories. The split is obtained from OFA. It contains 140/500/2068 samples for train/val/test set respectively. For the link-level task, the object is to predict whether two paper nodes are co-cited or not. We follow the setting of OFA (Liu et al., 2023a) and randomly split all edges into train/val/test sets with a ratio of 0.85/0.05/0.1.

PubMed. The PubMed dataset is a co-citation network, where nodes are papers related to diabetes mellitus. Edges mean the connected two papers are co-cited by other papers. The PubMed dataset contains 19717 nodes and 88648 edges. We collect the PubMed dataset and its raw text from OFA (Liu et al., 2023a). We evaluate the performance of the baseline and our proposed model on PubMed for both node-level and link-level tasks. For the node-level task, papers have 3 different categories. The goal is to classify the node into the correct paper category. We obtain the split directly from original source. It contains 60/500/19157 samples for train/val/test set respectively. For the link-level task, the object is to predict whether two paper nodes are co-cited or not. We follow the setting of OFA (Liu et al., 2023a) and randomly split all edges into train/val/test sets with a ratio of 0.85/0.05/0.1.

Arxiv. The Arxiv dataset is a citation network, where nodes are papers related to computer science and edges mean two papers have a citation relationship. The Arxiv dataset contains 169343 nodes and 1166243 edges. We collect the Arxiv dataset and its raw text from OGB (Hu et al., 2021b). We evaluate the node classification on the Arxiv dataset. The goal is to classify the paper node into the correct category from 40 possible categories. We obtain the split directly from OGB (Hu et al., 2021b). It contains 90941/29799/48603 samples for train/val/test set, respectively.

WikiCS. The WikiCS dataset is a graph obtained from Wikipedia. The nodes in WikiCS are Wikipedia terms and their descriptions. The edges mean there is a hyperlink between two terms. We collect the WikiCS dataset and its raw text from (Mernyei & Cangea, 2020). There are 11701 nodes and 216123 edges in the graph. We evaluate the performance of WikiCS on the node classification task. There are 10 different classes. We follow the same split as OFA (Liu et al., 2023a), which contains 580/1769/5847 samples for the train/val/test set, respectively.

1038 **Products**. The Products dataset is a co-purchase graph. The nodes in the graph represent product 1039 items from the Amazon platform, and the edges represent that two products are co-purchased together. 1040 We obtain the Products and their raw texts from TAPE (He et al., 2024a), which is a subset from the 1041 original ogbn-Products (Hu et al., 2021b) dataset. It contains 54025 nodes and 144638 edges. We 1042 evaluate the node classification performance on Products. The data from the original source contains 1043 47 different categories. However, we found that there are two classes with missing labels. To be consistent with previous literature, we adopt the approach in LLaGA to replace the label name with 1044 special symbols. There are 14708/1572/37745 samples for the train/val/test set, respectively. 1045

FB15K237. The FB15K237 is a knowledge graph generated from Free Base. Nodes in the dataset represent entities in the world and edges represent the relation between entities. We obtained the dataset from OFA (Liu et al., 2023a). The FB15K237 is used to evaluate the link classification. The dataset contains 237 unique classes. We follow the setting of OFA (Liu et al., 2023a) and split the dataset with a ratio of 0.85/0.05/0.1, which results in a total of 272115/17535/20466 samples for train/val/test set, respectively.

ExplaGraphs. The ExplaGraphs is a graph question answering dataset on commonsense concepts.
Nodes in the dataset represent a common sense concept and edges represent the relation between two concepts. We obtain the dataset from G-retriever (He et al., 2024b) The ExplaGraphs can be used for question-answering on graphs. We obtain the split directly from G-retriever (He et al., 2024b). It contains 1659/553/554 graph samples from the train/val/test set.

SceneGraphs. The SceneGraphs is a graph question answering dataset on scene graphs. Nodes in the dataset represent an object in an image and edges represent the relation between two objects. We obtain the dataset from G-retriever (He et al., 2024b) The SceneGraphs can be used for question-answering on graphs. We obtain the split directly from G-retriever (He et al., 2024b). It contains 59978/19997/20025 graph samples from the train/val/test set.

1062 MAG240M. The MAG240M dataset is a citation network generated from Microsoft Academic 1063 Graphs. The nodes represent academic papers and the links represent a citation relation between 1064 two papers. We obtained the dataset and raw text from OGB-lsc (Hu et al., 2021a). However, the original dataset is extremely large and contains nodes without text features (author and institution 1066 nodes), since we mainly use the dataset for pre-training, we further downsample the original dataset. Specifically, we only keep paper nodes and citation links between papers. Further, we downsample 1067 the edges in the following ways. First, we selected all nodes in the train/val/test split provided by 1068 OGB-lsc (Hu et al., 2021a). Next, we filter the edges through two rounds. In the first round, we 1069 only keep the edge if either the source or the target is in the selected nodes. If any node in the added 1070 edge is not in the selected nodes, we add it to the node set. Next, in the second round, we include 1071 additional edges where both the source and target are in the selected nodes (additional nodes are 1072 added in the first round). The procedure results in a total of 5875010 nodes and 26434726 edges. 1073

1074 Ultrachat200k. The Ultrachat200k is a question-answering dataset. each sample is a multi-round 1075 conversation obtained from the web. We obtained the Ultrachat200k from (Ding et al., 2023). 1076 However, the original dataset is not a network. To convert it to a graph dataset, we manually create 1077 a graph structure for it. Specifically, if the original sample has k round of conversation, we will 1078 generate k - 1 graph sample. The *i*-th graph will contain the first *i* round of conversation. Each node 1079 in the graph is either a question or an answer. The question and answer are linked by a directed edge 1079 indicating the order of the conversation. The conversation of i + 1 round will be the question-answer 1080 pair for this graph. Since we mainly use the dataset for pre-training. We only include *train-sft* subset. After the conversion, there are a total of 449929 graphs in total. 1082

Wikikg90m. Wikikg90m is an encyclopedic knowledge graph dataset extracted from Wikidata 1083 knowledge base. We obtain the original Wikikg90m from OGB-LSC (Hu et al., 2021a). It contains 1084 91,230,610 entities, 1,387 relations, and 601,062,811 edges.

WikiGraph. The WikiGraph dataset is designed to increase the diversity of the training texts. Hence, 1086 we use WikiText (Merity et al., 2022) dataset as the seed dataset. It contains plain sentences from 1087 Wikipedia pages. We generate graphs for sentences with more than 500 characters. Specifically, we 1088 first prompt an LLM to extract meaningful entities or concepts from a sentence, and these entities 1089 become the nodes in the graph. We then randomly pair concepts to generate edges. Again, we use 1090 LLM to generate a description of the relationship between the paired concepts and use the description 1091 as the edge text. 1092

1093

RELATED WORK EXTENDED D 1094

1095

Prompt Learning in Graph: The success of foundation models inspired many works to adapt their 1096 power to the graph domain. Earlier attempts designed a graph prompting mechanism such that a trained model can adapt to new data by fine-tuning a soft prompting vector (Liu et al., 2023c; Yu 1098 et al., 2023; Sun et al., 2023; Xia et al., 2024). GraphPrompt (Liu et al., 2023c; Yu et al., 2023) 1099 pretrains on link prediction tasks, and then finetune a prompt matrix for each downstream node or 1100 graph classification task. All in One (Sun et al., 2023) designs prompt tokens that are used to modify 1101 node features and then take a meta-learning paradigm for multi-task learning. Subsequent works 1102 extend graph prompts to allow in-context learning without weight update (Huang et al., 2023a; Galkin 1103 et al., 2023). However, these works only tackle limited types of tasks and do not generalize to new 1104 domains. Hence, researchers propose integrating LLM into the graph learning.

1105 GNNs and Transformers: In recent years, GNNs have become the most popular method for dealing 1106 with graph learning problems due to their extraordinary ability in structural learning. Particularly, 1107 Previous works (Xu et al., 2018; Morris et al., 2019) show that the expressive power of message-1108 passing GNNs can be as powerful as the 1-dimensional Weisfeiler-Lehman test, a powerful algorithm 1109 for graph isomorphism problems. Many recent works also try to design more powerful GNNs that 1110 beyond the 1-WL test (Zhang & Li, 2021; Kong et al., 2022; Feng et al., 2022; Huang et al., 2023b; Zhang et al., 2023b;a; Feng et al., 2023; Kong et al., 2023) for better structural ability like learning 1111 distance between nodes or counting cycles in graph. Some works try to combine the GNN with 1112 the transformer. particularly, GraphFormers (Yang et al., 2021) and GROVER (Rong et al., 2020) 1113 also insert a GNN layer between consecutive transformer layers for modeling graph inductive bias. 1114 Different from us, their transformer layers are randomly initialized and directly tuned on downstream 1115 tasks without text. 1116

1117

E ADDITIONAL DISCUSSIONS 1118

1119 **GRAPH STRUCTURE QUESTION EXAMPLE OF LLM** 1120 E.1

1121 We assessed the ability of LLMs to respond to questions related to graph structures, including shortest 1122 path distances and common neighbor counting. For this evaluation, graph edges were described using 1123 plain text, and the LLM was tasked with generating the answers. The results of this evaluation are 1124 presented in Table 1. These findings indicate that LLMs struggle to comprehend graph structures 1125 effectively. We include examples of the questions posed and the corresponding answers generated by 1126 the LLM in Table 7, to illustrate these challenges.

- 1127
- 1128 E.2 THEORETICAL ADVANTAGES OF GOFA'S GRAPH LANGUAGE ENCODER 1129

In GOFA, we innovatively integrate GNN layers into LLMs to help LLMs understand graph structures. 1130 This approach is theoretically more powerful and suitable for designing GFMs than using pure 1131 LLMs. Graph data have unique properties, such as node permutation invariance without fixed 1132 ordering (Keriven & Peyré, 2019), making sequential models like LLMs unsuitable for modeling 1133 graphs. For a graph with n nodes, the number of possible orders is n!, which means sequential

Question	Answer	Correct Answer
In the graph node 8 connects to 1, node 13 connects to 9, node 8 connects to 7, node 3 connects to 13, node 3 connects to 4, node 6 connects to 6, node 11 connects to 8, node 12 connects to 11, node 2 connects to 12, node 14 con- nects to 7, node 6 connects to 3, node 6 connects to 9, node 2 con- nects to 8, node 2 connects to 9, node 5 connects to 8, node 3 con- nects to 11, node 8 connects to 5, node 10 connects to 11, node 2 connects to 9, node 9 connects to 10, what is a shortest path be- tween node 8 and node 9?	To find the shortest path between node 8 and node 9, we can use Dijkstra's algorithm or any other shortest path algorithm. However, since this graph is small, we can find it manually. Here's one of the shortest paths between node 8 and node 9: Start at node 8. Move from node 8 to node 5 (neigh- bor). Move from node 5 to node 8 (neighbor). Move from node 8 to node 2 (neighbor). Move from node 2 to node 9 (neighbor). So, the shortest path between node 8 and node 9 is: $8 -> 5 -> 2 -> 9$.	8 -> 2 -> 9
In the graph node 8 connects to 1, node 13 connects to 9, node 8 connects to 7, node 3 connects to 13, node 3 connects to 4, node 6 connects to 6, node 11 connects to 8, node 12 connects to 11, node 2 connects to 12, node 14 con- nects to 7, node 6 connects to 3, node 6 connects to 9, node 2 con- nects to 8, node 2 connects to 9, node 5 connects to 8, node 3 con- nects to 11, node 8 connects to 5, node 10 connects to 11, node 2 connects to 9, node 9 connects to 10, what are common neighbors	To find the common neighbors be- tween nodes 13 and 5, we need to identify all nodes that are neigh- bors of both nodes 13 and 5. From the provided connections: Node 13 is connected to node 9 and node 3. Node 5 is connected to node 8. Therefore, the com- mon neighbor between node 13 and node 5 is node 8 .	No common neighbor

1134 Table 7: Comparison of LLM-generated answers with correct answers for graph structure questions. 1135

le in k n task graphs with a specific node ordering but cannot maintain this accuracy after nodes are reordered. 1173 1174 Methods like LLaGA (Chen et al., 2024) also fall into this category and are suboptimal if the task requires deep structure understanding. Instead, GNNs are a powerful choice widely accepted by the 1175 literature for encoding both features and the structure of graphs. They are permutation equivariant 1176 to graph order and can learn invariant structure information. Our GOFA, interleaving GNN layers 1177 into LLMs, naturally preserves this property. Specifically, for LLM layers, each node is processed 1178 individually, which is obvious that we can keep the permutation invariance. As GNN layers are 1179 permutation invariant, this conclude that the GOFA is permutation invariant to input graph. 1180

- 1181
- 1182

E.3 ADVANTAGES OF GOFA'S SELF-SUPERVISED LEARNING TASKS

1183 Our proposed self-supervised learning tasks are enlightened by existing graph and NLP SSL tasks. 1184 However, our tasks are novel compared to existing methods from several perspectives. 1185

In graph SSL, most prior work aims to recover original features or graph structure contrastively or 1186 generatively (Liu et al., 2022), using learned embeddings for downstream classifiers. In contrast, 1187 our tasks aim to learn embeddings that enable downstream natural language generation. Concretely,

1188 our SSL shortest path prediction task requires the model to output multiple actual paths (e.g., node 1189 $a \rightarrow$ node b \rightarrow node c) between two nodes in text format; this requires a more fine-grained and in-depth 1190 model understanding of the graph structure. Regular graph SSL tasks such as link prediction and 1191 shortest path distance prediction only cares about a simple objective (binary classification for link 1192 and single number for distance). Conversely, our generation-oriented design allows a unified task format to query into the graph from different aspects with different granularity (e.g. shortest path 1193 and common neighbor can be incorporated under the same natural language generation framework), 1194 whereas traditional SSL tasks inevitability lose much detailed information and may need artificial 1195 complicated design to accommodate multiple SSL targets. 1196

SSL in NLP (e.g. next-word-prediction) only takes texts as input. One may think of directly converting graphs to text and doing a similar SSL. However, as many previous works show (Wang et al., 2023), converting graphs directly to texts for LLM generation is ineffective. Hence, we design the sentence completion task directly on the graph to use connection information to help the model attend to correct nodes for subsequent generation.

In summary, our SSL design cares more about training the model to generate any answers in natural language format so that it can accommodate arbitrary tasks, which differs from traditional graph SSL that normally focuses on classification/regression (actually any graph SSL tasks can be incorporated into our natural language generation framework). Compared to NLP SSL, our novel SSL design focuses on sentence completion using neighboring sentence information rather than pure auto-regression, strengthening the model's power to leverage joint graph-text information.

1208

¹²⁰⁹ F EXPERIMENTAL SETTINGS

1210

1211 F.1 GENERAL SETTINGS 1212

Subgraph sampling: In the GOFA, for node/link/graph-level tasks, the input format is unified as a subgraph task. Namely, for node/link-level tasks, we will select a k-hop subgraph surrounding the target nodes as the input graph for the model. We follow a similar subgraph sampling strategy as OFA (Liu et al., 2023a). Specifically, for node-level tasks, we directly sample the k-hop subgraph rooted at the target node. Meanwhile, we set a threshold for maximum nodes per hop. If the nodes in a certain hop exceed the threshold, we will randomly sample maximum nodes from all nodes. For link-level tasks, we doing the sampling on both two nodes.

Implementations. Both the GOFA and all baselines are implemented using Python with Pytorch,transformers, and PyG (Fey & Lenssen, 2019) packages.

1222

1224

1223 F.2 DESIGN OF PRE-TRAINING TASKS

In this section, we describe the self-supervised pre-training of GOFA. The goal of the pre-training 1225 is to let the GOFA model obtain the ability to query graph structure and context but retain the 1226 ability to reason about plain text. Specifically, we perform the pre-training task using multiple 1227 existing graph datasets, including MAG240M (Hu et al., 2021a), Arxiv (Hu et al., 2021b), Pubmed, 1228 Wikikg90mv2 (Hu et al., 2021a), and Ultrachat200k (Ding et al., 2023) datasets. Further, we create 1229 another graph dataset called WikiGraph, whose graphs are generated from sentences in the pure 1230 textual WikiData dataset (Merity et al., 2022) using LLM. Details about the datasets can be found 1231 in Appendix C. We randomly generate a unique node ID (such as [Node A]) for each node in the 1232 training sample and append it to the original node text. This ID will serve as a basis for querying 1233 nodes in the graph. We design four pre-training tasks: sentence completion, structural understanding, question-answering, and information retrieval tasks. Figure 1 shows an example of each task. We 1234 describe the rationale of each task below and leave some implementation details to Appendix F. We 1235 also include an additional discussion of the advantages of our designed tasks in Appendix E.3. 1236

1237 Sentence completion task. The objective of the sentence completion task is to train GOFA to reason 1238 about the rest of the text in a node given both the existing text and the information in the rest of the 1239 graph. Given an input training sample, we randomly select n nodes in the graph as the target nodes. 1240 All selected nodes' texts are split into halves. The first half forms node text x(v), and the second 1241 half becomes the target y to generate. The length of the first half will also be randomly determined. 1242 Finally, the output representation of these n nodes will be directly input to the decoder (no prompt 1242 node will be connected) and we minimize the loss between model decoded text and target y. This sentence-completion pre-training task adapts LLMs' standard ability to the graph context.

Structural understanding tasks. The objective of the structural tasks is to pre-train GOFA to 1245 understand basic graph structural properties. In light of this, we design the shortest paths and common 1246 neighbors reasoning tasks between nodes. Specifically, For each training subgraph sample, we 1247 randomly sample n node pairs as the selected targets. For each selected node pair, we ask the model 1248 to compute the shortest path distance between two nodes and output all possible shortest paths 1249 between them using the assigned node IDs. Meanwhile, we also ask the model to output the number 1250 of common neighbors the two nodes have and the node IDs of their common neighbors. For the 1251 structural understanding task, a prompt node v_p will connect to both two nodes since our structural 1252 tasks need the model to reason about two nodes simultaneously. The text in the prompt node will be the corresponding question. Through these two tasks, the model is expected to gain the ability to 1253 identify basic graph structures, which are critical to downstream tasks. 1254

1255 Question answering task. Unlike language corpus, which naturally contains many question-and-1256 answer (QA) pairs, graph data usually only contain objective descriptions of entities. Nevertheless, 1257 for the model to be fluid in tasks, we need the model to understand user prompts and be sensitive to 1258 different tasks. Hence, we synthesize a QA-chain dataset from Ultrachat200k, as shown in Figure 1. 1259 A language QA sequence is converted to a chain graph where nodes with question texts alternate with nodes with answer texts, which are connected by directed edges to represent the conversation 1260 order. The last question becomes the text on prompt node v_p , which is connected to every node in the 1261 chain, and the last answer is the target text y (see Figure 1 QA-Chain Task for an example). This QA 1262 task provides QA pseudo-graphs missing from the common graph corpus, and we found it critical for 1263 enabling the model to be responsive to arbitrary tasks expressed in free-form text questions. 1264

1265 **Information retrieval task.** For most of the downstream tasks, GOFA requires a prompt node to link to all target nodes in the graph to solve related problems. To enable the prompt node to effectively 1266 maintain related information for solving the task in the decoding stage, we design an information 1267 retrieval task to realize these goals. Specifically, for each input graph, we randomly select n nodes and 1268 we connect a prompt node to these n nodes. Next, the information retrieval task is further divided into 1269 two parts: key-to-content and content-to-key. For key-to-content, we provide a node ID (randomly 1270 chosen from the selected n nodes) in the prompt node and ask the model to retrieve the text of that 1271 node. For the content-to-key task, we provide the content of one node (selected the same as above) in 1272 the prompt node and ask the model to return the correct node ID of that node. This task enhances the 1273 ability of GOFA to utilize our provided node IDs to retrieve and maintain correct information in the 1274 prompt node, which proves useful for many downstream tasks requiring information retrieval.

- 1275
- 1276 F.3 PRE-TRAIN IMPLEMENTATION DETAILS OF GOFA

1278 Dataset and task construction. As we discussed, we designed four different pre-training tasks for
 1279 GOFA . Here we describe some implementation details about each task and then discuss how we
 1280 construct each task on each dataset.

1281

1282 For the sentence completion task, the node text is split by the following rule: for each node, if the 1283 node text is less than 256 words, we set the maximum left-halve length to be the half of node sentence 1284 length. Otherwise, we set it to 128. Next, we randomly choose a length from 0 to maximum left 1285 length as the final cut point to cut the sentence into two pieces. For the shortest path task, we ask the 1286 model to output both the shortest path distance and all possible shortest paths. Since there may be 1287 multiple paths, to ensure the uniqueness of the answer, we first order all paths based on the node ID (the ascending order of alphabets) for nodes in each path and ask the model to learn this order. The 1288 construction of common neighbor task is similar. Finally, for information retrieval, given an input 1289 graph sample, we randomly select 2 to the number of nodes in the graph to be the target nodes. 1290

For pre-training datasets, we use multiple datasets including MAG240M, Arxiv, Pubmed,
Wikikg90mv2, Ultrachat200k, and WikiGraph. For MAG240M, Arxiv, and Pubmed datasets, each
training sample is a subgraph sampled around a node. Next, sentence completion, shortest path, and
common neighbor tasks are constructed. For each sample, there are 4 complete sentences, 3 shortest
path, and 3 common neighbor tasks. We will also construct information retrieval tasks on these
datasets. However, to ensure a moderated graph size, the information retrieval task will be constructed

Task	Question example	Answer example
Sentence completion	Complete the sentence of the tar- get node. Complete the sentence of the node[NODE.A].	The rest of the sentence in the tar- get node. The rest of the sentence in node [NODE.A].
Shortest paths	Compute the shortest path dis- tance between the target node [NODE.L] and node [NODE.B] and generate all shortest paths from the target node to the node [NODE.B]. Please separate nodes in the path with ->. If mul- tiple paths exist, generate all of them with an ascending order of node sequences and separate dif- ferent paths with ;.	The shortest path distance is 2. Shortest paths: [NODEID.L] -> [NODEID.G] -> [NODEID.B].
Common Neighbors	Is there any common neighbor be- tween the target node [NODE.L] and node [NODE.B]? If it exist, please give the total number and list all common neighbors in as- cending order of node, separate nodes with ;.	There is 1 common neighbor between two nodes, including [NODEID.G].
QA-Chain	What are the rules and restric- tions in place for COVID-19 in the city?	I don't have any live data regard- ing the covid-19 rules and restric- tions. Please check with the local authorities or health department for the latest guidelines and re- strictions in your city.
Information Retrieval	Please output the content of [NODE.A]. Given this node content: {node content}, please output the node id.	Content on [NODE.A]. [NODEID].

Table 8: Detailed question and answer example in pertaining task.

1332

1296

1333 1334

separately from the above tasks and also for both key-to-content and content-to-key tasks. For each 1335 information retrieval task sample, there will be only one task. For Wikikg90m, each training sample 1336 is a subgraph sampled around an edge. In Wikikg90m, we additionally include a link prediction 1337 task. That is, for each input graph, we randomly mask e edges and ask the model to recover the 1338 content in the edge. For each sample, there are 4 complete sentences, 2 shortest paths, and 2 common 1339 neighbor tasks, and 2 link prediction tasks. At the same time, the information retrieval task will also 1340 be generated separately. For WikiGraph, each sample is itself a graph. Similar to Wikikg90mv2, each sample consists of 4 complete sentences, 2 shortest paths, 2 common neighbor tasks, and 2 1341 link prediction tasks and information retrieval task will also be generated separately. Finally, for 1342 Ultracha200k, we only include question answer task and each sample only contains one task. The 1343 detailed task prompts and answer examples are shown in Table 8. 1344

Training details. The initial weight of the LLM compressor and decoder is obtained from ICAE (Ge et al., 2023). The initial weight of all GNN layers is randomly initialized. The value of all gates in the residual connection is set to 0 to ensure the initialized model performs the same as the original language model. During the training, we only tune the GNN layers. For each training epoch, the training corpus includes 500,000 MAG240M samples, 50,000 Arxiv samples, 5,000 PubMed samples, 100,000 Ultrachat200k samples, 80,000 WikiGraph samples, 100,000 Wikikg90mv2 samples. At

1350 the meantime, for MAG240M, Arxiv, Pubmed, WikiGraph, and Wikikg90mv2, we will include 1351 10,000 key-to-content and 10,000 content-to-key information retrieval tasks. This resulted in 935,000 1352 samples for each training epoch and we trained the model for 3 epochs. The training is conducted on 1353 8 NVIDIAA100_SXM4_80GB GPUs with DeepSpeed stage 2 (Rajbhandari et al., 2020) parallelism. 1354 The detailed training parameters are set the same for both two models and are listed in Table 9. We use AdamW optimizer with $\beta = (0.9, 0.95)$. We use a cosine annealing learning rate scheduler, and 1355 the minimum learning rate is 10% of the initial learning rate. We restarted the learning rate 2 times 1356 on one-third and two-thirds of the training. 1357

1	3	5	8
1	3	5	9

Table 9: Hyper-parameters for pretraining.

lr	weight_decay	batch_size	dropout	grad_clip	gradient_accum	llm_max_length	optimizer
0.0001	0.1	8	0.0	0.5	8	128	AdamW

1363 1364 1365

1367

F.4 ZERO-SHOT LEARNING

Setting. For the zero-shot learning, we select Cora-link, Cora-node, WikiCS, Products, ExplaGraphs, and SceneGraphs as evaluation datasets. For all datasets, we directly evaluate baselines and GOFA on the test set.

1371 **Baseline Details**: We compare the performance of GOFA with two categories of baseline methods. 1372 The first category includes models that directly utilize large language models (LLMs). For this, we select Llama2-7B and Mistral-7B (Jiang et al., 2023) as baselines. We input the content of all target 1373 nodes into these pre-trained models and concatenate the same prompt used in GOFA for evaluation. 1374 The second category consists of Graph LLM models that have zero-shot ability. We include OFA (Liu 1375 et al., 2023a), GraphGPT (Tang et al., 2023), UniGraph (He & Hooi, 2024), ZeroG (Li et al., 2024), 1376 and LLaGA (Chen et al., 2024) as baselines. For OFA, we extend the datasets by adding Products 1377 and ExplaGraphs and follow the original source code to train the model on Arxiv and FB15K237 for 1378 30 epochs, using Llama2-7B as the embedding model. All other settings remain consistent with the 1379 default OFA configuration, and we report the test performance accordingly. For GraphGPT, we use 1380 the results reported in the LLaGA paper. For UniGraph, we use the results from the original paper. 1381 For ZeroG, we use the results in UniGraph paper. For LLaGA, we rerun the source code, adapting 1382 the settings of ways to align with our experimental setup.

1383 **Detail of GOFA.** For the GOFA, we fine-tune the model from the pre-training checkpoint. In 1384 fine-tuning, we will train the parameters of GNN and LoRA layers in the LLM decoder. To com-1385 prehensively evaluate the performance of GOFA, We separately fine-tune the GOFA on different 1386 datasets. Specifically, we design two different settings. In the first setting, we fine-tune the model 1387 using the Arxiv and Pubmed datasets with both the node classification and link prediction tasks. In 1388 the second setting, we add mag240m and Wikikg90m additionally. We denote GOFA-T and GOFA-F, 1389 respectively. For GOFA-T, we sample 40000, 80000, 10000, 10000 for Arxiv link, Arxiv node, Pubmed link, and Pubmed node, respectively. For GOFA-F, we sample 10000, 10000, 40000, 1390 50000, 10000, 10000 for MAG240M, Wikikg90m, Arxiv_link, Arxiv_node, Pubmed_node, and 1391 Pubmed_link, respectively. For all evaluation and pre-training datasets, we design multiple prompt 1392 templates with instructions to let the model select the correct label from the provided label list. For 1393 each label in each dataset, we use the GPT-4 to generate a short description for the label. The detailed 1394 prompt examples for all datasets are shown in Table 10 and Table 11. For all MAG240M, Wikikg90m, 1395 and Arxiv, since it is hard to include all ways in the prompt, we randomly sampled 10 ways during 1396 the training for each sample. For each pre-training dataset, we randomly sample a fixed number of training samples in a random way. The detailed parameters for fine-tuning are listed in Table 12. All 1398 parameters not listed in the table are the same as the pre-training setting. For all training versions, we 1399 directly evaluate the model on the test set of all evaluation datasets. We evaluate the model on the test 1400 set. For datasets with less than 15000 test samples, we evaluate on the whole set. Otherwise, we only randomly select 15000 samples for evaluation, due to the time constraint. For evaluation, we will 1401 match the text output generated by the GOFA with the ground true label to compute the accuracy of 1402 the classification task. For the regression task, we will extract the number from the output text and 1403 compute the metric with the correct value.

Table 10: Prompt examples of GOFA for each training dataset in Zero-shot learning.

This is a citation network from microsoft academic graph platform. Nodes repre- sent academic papers and edges represent citation relationship. You are an expert in computer science. You need to choose the correct paper category based on the paper content and its citation network. For example, if the paper [NODEID] { <la- bel_description>, choose <label>;}. What is the most likely paper category for the target paper? Choose from the following: {<label>}. This is a co-citation network from the Pubmed platform focusing on diabetes mellitus. Nodes represent academic papers and edges represent two papers that are co-cited by other papers. You are a diabetes mellitus expert tasked with determining whether two given papers [NODEID1] and [NODEID2] are co-cited by another paper based on their content and network characteristics. Evaluate the following criteria: assess whether the topics of the two papers are similar, check if the shortest path distance between the two papers is small, and verify whether the papers have a large number of common neighbors in the citation network. If the answer to most of these questions is Yes, choose Yes; if the answer to most of these questions is No, choose No. This is a co-citation network from the Pubmed platform focusing on diabetes mellitus.</label></label></la-
This is a co-citation network from the Pubmed platform focusing on diabetes mellitus Nodes represent academic papers and edges represent two papers that are co-cited by other papers. You are a diabetes mellitus expert tasked with determining whether two given papers [NODEID1] and [NODEID2] are co-cited by another paper based on their content and network characteristics. Evaluate the following criteria: assess whether the topics of the two papers are similar, check if the shortest path distance between the two papers is small, and verify whether the papers have a large number of common neighbors in the citation network. If the answer to most of these questions is Yes, choose Yes; if the answer to most of these questions is No, choose No. This is a co-citation network from the Pubmed platform focusing on diabetes mellitus
This is a co-citation network from the Pubmed platform focusing on diabetes mellitus
Nodes represent academic papers and edges represent two papers that are co-cited by other papers. You are an expert on diabetes mellitus. You need to choose the correct paper category based on the paper content and its co-citation network. For example if the paper [NODEID] { <label_description>, choose <label>;}. What is the most likely paper category for the target paper? Choose from the following: {<label>}.</label></label></label_description>
This is a graph extracted from the entire Wikidata knowledge base. You are an expert in knowledge graph reasoning. You need to choose the correct relation type between two target entities based on their existing relations. For example, if two relations involve { <label_description>, choose <label>;}. What is the relationship between two target entities? Choose from the following list: {<label>}."</label></label></label_description>
This is a citation network from Arxiv platform focusing on the computer science area. Nodes represent academic papers and edges represent citation relationships. You are an expert in computer science. You need to choose the correct paper category based on the paper content and its citation network. For example, if the paper [NODEID] { <label_description>, choose <label>;}. What is the most likely paper category for the target paper? Choose from the following: {<label>}.</label></label></label_description>
This is a citation network from Arxiv platform focusing on the computer science area. Nodes represent academic papers and edges represent citation relationships. You are a computer science expert tasked with determining whether two given papers [NODEID1] and [NODEID2] are co-cited by another paper based on their content and network characteristics. Evaluate the following criteria: assess whether the topics of the two papers are similar, check if the shortest path distance between the two papers is small, and verify whether the papers have a large number of common neighbors in the citation network. If the answer to most of these questions is Yes, choose Yes; if the answer to most of these questions is No, choose No.

Table 11: Prompt examples of GOFA for each evaluation dataset in Zero-shot learning.

Dataset	Prompt
Cora-node	This is a co-citation network focusing on artificial intelligence, nodes represent academic papers and edges represent two papers that are co-cited by other papers. You are an expert in computer science. You need to choose the correct paper category based on the paper content and its co-citation network. For example, if the paper [NODEID] { <label_description>, choose <label>;}. What is the most likely paper category for the target paper? Choose from the following: {<label>}.</label></label></label_description>
Cora-link	This is a co-citation network focusing on artificial intelligence, nodes represent acad demic papers, and edges represent two papers that are co-cited by other papers. You are a computer science expert tasked with determining whether two given papers are co-cited by another paper based on their content and network characteristics Evaluate the following criteria: assess whether the topics of the two papers are similar check if the shortest path distance between the two papers is small, and verify whether the papers have a large number of common neighbors in the citation network. If the answer to most of these questions is Yes, choose Yes; if the answer to most of these questions is No, choose No.
WikiCS	This is a Wikipedia graph focusing on computer science. Nodes represent Wikipedia terms and edges represent two terms that have hyperlinks. You are an expert in computer science. You need to choose the correct category of Wikipedia term based on the term content. For example, if the term [NODEID] { <label_description>, choose <label>;}. What is the most like category for this Wikipedia entry? Choose from the following: {<label>}.</label></label></label_description>
Products	This is a co-purchase network from the Amazon platform. Nodes represent the products sold on Amazon and edges represent two products that are co-purchased together. For example, if the product [NODEID] { <label_description>, choose <label>;}. What is the most like category for this product? Choose from the following: {<label>}.</label></label></label_description>
FB15K237	This is a knowledge graph from the FreeBase. Nodes represent knowledge entities and edges represent relations between two entities. You are an expert in knowledge graph reasoning. You need to choose the correct relation type between two target entities based on their existing relations. For example, if two relations { <label_description> choose <label>;}. What is the relationship between two target entities? Choose from the following list: {<label>}."</label></label></label_description>
ExplaGraphs	This is a graph constructed from commonsense logic. Nodes represent commonsense objects and edges represent the relation between two objects. You are a logic expert tasked with analyzing the logical relationship between two arguments related to connected entities. Determine if the arguments support or counter each other based on their logical coherence. If there is no logical conflict between the two arguments and they are in agreement, choose Support; if the arguments exhibit a logical conflict or contradiction, choose Counter.
SceneGraphs	This is a scene graph generated from an image. Nodes represent an object in the image

Table 12. Hyper r	arameters for zer	o shot instru	ction fine tuning
Table 12: Hyper-L	arameters for zer	o-snot mstru	cuon nne-tuning.

lr	weight_decay	gradient_accum	llm_max_length
0.0001	0.1	64	256

1518 F.5 SUPERVISED-LEARNING

1520

1521

1525

Table 13: Hyper-parameters for supervised fine-tuning.

lr	weight_decay	grad_clip	gradient_accum	llm_max_length
0.0001	0.1	0.5	32	256

Setting. For the supervised-learning setting, we select Cora (node/link), PubMed (node/link), Arxiv,
WikiCS, WN18RR, FB15K237, and Products datasets for the evaluation. For all datasets, we utilize
the default split described in Appendix C. To ensure a fair comparison, we employ subgraph sampling
for GOFA and all baseline methods. For all datasets, the sampling hop is 3 and the maximum nodes
per hop are 5.

1531 **Detail of baselines.** For the traditional GNN methods, we include GCN (Kipf & Welling, 2017) 1532 and GAT (Veličković et al., 2018). To ensure a fair comparison, we use Llama2-7B to convert raw 1533 texts in all datasets to sentence embedding and use this as the model's input node/edge features. We 1534 re-implement both methods in order to adapt the original method with subgraph input. Specifically, for but node/link-level tasks, we will add labeling trick (Zhang et al., 2021) to the target nodes at 1535 the beginning. After message passing, we will use the summation pooling on all target nodes and 1536 use the result embedding for the prediction. For traditional GNN methods, we train and evaluate 1537 each dataset independently. For all datasets, we search the number of layers and dropout parameters. 1538 For each parameter set, we repeat the experiment 4 times select the parameter set with the best 1539 validation performance, and report the performance on the test set. For constrastive learning methods, 1540 we include DGI (Veličković et al., 2018) and BGRL (Thakoor et al., 2021). We directly report 1541 results from UniGraph (He & Hooi, 2024). For the graph foundation model, we include OFA (Liu 1542 et al., 2023a) and UniGraph (He & Hooi, 2024) as the baseline. The OFA is simultaneously trained 1543 and evaluated on all datasets. To ensure a fair comparison, we get their code from the original 1544 source and train the model on Cora (node/link), PubMed (node/link), Arxiv, WikiCS, WN18RR, 1545 and FB15K237 dataset using the Llama2-7b as base LLM model. Similarly, for OFA, we use the same subgraph sampling parameters as all other methods. For other parameters, we use the default 1546 parameter provided in their code. We only run the model one time and report the final performance. 1547 For UniGraph, we directly report results from their original paper. 1548

1549 **Detail of GOFA**. For the GOFA, we fine-tune the model from the pre-training checkpoint. In fine-1550 tuning, we will train the parameters of GNN and LoRA layers in the LLM decoder. We simultaneously fine-tune the model on the train set of Cora-node, Cora-link, PubMed-node, PubMed-link, Arxiv, 1551 WikiCS, WN18RR, FB15K237, and Products. For each dataset, we will randomly sample a fixed 1552 number of training samples for each epoch with random sampling. The sample numbers for each 1553 dataset is 3000, 40000, 3000, 80000, 105000, 12000, 60000, 120000, and 38000, respectively. We 1554 fine-tune the model for 1 epochs. The detailed parameters for fine-tuning are listed in Table 13. For 1555 each dataset, we create a prompt for the LLM decoder to generate the desired answer. In a supervised 1556 setting, we ask the LLM model directly to generate the correct answer, instead of doing the selection 1557 from the given list. The detailed prompt for each dataset is listed in Table 14. For evaluation, we will match the text output generated by the GOFA with the ground true label to compute the accuracy of the classification task. We evaluate the model on the test set. For datasets with less than 15000 test samples, we evaluate on the whole set. Otherwise, we only randomly select 15000 samples for 1561 evaluation, due to the time constraint.

1562

1563

1564

1565

Table 14:	Detailed prompt of GOFA for each dataset in supervised learning.		
Dataset	Prompt		
Cora-node	This is a co-citation network focusing on artificial intelligence, nodes represent academic papers and edges represent two papers are co-cited by other papers. What is the most likely paper category for the target paper? Please directly answer the category.		
Cora-link	This is a co-citation network focusing on artificial intelligence, nodes represent academic papers and edges represent two papers are co-cited by other papers. Is the two target papers co-cited or not? Please only answer yes or no.		
PubMed-node	This is a co-citation network from Pubmed platform focusing on dia betes mellitus. Nodes represent academic papers and edges represen two papers are co-cited by other papers. What is the most likely paper category for the target paper? Please directly answer the category.		
PubMed-link	This is a co-citation network from Pubmed platform focusing on dia betes mellitus. Nodes represent academic papers and edges represen two papers are co-cited by other papers. Is the two target papers co-cited or not? Please only answer yes or no.		
Arxiv	This is a citation network from arxiv platform focusing on the computer science area. Nodes represent academic papers and edges represen citation relationships. What is the most likely paper category for the target Arxiv paper? please directly answer the category.		
WikiCS	This is a Wikipedia graph focusing on computer science. Noder resent Wikipedia terms and edges represent two terms have hype What is the most likely category for this Wikipedia term? Please a answer the category.		
WN18RR	This is a knowledge graph from WordNet. Nodes represent an English word and edges represent the relationship between two words. What is the relationship between two target words? Please directly answer the relationship.		
FB15K237	This is a knowledge graph from freebase. Nodes represent knowledge entities and edges represent relations between two entities. What is the relationship between two target entities? Please directly answer the relationship.		
Products	This is a co-purchase network from the Amazon platform. Nodes repre sent the products sold on Amazon and edges represent two products are co-purchased together. What is the most like category for this product? Please directly answer the category.		