Revisiting the Graph Reasoning Ability of Large Language Models: Case Studies in Translation, Connectivity and Shortest Path

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Abstract

Large Language Models (LLMs) have achieved great success in various reasoning tasks. However, their capacity for graph reasoning remains poorly understood. Although recent theoretical analyses suggest that LLMs can, in principle, perform complex graph tasks, empirical evaluations reveal numerous failures. To bridge this gap, we revisit the graph reasoning ability by introducing a new, balanced, and comprehensive benchmark. Through systematic experimentation, we identify key factors influencing performance, including node connectivity types, graph sizes, graph descriptions, and node naming methods. Moreover, we also demonstrate the impact of training data, model size and fine-tuning on graph reasoning. All the implementations and datasets are publicly available[1].

1 Introduction

Large Language Models (LLMs) have shown remarkable achievements in a multitude of reasoning tasks, ranging from mathematical, commonsense and symbolic problem-solving (Luo et al., 2023; Creswell et al., 2023), to more specialized applications like dialogue systems (Ouyang et al., 2022), program debugging (Surameery and Shakor, 2023) and scientific discovery (Boiko et al., 2023). In this work, we focus on graph reasoning capability, where LLMs employ an explicit graph, sourced either from the input data or external resources, to infer the outcome. This reasoning ability is crucial and can be applied across various domains, such as improving question-answering system by a domain-specific knowledge graph (Huang et al., 2022), facilitating planning in autonomous agents through the tool relation graph (Liu et al., 2024), and enhancing robot navigation via physical maps (Creswell et al., 2022).

Figure 1: The overview of datasets in accuracy and distribution across different connectivity types. We evaluate GPT-3 on determining whether a path exists between two nodes. Previous work (Wu et al., 2024) primarily focused on 1-hop and 2-hop connections, resulting in high accuracy. However, it overlooked the fact that accuracy tends to drop when extending to 3, 4, and 5-hop connections.

There are recent studies initially exploring the LLM's graph reasoning capability. On the one hand, the theoretical work (Feng et al., 2024) proved that LLMs have the ability to mimic a powerful decision-making framework (i.e., dynamic programming), to solve the complex tasks. This suggests that LLMs are capable of handling certain graph reasoning tasks that can be formulated as decision-making problems, including breadth-first search for graph connectivity, and the Dijkstra for shortest path problem. On the other hand, recent empirical studies, such as GPT4Graph (Guo et al., 2023) and NLGraph (Wang et al., 2024a), found that LLMs could fail in these graph tasks. This discrepancy between theoretical expectations and practical observations indicates a critical gap in our comprehension of LLMs' graph reasoning abilities. In light of this, we aim to delve deeper into

[1]codes available: https://anonymous.4open.science/r/LLM-graph-evaluation-5E2C
datasets available: https://drive.google.com/file/d/1tBQVW1ThflqdAV7iGW9oCpeHhwB8xghK/view?usp=sharing.

fundamental graph tasks to uncover the limitations inherent in LLMs, assess the impact of these limitations in real-world graphs, and propose possible explanations to understand the discrepancy.

In this work, we re-evaluate three fundamental graph reasoning tasks: graph description translation, graph connectivity, and the shortest path problem. First, we check whether LLMs can comprehend graph structures through the translation of varied graph descriptions (See Section 3.1). We summarize the three most popular graph description methods and evaluate the translation tasks among them. Although it is a simple reasoning task and LLMs could achieve high performance, LLMs are not entirely error-free. Then, we explore graph connectivity and examine LLMs systematically by considering varying connectivity lengths between nodes, diverse types of disconnections and different graph descriptions (See Section 4). Existing works (Wang et al., 2024a; Luo et al., 2024) primarily focus on the influence of graph size while considering only a limited range of connectivity types, leading to biased evaluations in connectivity tasks, as demonstrated in Figure 1. To address this, we construct a balanced and comprehensive dataset. Our investigations on this dataset indicate that in addition to graph size, node connectivity types and graph descriptions also play significant roles, and we extend those insights to the shortest path and real-world application tasks. In Section 5, we further explore the effects of model size and training data scale on graph reasoning, demonstrating that LLMs have the potential to excel in reasoning tasks given sufficient data and large-scale parameters. Finally, we reveal that LLMs may adopt different reasoning approaches depending on the form of the graph descriptions provided.

2 Related work and Background

2.1 Evaluation on graph reasoning tasks

Recent efforts have been made on graph reasoning evaluations (Guo et al., 2023; Fatemi et al., 2023; McLeish et al., 2024). NLGraph (Wang et al., 2024a) evaluates LLMs across the 8 fundamental graph reasoning tasks, suggesting that LLMs have preliminary graph reasoning abilities. GraphInstruct (Luo et al., 2024) extends the graph reasoning benchmark to 21 classical graph tasks and introduces a step masking method to enhance the graph reasoning abilities of LLMs. Additionally, VisionGraph (Li et al., 2024) provides a multi-modal version of the graph reasoning task benchmark, extending its applicability beyond text.

2.2 Graph connectivity in theory

LLMs, through their transformer architecture, have demonstrated essential capabilities for reasoning tasks (Giannou et al., 2023; Yang et al., 2023; Sanford et al., 2024b). Specifically, for the graph reasoning tasks, de Luca and Fountoulakis (2024) suggest that looped transformers are able to simulate every step in a graph algorithm. Sanford et al. (2024a) reveal that a single-layer transformer is sufficient for a naive graph connectivity task.

2.3 LLMs for graphs in the applications

Despite LLMs having capabilities in graph reasoning tasks in theory, there remains a gap between text understanding and graph reasoning (Chai et al., 2023; Zhao et al., 2023). Therefore, some recent work approves the use of additional tools to help LLMs understand graphs. Recent studies have validated the use of extra tools to enhance LLMs' comprehension of graphs. GraphEmb (Perozzi et al., 2024) employs an encoding function to augment prompts with explicit structured information. Additionally, GraphWiz (Chen et al., 2024) fine-tunes LLMs using graph reasoning datasets to achieve higher performance in graph tasks. However, when LLMs are pretrained using text data, their limitations in graph reasoning tasks remain unclear. In this work, we do a comprehensive study on the failures of LLMs in graph reasoning tasks. We summarize and analyze the potential reasons why LLMs fail in graph reasoning only using text prompts.

2.4 Theoretical support for graph reasoning tasks

Feng et al. (2024) prove that if a task can be deconstructed into subtasks, it can be solved by LLMs. Based on this, Wu et al. (2024) offer insights into transforming message-passing processes among graphs into subtasks of message-passing among nodes using transition functions, suggesting that LLMs are capable of handling graph decision tasks. Specifically, it can be theoretically proven that graph connectivity and shortest-path tasks are two examples of problems solvable by LLMs.

Suppose that the structure of a graph can be represented as $\mathcal{G} = (\mathbf{X}, \mathbf{E}, \mathcal{E})$, where $\mathbf{X}$ is the set of nodes, $\mathbf{E}$ is the edge set, and $\mathcal{E}$ is the feature set of the edges. For the graph connectivity task, we start from node n_i and end at node

n_j. The transition function $F(i,j)$ for the graph connectivity task can be formulated as: $F(i,j) = \mathbb{1}_{k\in\mathcal{N}_{v_j}}(F(i-1,k) \cap F(k,j))$, where $\mathcal{N}_{v_j}$ denotes the neighbors of node node v_j and $\mathbb{1}$ means whether the connection is existing. Consequently, we can deconstruct the graph connectivity tasks into subtasks, which have been proven to be solved by LLMs in Feng et al. (2024).

Theoretical results suggest that LLMs are capable of solving fundamental graph reasoning tasks, such as graph connectivity and shortest-path tasks. However, we find that they fail in practice.

3 Limitations of LLMs in graph reasoning

In this section, we empirically revisit the graph reasoning ability via case studies. In particular, we introduce three fundamental graph tasks: graph description translations in Section 3.1, graph connectivity in Section 4, and the shortest path task in Section 4.5. Finally, we summarize and analyze our findings in Section D.3.

3.1 Graph description translation

3.1.1 Graph Descriptions

To begin with, we first describe the graph properties denoted as: *G describes a [attribute] graph among* $x \in \mathbf{X}$, where [attribute] defines the graph types, such as undirected, directed, or knowledge graphs. Then, we use different graph descriptions to introduce their structures.

We summarize three types of graph structure description methods that have been widely used by the previous works (Fatemi et al., 2023; McLeish et al., 2024) as shown in Figure 2. They are (1) Adjacency Matrix: describing the adjacency matrix of a graph; (2) Node List: referring to the neighbors of a central node on a graph, and (3) Edge List: listing every edge of a graph. Adjacency Matrix is denoted as $\mathbf{A} \in \mathcal{R}^{N\times N}$, where N is the number of nodes. In the text description, it encodes a paragraph by $N \times N$ binary tokens.

Node List uses the neighbors of a central node to describe a graph. For instance, consider the set of sentences $S_N = \{s_1, s_2, \ldots, s_N\}$, which describes the graph via the neighbors $[u]$ of node v_i with the edge feature ϵ. A single sentence is as follows:

$$s_i = \text{Node } v_i \text{ [relation] Nodes } \{[u,\epsilon]_{u\in\mathcal{N}_{v_i},\epsilon\in\mathcal{E}(v_i,u)}\}.$$

Note that the [relation] varies across different types of graphs. In undirected graphs, we use the relation "is connected to," whereas in directed graphs,

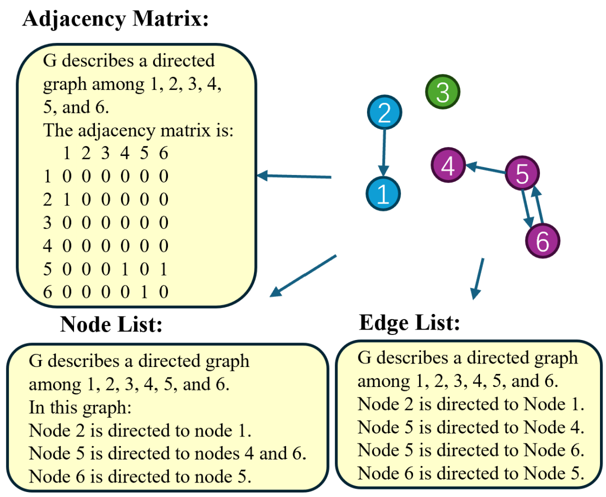

Figure 2: Three types of graph descriptions. A graph can be described by an adjacency matrix, edge list, and neighborhood node sets.

we use "is directed to." In knowledge graphs, the relation can be any specified type.

Edge List describes a graph by listing the edges in a graph. The set of description sentences is denoted as: $S_{N_E} = \{s_1, s_2, \ldots, s_{N_E}\}$, where N_E is the number of edges and s_i represents an edge, which is defined as:

$$s_i = \text{Node } v_i \text{ [relation] Node } v_j, \epsilon_{ij}.$$

The examples of the graph descriptions are shown in Appendix A.

3.1.2 Translations on graph descriptions

If LLMs can comprehend the structures of a graph, such understanding should be independent of the methods used to describe the graph. Therefore, to verify the ability of LLMs to understand the structural information of a graph, we design a graph translation description task. This task requires LLMs to use the input graph description to generate various descriptions. After that, we will compare these descriptions to determine if they represent the same graph structure.

Note that the number of tokens in the Adjacency Matrix depends on the number of nodes. This suggests that the Adjacency Matrix may require more tokens in dense graphs than Node or Edge Descriptions, limiting its applicability in the real world when the graph size is large. Therefore, we only apply the Adjacency Matrix as the target format in the graph description translation task while employing Node List and Edge List as both source and target descriptions. Similarly, we use Node List and Edge List for graph connectivity and shortest-path tasks in Section 4 and Section 4.5.

As suggested by the previous study, such as NLGraph (Wu et al., 2024) and GraphInstruct (Luo et al., 2024), increasing the graph size will challenge LLMs to understand graph structures. Thus, following the previous work, we use node numbers to indicate difficulty levels. In particular, we randomly generate 100 graphs with node numbers ranging from 5 to 25, and divide them into two datasets: one containing 50 graphs with node counts ranging from 5 to 15, labeled as "Easy", and another containing 50 graphs with node counts from 16 to 25, labeled as "Hard".

We employ GPT-4 and LLAMA3.0-70B with the zero-shot setting and 0 temperature in the experiment. As the Adjacency Matrix is constrained by sentence length, we only predict the Adjacency Matrix on the dataset with smaller graphs. In the evaluation, we use the accuracy metrics. If the translations are completely correct, we categorize them as correct predictions. The results are summarized in the Table 1.

Table 1: Using LLMs to predict the translation among different descriptions. The scores are (GPT-4/LLAMA3.0-70B)

Dataset 1	# Graph 50	Avg. Node 10.6	Avg. Edge 33.56
Source\Target	**Adjacency**	**Nodes**	**Edges**
Nodes	0.88 / 0.68	1.00 / 0.94	0.94 / 0.88
Edges	0.88 / 0.66	0.94 / 0.74	1.00 / 0.88
Dataset 2	**# Graph** 50	**Avg. Node** 20.49	**Avg. Edge** 110.35
Source\Target	**Adjacency**	**Nodes**	**Edges**
Nodes	-	1.00 / 0.90	0.66 / 0.74
Edges	-	0.50 / 0.32	0.92 / 0.70

The results indicate that LLMs struggle with graph description translations. LLMs achieve reliable accuracy only when the source and target descriptions are identical; however, they fail when translating between different types of descriptions. For example, LLMs show high accuracy in repeating the Node description, with both the source and target being Node descriptions. However, their performance significantly declines when Edge Description is used. Similarly, while LLMs can summarize edge information effectively using Edge description, they struggle to summarize edge information from Node description. Those suggest that LLMs may not fully understand graph structures.

Furthermore, performance is also related to the sequence length. Although LLMs perform adequately with smaller-scale graphs, their effectiveness decreases as the graph size increases. Additionally, as Adjacency Matrix descriptions require more tokens in the output, accuracy significantly decreases when predicting adjacency matrices. These findings align with similar limitations observed in general long-form text-generation tasks (Ji et al., 2023).

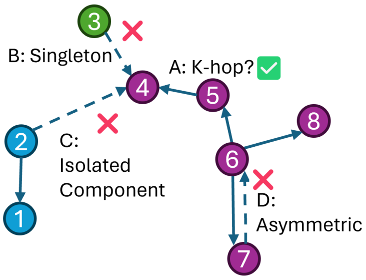

Figure 3: Different types of connectivity. The directed graph consists of 8 nodes, where solid lines represent the existence of directed edges, and dotted lines indicate no edge exists. Four connectivity types include: (A) K-hop: nodes 5 and 6 connect to node 4 within 1-hop and 2-hops, respectively. (B) Singleton: node 3 is an isolated node and not attached to node 4; (C) Isolated Components: nodes 2 and 4 belong to separate components with no path-connected edge; (D) Asymmetric: node 6 is directed towards node 7 but lacks any connection in an asymmetric configuration.

The experiments suggest that LLMs often generate content that is logically inconsistent with the input and the instructions, indicating that these failures may be due to faithfulness hallucinations. The appendix I provides examples of these failures in description translation, where LLMs occasionally ignore certain edges or introduce non-existent ones, diverging from the input. Since translation tasks do not require complex reasoning but still exhibit hallucinations, it is possible that more complex reasoning tasks may also be prone to similar hallucinations in graph understanding.

4 Revisit graph connectivity task

4.1 Connectivity types

Previous studies suggest that large language models (LLMs) possess essential capabilities for graph connectivity tasks (Wang et al., 2024a; Luo et al., 2024), yet they still fail in some instances. To further investigate the graph connectivity task, we begin by analyzing the samples where failures occurred based on those two baseline datasets.

We first categorize the types of connectivity samples. For the samples of connected nodes, we classify them according to the path length, which is denoted as K-hops. Besides, for the samples of unconnected nodes, we label them into three categories: Singleton, Isolated Components (IC), and

Table 2: Connectivity evaluation on the undirected graph datasets

Difficulty	Model	Des.	k-hop, 1≤k≤2			k-hop, 3≤k≤4			5-hop			Singleton	I.C.	AVG. ACC	AVG. F_{acc}
			ACC	F_{acc}	PCR	ACC	F_{acc}	PCR	ACC	F_{acc}	PCR	F_{acc}	F_{acc}		
Easy	LLAMA3	Node	1.00	0.99	0.99	1.00	0.96	0.98	1.00	0.92	0.96	1.00	0.33	0.73	0.71
		Edge	1.00	0.94	0.88	1.00	0.96	0.98	0.98	0.78	0.94	1.00	0.44	0.77	0.73
	GPT-3	Node	1.00	0.98	0.82	0.88	0.87	0.93	0.78	0.72	0.87	0.92	0.13	0.60	0.59
		Edge	1.00	0.96	0.80	0.82	0.80	0.93	0.88	0.72	0.90	0.94	0.17	0.61	0.58
	GPT-4	Node	1.00	0.93	0.99	1.00	0.93	0.99	1.00	0.94	0.97	1.00	0.53	0.81	0.78
		Edge	1.00	0.93	0.98	1.00	0.90	0.98	0.98	0.88	0.97	0.98	0.69	0.87	0.83
Medium	LLAMA3	Node	1.00	0.94	0.90	1.00	0.93	0.96	0.94	0.82	0.93	1.00	0.36	0.74	0.70
		Edge	1.00	0.96	0.83	0.96	0.81	0.90	0.94	0.62	0.94	0.98	0.35	0.72	0.65
	GPT-3	Node	1.00	0.97	0.72	0.81	0.74	0.84	0.76	0.62	0.79	0.94	0.16	0.60	0.56
		Edge	1.00	0.96	0.72	0.72	0.60	0.90	0.76	0.52	0.83	0.96	0.18	0.59	0.53
	GPT-4	Node	1.00	0.89	0.98	1.00	0.85	0.97	1.00	0.94	0.92	0.98	0.42	0.77	0.71
		Edge	1.00	0.91	0.97	1.00	0.90	0.93	0.96	0.74	0.94	0.96	0.44	0.77	0.71
Hard	LLAMA3	Node	1.00	0.98	0.90	1.00	0.83	0.94	0.96	0.64	0.94	0.96	0.2	0.67	0.60
		Edge	1.00	0.92	0.78	0.92	0.59	0.86	0.94	0.42	0.92	0.84	0.2	0.64	0.51
	GPT-3	Node	1.00	0.92	0.65	0.76	0.67	0.85	0.80	0.50	0.77	0.98	0.14	0.59	0.52
		Edge	1.00	0.92	0.66	0.65	0.47	0.86	0.74	0.38	0.81	1.00	0.18	0.58	0.49
	GPT-4	Node	1.00	0.87	0.98	0.99	0.84	0.93	0.98	0.76	0.90	1.00	0.30	0.72	0.64
		Edge	1.00	0.86	0.94	0.93	0.69	0.87	0.90	0.58	0.90	0.92	0.34	0.71	0.60

Asymmetric, as shown in Figure 3. Singleton denotes that one node is isolated. Isolated Components indicate that these two nodes belong to separate components in the graph. Note that a Singleton is a special case of Isolated Components. The distinction lies in the representations using Node List and Edge List, where the isolated node is not included in the descriptions of the graph structure, such as Node 3 in Figure 2. Asymmetric is designated for directed graphs, highlighting situations where a path exists from one node to another, but the reverse path does not exist, indicating a one-way connectivity.

We calculate the distribution of connectivity types in the baseline datasets, as shown in Table 11 of Appendix C.1, and subsequently conduct the experiment on them. The results, presented in Table 6 of Appendix C.2, indicate that the baseline datasets lack a balanced distribution across different connectivity types. More importantly, LLMs exhibit varying performances across these types. Thus, it is crucial to establish a balanced dataset to better evaluate different graph connectivities.

4.2 Dataset Construction

In previous work, NLGraph (Wang et al., 2024a) included only an undirected graph dataset for the connectivity task, and GraphInstruct (Luo et al., 2024) featured an unbalanced distribution as shown in Appendix C.1, Table 11. Therefore, based on these studies, we need to consider factors such as the number of nodes in graphs, edge directions, and types of connectivity.

Following previous studies (Wu et al., 2024; Luo et al., 2024), we indicate the difficulty levels of graphs based on the number of nodes, labeling them as Easy, Medium, and Hard. For each level, we initially generate all possible graphs with a certain number of nodes and then randomly select graphs and corresponding node pairs to formulate test pairs of the questions. For samples connected within K-hops, we collect 50 samples for each k where $k \in [1, 2, 3, 4, 5]$. For negative samples, we selected 200 Isolated Component samples and 50 Singleton samples from the undirected graph dataset. Similarly, for the directed graph dataset, we chose 100 Connected pairs, 100 Asymmetric samples, and 50 Singleton samples. The details can be found in Table 11 of Appendix C.1.

4.3 Evaluation Metrics

Instead of only evaluating the accuracy of graph connectivity, we also want to check if the reasoning path to make the prediction can support the prediction. Thus, the prompt is defined as follows: "If a path exists, present the path formatted as "Node #1 -> Node #2."; If no path is found, state "No path.". Therefore, to evaluate the reliability of such paths, we design two novel metrics, $\text{Fidelity}_{\text{Acc}}$ (F_{acc}) and Path Consistency Ratio (PCR), which are used to analyze the correctness of reasoning paths. F_{acc} evaluates whether the reasoning path to infer the answer is correct or not. The formulation is denoted as: $F_{acc} = \frac{1}{M} \sum_{i=1}^{M} (\hat{y}_i = y_i) \wedge (\hat{p}_i \in \mathbf{P})$, where $\hat{y}_i$ denotes the predicted answer, y_i the ground truth answer, $\hat{p}_i$ the predicted path, and $\mathbf{P}$ the set of reachable paths. M is the number of data samples. F_{acc} correctly identifies the answer only when both

Table 3: Connectivity evaluation on the directed graph datasets

Difficulty	Model	Des.	k-hop, 1≤k≤2			k-hop, 3≤k≤4			5-hop			Singleton	Isolated C.	Asymmetric	AVG. ACC	AVG. F_{acc}
			ACC	F_{acc}	PCR	ACC	F_{acc}	PCR	ACC	F_{acc}	PCR	F_{acc}	F_{acc}	F_{acc}		
Easy	GPT-3	Node	0.99	0.92	0.88	0.85	0.58	0.93	0.92	0.36	0.95	0.96	0.13	0.37	0.66	0.53
		Edge	1.00	0.93	0.94	0.89	0.47	0.95	0.92	0.30	0.96	0.94	0.15	0.36	0.67	0.51
	GPT-4	Node	0.99	0.98	0.94	0.95	0.81	0.96	0.88	0.66	0.96	1.00	0.84	0.85	0.91	0.86
		Edge	0.99	0.97	0.99	0.88	0.72	0.97	0.76	0.44	0.99	0.98	0.65	0.84	0.85	0.78
Medium	GPT-3	Node	1.00	0.87	0.67	0.81	0.40	0.75	0.78	0.38	0.88	1.00	0.17	0.48	0.67	0.52
		Edge	0.99	0.84	0.80	0.79	0.30	0.90	0.78	0.32	0.97	1.00	0.18	0.42	0.65	0.48
	GPT-4	Node	1.00	0.94	0.95	0.86	0.55	0.94	0.74	0.50	0.82	1.00	0.70	0.67	0.82	0.72
		Edge	0.98	0.88	0.96	0.79	0.43	0.92	0.70	0.38	0.91	1.00	0.53	0.75	0.78	0.66
Hard	GPT-3	Node	0.98	0.81	0.53	0.65	0.25	0.71	0.80	0.26	0.77	1.00	0.10	0.55	0.64	0.47
		Edge	0.93	0.75	0.74	0.64	0.19	0.86	0.84	0.16	0.89	0.98	0.18	0.57	0.65	0.45
	GPT-4	Node	0.96	0.88	0.91	0.81	0.44	0.81	0.68	0.36	0.76	0.98	0.70	0.53	0.77	0.64
		Edge	0.96	0.80	0.93	0.85	0.40	0.83	0.76	0.38	0.82	0.98	0.41	0.59	0.74	0.58

the connective prediction and the path prediction are accurate. The range of F_{acc} is $[0, 1]$, where a higher score indicates greater consistency with the ground truth. A high accuracy with a low F_{acc} score suggests that the reasoning paths cannot well support connectivity predictions, which could indicate that LLMs are hallucinating.

Multiple reachable paths exist within a graph. LLMs demonstrate superior reasoning abilities if they can identify a shorter path. To assess the paths LLMs select for reasoning, we introduce the Path Consistency Ratio (PCR): $\mathrm{PCR} = \frac{1}{M}\sum_{i=1}^{M}\frac{|p_i|}{|\hat{p}_i|}$, $|\hat{p}_i|$ represents the number of nodes in the path, while $|p_i|$ denotes the number of nodes in the shortest path. We evaluate PCR only when the LLMs give the correct path. A higher score indicates that the LLMs are more adept at selecting the shortest path between two nodes.

4.4 Results

We select three representative large language models, GPT-3 (GPT-3.5-turbo-0301), GPT-4 (GPT-4-0125-preview) and LLAMA 3 (LLAMA3.0-70B).

Undirected Graph Results We start with the undirected graph datasets and show the results in Table 2. First of all, GPT-4 has better reasoning ability compared with GPT-3 and LLAMA 3 across all cases, regardless of the graph difficulty, graph description or the categories of connectivity.

Secondly, we have following observations by comparing different connectivity situations: (1) The difficulty of reasoning increases as the path length extends (i.e., K-hop), peaking in the isolated component (where K can be viewed as infinite). As a result, both ACC and F_{acc} exhibit a corresponding decline. (2) The value of PCR is stable and almost larger than 0.9 via GPT-4, indicating a tendency of GPT-4 to find some shorter paths when judging the connectivity. (3) The Singleton scene is particular because it is not affected by the difficulty changes and always performs well. This suggests that LLMs may have a shortcut in graph understanding: nodes not mentioned in the graph description are considered isolated and no connection with others. (4) Node Lists generally perform better than Edge Lists in most cases. This is because the search space differs when various description methods are used to search nodes within the next-token prediction framework. For the Node Lists, it is easy to find all the positions of neighbor nodes, which costs $\mathcal{O}(|N|)$. However, it takes $\mathcal{O}(|E|)$ for Edge Lists. Therefore, the overall algorithmic complexity is different, where the Node Lists should be $\mathcal{O}(|N|^2)$ while the Edge Lists should be $\mathcal{O}(|N||E|)$.

Interestingly, LLMs demonstrate enhanced performance with node descriptions when k is larger, e.g., 5-hops, while they perform better in the isolated component scene when provided with edge descriptions. This suggests that LLMs may not consistently apply the same strategy for analyzing graph connectivity. Instead, the approach adopted by LLMs is shaped by the input context provided.

Directed Graph Results Next, we evaluate the connectivity on the directed graphs shown in Table 3. Some key observations are similar to those of undirected graph datasets. However, LLMs have lower performance on directed graphs across almost all sub-datasets, yet they maintain high performance on subsets with k≤2 and Singleton subsets.

We also note distinct performance differences between GPT-3 and GPT-4 on the Asymmetric dataset. GPT-3's accuracy increased from 0.4 to 0.55, whereas GPT-4's decreased from 0.8 to 0.55. Given that an accuracy of 0.55 is nearly equivalent to random guessing in a binary task for asymmetric detection, it suggests that LLMs might engage in random reasoning within the Hard dataset. Furthermore, descriptions using Node Lists outperform those using Edge Lists. Since an Edge List simply describes two nodes in one sentence, LLMs may meet hallucination in determining whether

Table 4: Results on the shortest path problem

Dataset Subdataset	Des.	undirected graphs unweighted	undirected graphs weighted	directed graphs unweighted	directed graphs weighted
1≤k≤2 hops	Node	0.88	0.80	0.93	0.76
	Edge	0.89	0.70	0.91	0.71
3≤k≤4 hops	Node	0.87	0.52	0.64	0.45
	Edge	0.81	0.47	0.51	0.38
5-hops	Node	0.88	0.54	0.48	0.40
	Edge	0.76	0.44	0.42	0.26
Singleton	Node	1.00	0.98	0.98	0.96
	Edge	0.98	0.98	0.94	0.96
Isolated C.	Node	0.46	0.47	0.63	0.67
	Edge	0.61	0.51	0.52	0.69
Asymmetric	Node	-	-	0.59	0.62
	Edge	-	-	0.65	0.66
AVG	Node	0.72	0.60	0.70	0.64
	Edge	0.76	0.58	0.65	0.61

the relationship "A is B" is equivalent to "B is A" (Berglund et al., 2023).

4.5 The shortest-path problem

The shortest-path problem is another essential task theoretically proven to be achievable by LLMs, yet it fails in practice. Compared to the graph connectivity task, it is more challenging because it requires not only determining whether nodes are connected but also calculating edge weights to identify the shortest path among multiple potential solutions. Next, we explore if the varied performance of LLMs across different connectivity types is also applicable to the shortest-path problem. The details of experiment settings are in Appendix D.1.

We use GPT-4 to illustrate an example of the shortest-path problem. Table 4 displays the results of LLMs' performance. The findings for the shortest path problem align with our observations from graph connectivity, where performance diminishes as the path length (k-hop) increases. Moreover, undirected graphs consistently outperform directed graphs. We observe a significant difference in LLM performance between datasets with weighted edges and those without. This suggests that LLMs might overlook or misrepresent edge weights in the text.

4.6 Entity connection on the knowledge graph

To determine whether our findings can apply to real-world applications, we performed the entity connection on the knowledge graph using WN18RR (Shang et al., 2019) dataset. The details of dataset construction are provided in Appendix A.

We use GPT-4 to evaluate the connections, and summarize the results in Table 5. The performance trends align with Section 4.4 and Section 4.5. Specifically, the performance declines with K increasing in the K-hop setting, and Node List descriptions outperform Edge List descriptions. Notably, LLMs demonstrate improved performance with meaningful node naming. Furthermore, incorporating BFS into the prompt results in significant improvements. Detailed analyses are provided in Appendix D.3.2 and Appendix D.3.1.

5 Other factors for graph reasoning

5.1 Impact of training data and model scale

To explore the impact of training data and model scale on LLMs' graph reasoning, we train GPT-2 from scratch to perform k-hop reasoning. Specifically, we use the Medium (M), Small (S), and Baby (B) versions, as statistics are outlined in Table 15. We create a new dataset different from the previous sections, focusing on K-hop connections within directed graphs consisting of 5 to 15 nodes. The training dataset contains 210,000 unique question-answer pairs, with 20,000 reserved for validation and 10,000 for testing.

We focus on 3-hop and 5-hop connections, requiring GPT-2 to solve the shortest path problem using simplified graph descriptions. An example is shown in Table 14. Additional training details are provided in Appendix G.1.

To analyze the effect of the training data scale, we vary the amount of training data from 1,000 to 180,000 and report the test loss on the test set. Besides, we also evaluate various versions of GPT-2 and different graph descriptions. The results are shown in Figure 4 and Figure 5.

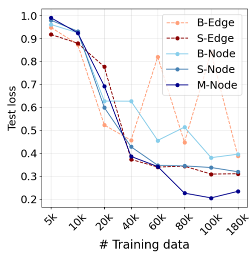

Figure 4: 3-hop results

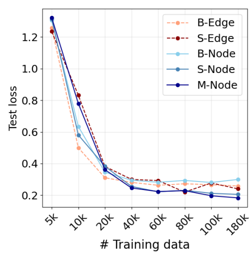

Figure 5: 5-hop results

We observe that the reasoning ability of LLMs is strongly correlated with both the scale of the training data and the models, regardless of using Node List or Edge List. The test loss decreases significantly for both 3-hop and 5-hop reasoning tasks, demonstrating that GPT-2 architectures can perform reasoning tasks with sufficient model size and training data. The final test accuracy achieved about 80%. Moreover, Node List is more stable than Edge List, likely because the Edge List contains longer sentences (up to 400 characters) compared to the Node List (up to 200 characters). This increased length may hinder the transformer's ability to process the long context (Tay et al., 2020).

Table 5: Entity connection on the knowledge graph

Node Naming	Des.		1-hop	2-hop	3-hop	4-hop	k-hop, k>5	Asymmetric	AVG. scores
ID names	Edge	ACC	1.0000	1.0000	0.9808	0.7805	0.6538	0.1750	0.7166
		F_{acc}	0.6400	0.6489	0.4808	0.1220	0.0000	0.1750	0.3810
	Node	ACC	1.0000	0.9892	0.8868	0.6429	0.5167	0.3216	0.7369
		F_{acc}	0.7664	0.7849	0.4906	0.2143	0.0000	0.3126	0.4981
Entity names	Edge	ACC	1.0000	1.0000	1.0000	0.9524	0.9153	0.0754	0.7258
		F_{acc}	0.9700	0.8085	0.5283	0.3333	0.0508	0.0754	0.4685
	Node	ACC	1.0000	0.9681	0.9811	0.9048	0.8167	0.2374	0.7717
		F_{acc}	0.9907	0.8298	0.5472	0.2857	0.0333	0.2374	0.5416
Entity names + BFS COT	Edge	ACC	1.0000	0.9894	0.9811	0.9048	0.9500	0.1717	0.7637
		F_{acc}	0.9907	0.8404	0.5660	0.2619	0.0333	0.1717	0.5147
	Node	ACC	1.0000	1.0000	0.9245	0.8571	0.8333	0.4343	0.8521
		F_{acc}	0.9813	0.8830	0.5660	0.3333	0.0333	0.4343	0.6380

Additionally, we evaluate the impact of data on fine-tuning. We use Llama3.2-3B as the backbone model, apply LoRA for fine-tuning to enhance shortest-path reasoning, and demonstrate a similar effect with increasing the training data. The whole details are shown in Appendix G.2.

5.2 Different reasoning processes in Node List and Edge List

To gain deeper insights into how the LLM performs reasoning on a graph, we drew inspiration from syntax analysis in language models (Jawahar et al., 2019) to the reasoning tasks. Specifically, we applied t-SNE clustering to the outputs of various attention layers in a small-scale GPT-2 model at different reasoning steps. We define special labels for the nodes in the sentence. The details are illustrated in Appendix H. To analyze the reasoning process, we selected 200 correct samples from the test set. The results are presented in Figure 6. The Appendix Figure 10 and Figure 11 provides more comprehensive results.

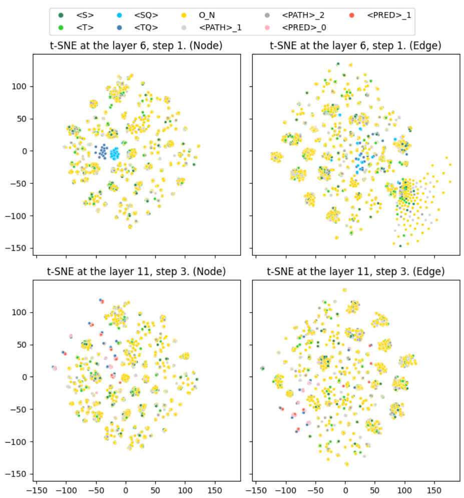

Figure 6: t-SNE results on the different layers and steps

The observations can be summarized as follows: (1) GPT-2 learns the node combination patterns in both Node and Edge Lists. In the final layer, the model reorganizes these combinations to identify the source (light blue), target (deep blue), and predicted nodes (red). The observed pattern combination phenomenon suggests that, rather than directly extracting path information from the given sentences, the GPT model relies on learned relationships among different nodes. This reliance also explains the accuracy drop in the connectivity task when node IDs are replaced with random numbers or characters, as such disruptions interfere with the model's learned combinations. (2) GPT-2 exhibits different reasoning processes when using Node List and Edge List as graph descriptions. With the Node List, GPT-2 easily captures the source and target nodes in the middle layers, subsequently identifying path patterns based on the source and target in the question. In contrast, when using the Edge List, the model tends to skip this intermediate step, instead directly matching the source and target nodes to its learned node combination patterns.

6 Conclusion

In this paper, we focus on the graph reasoning ability of LLMs. Recently, there exists a discrepancy between theoretical potential and poor empirical performance. To bridge this gap, we construct a balanced and comprehensive benchmarking, and conclude that graph reasoning ability is influenced by various node connectivity types, graph sizes, graph descriptions, and node naming methods. Moreover, we also demonstrate the impacts of training data, model size and fine-tuning on graph reasoning ability. These findings offer valuable insights to enhance LLMs in graph reasoning tasks.

Limitation: Our computational resources are limited, which poses challenges in fully exploring the upper bounds of training or fine-tuning LLMs for graph reasoning tasks.

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A Example of different descriptions

Here we list the examples of descriptions utilized in the experiment. Examples are listed as node descriptions and edge descriptions on directed or undirected graphs, with or without weights on edges.

Node Description for Undirected Graph:

Edge Description for Undirected Graph:

G describes an undirected graph among node 0, 1, 2, 3, and 4.
Node 0 is connected to Node 1.
Node 1 is connected to Node 2.
Node 1 is connected to Node 3.
Node 2 is connected to Node 3.
Node 3 is connected to Node 4.

Node Description for Directed Graph:

G describes a directed graph among 0, 1, 2, 3, and 4.
In this graph:
Node 0 is directed to Node 1.
Node 1 is directed to Node 2, 3.
Node 2 is directed to Node 3.
Node 3 is directed to Node 4.

Edge Description for Directed Graph:

G describes a directed graph among node 0, 1, 2, 3, and 4.
Node 0 is directed to Node 1.
Node 1 is directed to Node 2.
Node 1 is directed to Node 3.
Node 2 is directed to Node 3.
Node 3 is directed to Node 4.

Node Description for Undirected Weighted Graph:

G describes an undirected graph among 0, 1, 2, 3, and 4.
In this graph:
Node 0 is connected to nodes 1 (weight: 8), 2 (weight: 1).
Node 1 is connected to node 0 (weight: 8).
Node 2 is connected to node 0 (weight: 1).

Edge Description for Undirected weighted Graph:

G describes an undirected graph among node 0, 1, 2, 3, and 4.
Node 0 is connected to Node 1 with weight 8.
Node 0 is connected to Node 2 with weight 1.

Directivity	Model	Difficulty	Des.	1-hop	2-hop	3-hop	4-hop	5-hop	6-hop	Singleton	Isolated C.	Asymmetric	k-hop k>6
Dataset				GraphInstruct									
Undirected	GPT-4	Tiny	Node	1.00	1.00	1.00	0.83	1.00	-	-	0.60	-	-
			Edge	1.00	1.00	1.00	0.83	1.00	-	-	0.60	-	-
		Easy	Node	1.00	1.00	1.00	1.00	1.00	1.00	-	0.35	-	1.00
			Edge	1.00	1.00	1.00	1.00	0.67	1.00	-	0.41	-	1.00
		Med	Node	1.00	1.00	1.00	1.00	1.00	1.00	-	0.12	-	1.00
			Edge	1.00	1.00	1.00	1.00	1.00	1.00	-	0.71	-	0.67
		Hard	Node	1.00	1.00	1.00	1.00	1.00	-	-	0.04	-	0.75
			Edge	1.00	1.00	1.00	1.00	1.00	-	-	0.36	-	0.50
	GPT-3	Tiny	Node	1.00	0.88	0.36	0.00	0.00	-	-	0.00	-	-
			Edge	1.00	0.79	0.18	0.33	0.00	-	-	0.40	-	-
		Easy	Node	0.98	0.91	0.92	0.64	0.67	1.00	-	0.56	-	1.00
			Edge	1.00	0.91	0.75	0.45	0.33	1.00	-	0.50	-	0.00
		Med	Node	1.00	0.98	0.84	0.67	1.00	0.00	-	0.67	-	0.00
			Edge	0.97	0.96	0.63	1.00	1.00	0.50	-	0.42	-	0.00
		Hard	Node	1.00	0.98	0.85	0.80	0.50	-	-	0.36	-	1.00
			Edge	1.00	0.96	0.90	0.60	1.00	-	-	0.30	-	0.75
Directed	GPT-4	Tiny	Node	1.00	0.92	0.14	-	-	-	-	1.00	0.95	-
			Edge	1.00	0.85	0.43	-	-	-	-	1.00	0.97	-
		Easy	Node	1.00	0.93	1.00	0.67	-	-	-	-	0.91	-
			Edge	1.00	0.64	0.83	0.33	-	-	-	-	0.91	-
		Med	Node	0.78	0.71	0.60	1.00	1.00	-	-	-	0.82	-
			Edge	0.89	0.71	1.00	0.50	1.00	-	-	-	0.78	-
		Hard	Node	0.90	0.88	0.60	1.00	1.00	1.00	-	-	0.77	-
			Edge	1.00	0.88	0.60	1.00	1.00	1.00	-	-	0.83	-
	GPT-3	Tiny	Node	0.94	0.92	1.00	-	-	-	-	1.00	0.26	-
			Edge	1.00	1.00	0.71	-	-	-	-	1.00	0.27	-
		Easy	Node	0.77	0.93	0.83	1.00	-	-	-	-	0.19	-
			Edge	1.00	0.93	0.83	1.00	-	-	-	-	0.31	-
		Med	Node	1.00	1.00	1.00	0.50	1.00	-	-	-	0.33	-
			Edge	1.00	0.79	0.80	1.00	1.00	-	-	-	0.42	-
		Hard	Node	1.00	0.88	1.00	0.00	1.00	1.00	-	-	0.22	-
			Edge	1.00	0.88	0.90	0.00	0.50	1.00	-	-	0.37	-

Table 6: Baseline result of zero-shot accuracy on GraphInstruct dataset.

Difficulty	Model	Des.	k-hop, $1\leq k\leq 2$			k-hop, $3\leq k\leq 4$			5-hop			Singleton	Isolated C.	AVG. ACC	AVG. F_{acc}
			ACC	F_{acc}	PCR	ACC	F_{acc}	PCR	ACC	F_{acc}	PCR	F_{acc}	F_{acc}		
Tiny	GPT-3	Node	1.00	0.99	0.90	0.82	0.82	0.95	1.00	1.00	1.00	-	0.00	0.93	0.92
		Edge	1.00	0.96	0.87	0.65	0.65	0.96	1.00	1.00	1.00	-	0.00	0.91	0.87
	GPT-4	Node	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	-	0.80	0.99	0.99
		Edge	1.00	0.98	0.99	1.00	1.00	1.00	1.00	1.00	1.00	-	0.80	0.99	0.97
Easy	GPT-3	Node	1.00	0.97	0.85	1.00	0.91	0.95	1.00	1.00	0.94	-	0.09	0.79	0.75
		Edge	1.00	0.93	0.80	0.87	0.61	0.82	1.00	0.67	0.77	-	0.00	0.75	0.66
	GPT-4	Node	1.00	0.97	0.99	1.00	1.00	1.00	1.00	1.00	1.00	-	0.68	0.92	0.90
		Edge	1.00	0.98	0.99	1.00	1.00	0.99	1.00	1.00	0.94	-	0.74	0.94	0.92
Medium	GPT-3	Node	0.99	0.98	0.69	1.00	1.00	0.90	1.00	0.00	0.00	-	0.00	0.68	0.66
		Edge	0.99	0.86	0.72	0.96	0.68	0.88	1.00	0.50	1.00	-	0.02	0.68	0.57
	GPT-4	Node	1.00	0.92	0.98	1.00	0.80	0.99	1.00	1.00	1.00	-	0.56	0.86	0.79
		Edge	1.00	0.98	0.96	1.00	0.88	0.98	1.00	1.00	1.00	-	0.77	0.93	0.90
Hard	GPT-3	Node	1.00	0.94	0.63	1.00	0.76	0.85	1.00	0.00	0.00	-	0.10	0.71	0.63
		Edge	1.00	0.78	0.56	1.00	0.56	0.81	1.00	0.00	0.00	-	0.08	0.70	0.51
	GPT-4	Node	1.00	0.87	0.94	1.00	1.00	0.93	1.00	0.50	0.71	-	0.34	0.79	0.72
		Edge	1.00	0.87	0.90	1.00	0.96	0.93	1.00	1.00	1.00	-	0.62	0.88	0.81

Table 7: Undirected Baseline result of ACC and F_{acc}.

Difficulty	Model	Des.	k-hop, $1\leq k\leq 2$			k-hop, $3\leq k\leq 4$			5-hop			Singleton	Isolated C.	Asymmetric	AVG. ACC	AVG. F_{acc}
			ACC	F_{acc}	PCR	ACC	F_{acc}	PCR	ACC	F_{acc}	PCR	F_{acc}	F_{acc}	F_{acc}		
Tiny	GPT-3	Node	1.00	0.05	0.62	1.00	0.00	0.00	-	-	-	-	-	0.06	0.20	0.06
		Edge	1.00	0.94	0.99	1.00	0.71	0.95	-	-	-	-	1.00	0.04	0.25	0.22
	GPT-4	Node	1.00	1.00	0.96	1.00	0.86	1.00	-	-	-	-	1.00	0.88	0.90	0.90
		Edge	1.00	1.00	1.00	1.00	1.00	1.00	-	-	-	-	1.00	0.85	0.88	0.88
Easy	GPT-3	Node	1.00	0.00	0.00	1.00	0.00	0.00	-	-	-	-	-	0.04	0.17	0.03
		Edge	0.96	0.89	0.93	1.00	0.78	0.83	-	-	-	-	-	0.07	0.28	0.26
	GPT-4	Node	1.00	0.96	1.00	1.00	0.89	1.00	-	-	-	-	-	0.87	0.90	0.89
		Edge	1.00	1.00	0.95	1.00	0.67	0.95	-	-	-	-	-	0.81	0.86	0.84
Medium	GPT-3	Node	1.00	0.00	0.00	-	-	-	-	-	-	-	-	0.08	0.19	0.07
		Edge	1.00	0.70	0.88	1.00	0.29	0.51	1.00	0.00	0.00	-	-	0.10	0.32	0.22
	GPT-4	Node	0.96	0.83	0.87	1.00	0.43	1.00	1.00	0.00	0.00	-	-	0.67	0.74	0.68
		Edge	1.00	0.87	0.91	1.00	0.57	0.97	1.00	0.00	0.00	-	-	0.67	0.75	0.70
Hard	GPT-3	Node	1.00	0.00	0.00	1.00	0.00	0.00	-	-	-	-	-	0.17	0.32	0.14
		Edge	1.00	0.70	0.74	1.00	0.36	0.85	1.00	0.50	1.00	-	-	0.12	0.37	0.26
	GPT-4	Node	1.00	0.74	0.93	0.91	0.45	0.82	1.00	0.00	0.00	-	-	0.59	0.70	0.60
		Edge	1.00	0.81	0.95	1.00	0.73	0.87	1.00	0.50	0.83	-	-	0.67	0.76	0.70

Table 8: Directed Baseline result of ACC and F_{acc}. '-' indicates no data.

	Subdataset	Des.	0-shot	few-shot	0-dijkstra	cot-dijkstra
unweighted	1≤k≤2 hops	Node	0.88	0.91	0.92	0.96
		Edge	0.89	0.82	0.87	0.96
	3≤k≤4 hops	Node	0.87	0.90	0.87	0.94
		Edge	0.81	0.86	0.83	0.85
	5-hops	Node	0.88	0.78	0.78	0.86
		Edge	0.76	0.68	0.74	0.82
	Singleton	Node	1.00	1.00	0.86	1.00
		Edge	0.98	1.00	0.84	0.96
	I.C.	Node	0.46	0.52	0.58	0.70
		Edge	0.61	0.37	0.64	0.74
	AVG	Node	0.72	0.75	0.75	0.84
		Edge	0.76	0.65	0.75	0.81
Weighted	1≤k≤2 hops	Node	0.80	0.75	0.75	0.81
		Edge	0.70	0.66	0.65	0.73
	3≤k≤4 hops	Node	0.52	0.58	0.59	0.65
		Edge	0.47	0.47	0.48	0.64
	5-hops	Node	0.54	0.48	0.54	0.58
		Edge	0.44	0.52	0.44	0.50
	Singleton	Node	0.98	0.92	0.80	0.84
		Edge	0.98	1.00	0.76	0.98
	I.C.	Node	0.47	0.39	0.35	0.53
		Edge	0.51	0.32	0.46	0.57
	AVG	Node	0.60	0.56	0.54	0.65
		Edge	0.58	0.51	0.53	0.65

Table 9: Shortest path result with strategy

Connectivity types	# Sample	AVG. # Node	AVG. # Edge
1-hop	107	82	199
2-hop	64	104	257
3-hop	53	139	347
4-hop	42	145	363
k-hop (k≥5)	60	201	521
Asymmetric	198	49	106

Table 10: Knowledge graph dataset.

Node Description for Directed weighted Graph:

G describes a directed graph among node 0, 1, 2, 3, and 4.
In this graph:
Node 0 is directed to Node 1 (weight: 8), 2 (weight: 1).

Edge Description for Directed weighted Graph:

G describes a directed graph among node 0, 1, 2, 3, and 4.
Node 0 is directed to Node 1 with weight 8.
Node 0 is directed to Node 2 with weight 1.

Knowledge graph Node:

G describes a knowledge graph among entity: "hairpiece", "wig", "dress", "overdress", "attire", "clothing", and "clothing".

Entity "hairpiece" is directed to entity "attire" (relation hypernym).

Entity "wig" is directed to entity "hairpiece" (relation hypernym).

Entity "dress" is directed to entity "attire" (relation derivationally related form), "dress" (relation verb group), "overdress" (relation also see), and "clothing" (derivationally related form) .

Entity "overdress" is directed to entity "attire" (relation derivationally related form), "dress" (relation verb group).

Entity "attire" is directed to entity "overdress" (relation derivationally related form), "clothing" (relation hypernym), "dress" (derivationally related form).

Entity "clothing" is directed to entity "dress" (relation derivationally related form).

Knowledge graph Edge:

G describes a knowledge graph among entity: "hairpiece", "wig", "dress", "overdress", "attire", "clothing", and "clothing". Entity "hairpiece" is hypernym of entity "attire".

Entity "wig" is hypernym of entity "hairpiece".

Entity "dress" is derivationally related form of entity "attire".

Entity "dress" is verb group of entity "dress".

Entity "dress" is also see of entity "overdress".

Entity "dress" is derivationally related form of entity "clothing".

Entity "overdress" is derivationally related form of entity "attire".

Entity "overdress" is verb group of entity "dress".

Entity "attire" is derivationally related form of entity "overdress".

Entity "attire" is hypernym of entity "clothing".

Entity "attire" is derivationally related form of entity "dress".

Entity "clothing" is derivationally related form of entity "dress".

B Few-shot and CoT examples

Here are examples of how to use few-shot and CoT prompting in graph connectivity and shortest path tasks.

B.1 Connectivity examples

Few-shot:

Q: Given a directed graph: G describes a directed graph among 0, 1, 2, 3, and 4.
In this graph:
Node 0 is directed to nodes 1, 3.
Node 1 is directed to nodes 2, 0, 4.
Node 2 is directed to nodes 3.
Node 3 is directed to nodes 4, 0, 1.
Is there a directed path from node 0 to node 3 If the path exist, give "Exist path" the path in the form of "Node #1 -> Node #2". Otherwise, give "No path"
A: Exist path: 0 -> 3.

BFS-CoT:

Q: Determine if there is a path between two nodes in the graph. The graph is: G describes an undirected graph among 0, 1, 2, 3, 4, and 5. In this graph: Node 0 is connected to node 1. Node 1 is connected to nodes 0, 2. Node 2 is connected to nodes 1, 3. Node 3 is connected to nodes 2, 4. Node 4 is connected to nodes 3, 5. Node 5 is connected to node 4. The question is: Does a path

		1-hop	2-hop	3-hop	4-hop	5-hop	Singleton	Isolated C.	Asymmetric
	Dataset	GraphInstruct Dataset (Tiny/Easy/Med/Hard)							
Undirected	# Sample	51 / 41 / 37 / 29	43 / 45 / 50 / 49	11 / 12 / 19 / 20	6 / 11 / 6 / 5	1 / 3 / 2 / 2	- / - / - / -	5 / 34 / 52 / 50	-
	AVG. # Node	6 / 12 / 21 / 30	6 / 12 / 21 / 30	6 / 12 / 20 / 31	6 / 11 / 22 / 31	7 / 14 / 20 / 28	- / - / - / -	7 / 12 / 20 / 31	-
	AVG. # Edge	8 / 24 / 77 / 181	7 / 22 / 68 / 125	5 / 14 / 37 / 62	6 / 10 / 33 / 49	7 / 14 / 20 / 28	- / - / - / -	7 / 12 / 20 / 31	-
Directed	# Sample	18 / 13 / 9 / 10	13 / 14 / 14 / 17	7 / 6 / 5 / 10	- / 3 / 2 / 1	- / - / 1 / 2	- / - / - / -	1 / - / - / -	144 / 116 / 98 / 100
	AVG. # Node	6 / 12 / 21 / 30	6 / 12 / 21 / 31	7 / 12 / 20 / 29	- / 15 / 20 / 31	- / - / 19 / 32	- / - / - / -	6 / - / - / -	6 / 11 / 21 / 31
	AVG. # Edge	15 / 44 / 117 / 194	15 / 38 / 123 / 220	14 / 30 / 80 / 140	- / 28 / 50 / 56	- / - / 47 / 70	- / - / - / -	4 / - / - / -	10 / 24 / 45 / 73
	Dataset	NLGraph Dataset (Easy/Med/Hard)							
Undirected	# Sample	137 / 417 / 163	36 / 146 / 152	3 / 30 / 21	- / 5 / 4	- / 2 / -	51 / 106 / 42	125 / 494 / 298	-
	AVG. # Node	7 / 19 / 31	8 / 19 / 31	9 / 19 / 30	- / 17 / 32	- / 20 / -	7 / 17 / 31	7 / 19 / 31	-
	AVG. # Edge	11 / 78 / 138	8 / 47 / 103	7 / 26 / 56	- / 24 / 44	- / 20 / -	7 / 49 / 127	11 / 71 / 103	-
	Dataset	Our Dataset with Unweighted Edge Graphs (Easy/Med/Hard)							
Undirected	# Sample	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	200 / 200 / 200	-
	AVG. # Node	10 / 21 / 30	10 / 21 / 31	11 / 21 / 30	11 / 20 / 31	11 / 20 / 30	11 / 20 / 31	11 / 21 / 31	-
	AVG. # Edge	32 / 104 / 229	33 / 112 / 215	26 / 83 / 158	21 / 51 / 146	17 / 43 / 90	35 / 93 / 198	20 / 60 / 113	-
Directed	# Sample	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	100 / 100 / 100	100 / 100 / 100
	AVG. # Node	10 / 20 / 30	10 / 20 / 31	10 / 20 / 31	10 / 20 / 31	11 / 20 / 30	10 / 21 / 31	11 / 21 / 31	11 / 21 / 31
	AVG. # Edge	64 / 191 / 514	57 / 191 / 479	49 / 170 / 409	38 / 131 / 251	32 / 89 / 185	45 / 162 / 466	35 / 102 / 188	57 / 120 / 279
	Dataset	Our Dataset Wtih Positive Weighted Edge Graphs (Easy/Med/Hard)							
Undirected	# Sample	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	200 / 200 / 200	-
	AVG. # Node	10 / 20 / 30	10 / 20 / 30	10 / 20 / 30	11 / 20 / 30	11 / 20 / 30	11 / 20 / 30	11 / 20 / 30	-
	AVG. # Edge	32 / 104 / 231	33 / 109 / 221	26 / 81 / 192	21 / 54 / 119	19 / 42 / 96	30 / 91 / 233	18 / 56 / 115	-
Directed	# Sample	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	50 / 50 / 50	100 / 100 / 100	100 / 100 / 100
	AVG. # Node	10 / 20 / 30	10 / 20 / 30	10 / 20 / 30	10 / 20 / 30	11 / 20 / 30	10 / 20 / 30	10 / 20 / 30	10 / 20 / 30
	AVG. # Edge	55 / 184 / 386	55 / 205 / 503	49 / 173 / 356	36 / 97 / 222	31 / 99 / 177	46 / 192 / 437	32 / 91 / 194	47 / 121 / 250
	Dataset	Ours Dataset with Directed Negative Weighted Edge Graphs (Easy)							
Directed	# Sample	50	50	50	50	50	50	100	100
	AVG. # Node	10	10	10	10	10	10	10	10
	AVG. # Edge	30	30	28	27	25	22	20	26

Table 11: The summary table of datasets used in the connectivity task including the baseline dataset NLGraph and GraphInstruct. Our dataset is generated for various types of node connections

exist between node 1 and node 5? If a path exists, present the BFS path formatted as "Node #1 -> Node #2." If no path is found, state "No path." This problem will be addressed using Breadth-First Search (BFS). Let's think step by step. A: 1. Node 1 is directely connected with nodes 0, 2. 2. From node 0, we can reach nodes 1. 3. From node 2, we can reach nodes 1, 3. 4. From node 3, we can reach nodes 2, 4. 5. From node 4, we can reach nodes 3, 5. 6. From node 5, we have reached our target. So a path from node 1 to node 5 does exist. The BFS path taken in this search is: Node 1 -> Node 2 -> Node 3 -> Node 4 -> Node 5.

Dijkstra-CoT:

Q: Given a directed graph: G describes a directed graph among 0, 1, 2, 3, and 4.
In this graph:
Node 0 is directed to nodes 1 (weight: 6), 4 (weight: 6), 3 (weight: 6), 2 (weight: 1).
Node 1 is directed to nodes 2 (weight: 4), 4 (weight: 3).
Node 2 is directed to nodes 3 (weight: 7), 1 (weight: 4), 0 (weight: 5).
Node 3 is directed to nodes 4 (weight: 6), 0 (weight: 6).
Node 4 is directed to nodes 1 (weight: 6), 3 (weight: 9), 0 (weight: 5).
Does a path exist from node 4 to node 2? If so, provide the shortest path formatted as "Node #1 -> Node #2." If not, state "No path.". Let's think step by step using Dijkstra's Algorithm.
A: To determine if there is a path from node 4 to node 2 and find the shortest path if it exists, we can use Dijkstra's Algorithm. Let's apply the algorithm step by step:

Initialization
- Start with node 4.
- Set the distance to node 4 (the starting node) to 0 and to all other nodes to infinity.
- Keep a priority queue to select the node with the smallest tentative distance that hasn't been permanently set yet.
- Mark all nodes as unvisited.

Step by Step Process
1. Select node 4 (smallest distance in the priority queue). From node 4, we can reach nodes 1, 3 and 0. We update the distances to nodes 1, 3 and 0.
- Distance to node 1 (from node 4) is 6, which is better than the previous, update the priority queue.
- Distance to node 3 (from node 4) is 9, which is better than the previous, update the priority queue.
- Distance to node 0 (from node 4) is 5, which is better than the previous, update the priority queue.

2. Select node 0 (next smallest distance in the priority queue). From node 0, we can reach nodes 1, 4, 3 and 2. However, nod and 4 has already been selected. We update the distances to nodes 1, 3 and 2.
- Distance to node 1 (from node 0) is 11, which is not better than the previous, and will not update the priority queue.
- Distance to node 3 (from node 0) is 11, which is not better than the previous, and will not update the priority queue.
- Distance to node 2 (from node 0) is 6, which is better than the previous, update the priority queue.

3. Select node 1 (next smallest distance in the priority queue). From node 1, we can reach nodes 2 and 4. However, node 4 has already been selected. We update the distance to node 2.

- Distance to node 2 (from node 1) is 10, which is not better than the previous, and will not update the priority queue.

4. Select node 2 (next smallest distance in the priority queue). From node 2, we can reach nodes 3, 1 and 0. However, nodes 1 and 0 have already been selected. We update the distance to node 3.
- Distance to node 3 (from node 2) is 13, which is not better than the previous, and will not update the priority queue.

5. Select node 3 (next smallest distance in the priority queue). From node 3, we can reach nodes 4 and 0. However, nodes 4 and 0 have already been selected. We have nothing to update.

Conclusion
A path exists from node 4 to node 2.
Answer: Node 4 -> Node 0 -> Node 2.

C Graph Connectivity task

C.1 Dataset

Table 11 shows the dataset information for all datasets we used. We separated the dataset according to the connectivity type to ensure clear display of whether or not the dataset is uniformly distributed. The table helps illustrate that our dataset aims to balance the distribution on connectivity type as uniform as possible (with 50 samples for most types), as well as the balance of positive and negative cases (250 samples for both connective and non-connective cases).

C.2 Results

Table 6 shows the zero-shot accuracy result of baseline datasets. The result is separated by connectivity type in columns. However, due to the variability of distribution, significant numbers of grids remain empty. Table 7 and Table 8 are novel evaluations of undirected and directed baseline datasets with ACC and F_{acc}.

D Shortest-path task

D.1 Experimental setup

We study the shortest-path problem using the Easy datasets from the unweighted graphs as mentioned in Section 4. For the weighted graphs, we applied similar strategies that were used in undirected graph generations to generate the directed and undirected graph datasets. The directed graph datasets include two types, whether there are negative edges in the graphs. Appendix C.1 Table 11 shows the details. The graph structure descriptions are shown in Appendix A

D.2 Result

Table 9 records the shortest path accuracy on various prompting methods. Weighted graph in this table only have positive weights.

D.3 Analysis of other factors

D.3.1 Impact of the algorithm prompts

In-context learning approaches, including Chain-of-Thought (CoT) (Wei et al., 2022) and zero-Chain-of-Thought (0-CoT) (Kojima et al., 2022), have been widely utilized in LLMs to enhance their reasoning capabilities. Meanwhile, specifically in graph-related tasks, previous works combined the prompts with the graph algorithms. However, they do not demonstrate consistent improvement (Wang et al., 2024a). In this subsection, we revisit these approaches in detail.

We consider several graph algorithms in the experiments. For the graph connectivity task, we focus on the Breadth-First Search (BFS) and we employ the Dijkstra algorithms to soleve the shortest path problem. We utilize Node descriptions to search the connectivity and shortest pathes in Easy setting by GPT-4. The prompts examples are shown in Appendix B. The results are detailed in Table 12.

The observations can be summarized as follows: (1) In the connectivity task, few-shot examples help LLMs recognize isolated components. This is because few-shot examples enable the LLMs to correctly output 'No connection' when they do not find a connected path. (2) In the shortest path cases, few-shot examples do not consistently lead to better performance. However, performance improves when the Dijkstra-CoT method is applied. This suggests that while LLMs may use multiple strategies to make decisions, but a specific algorithm can guide them toward a unique solution.

D.3.2 The influence of node names

Fatemi et al. (2023) suggest that different naming methods for graphs can yield varied results. This variation is attributed to the graph node IDs occupying the same space as the pre-trained data of LLMs. Thus, we further evaluated the impact of naming conventions on nodes for the connectivity task. Table 13 summarizes the results for GPT-4 on the Easy subset of the undirected graph dataset. "Ordered ID" refers to nodes named sequentially

Table 12: Algorithm CoT applied in the graph connectivity and shortest path

Dataset	prompt	Connectivity task (F_{acc}) k-hop, 1≤k≤2	k-hop, 3≤k≤4	5-hop	Singleton	I.C.	AVG.
Undirected	0-shot	0.93	0.93	0.94	1.00	0.53	0.78
	few-shot	0.92	0.93	0.96	1.00	0.87	0.92
	BFS-CoT	0.95	0.98	1.00	1.00	0.88	0.93
		Shortest path (ACC)					
undirected	0-shot	0.88	0.87	0.88	1.00	0.46	0.72
	few-shot	0.91	0.90	0.78	1.00	0.52	0.75
	Dijkstra-CoT	0.96	0.94	0.86	1.00	0.70	0.84
weighted undirected	0-shot	0.80	0.52	0.54	0.98	0.47	0.60
	few-shot	0.75	0.58	0.48	0.92	0.39	0.56
	Dijkstra-CoT	0.81	0.65	0.58	0.84	0.53	0.65

Table 13: Results for different node ID naming methods

Naming	Des.	k-hops, 1≤k≤2 ACC	k-hops, 1≤k≤2 F_{acc}	k-hops, 1≤k≤2 PCR	k-hop, 3≤k≤4 ACC	k-hop, 3≤k≤4 F_{acc}	k-hop, 3≤k≤4 PCR	5-hop ACC	5-hop F_{acc}	5-hop PCR	Singleton F_{acc}	Isolated C. F_{acc}	AVG. ACC	AVG. F_{acc}
Ordered ID	Node	1.00	0.93	0.99	1.00	0.93	0.99	1.00	0.94	0.97	1.00	0.53	0.81	0.78
	Edge	1.00	0.93	0.98	1.00	0.90	0.98	0.98	0.88	0.97	0.98	0.69	0.87	0.83
Random ID	Node	1.00	0.81	1.00	1.00	0.85	1.00	1.00	0.92	0.97	1.00	0.41	0.77	0.69
	Edge	1.00	0.89	0.98	0.99	0.88	0.97	0.96	0.70	0.94	1.00	0.59	0.83	0.76
Random characters	Node	1.00	0.83	0.99	1.00	0.86	1.00	1.00	0.94	0.99	0.98	0.43	0.77	0.70
	Edge	1.00	0.88	0.98	0.99	0.88	0.98	0.94	0.88	0.96	0.98	0.55	0.81	0.76

as "1, 2, 3, ...", "Random ID" denotes nodes named using random numbers up to 10,000, and "Random character" represents nodes named with random five-character strings. The results indicate that naming nodes in sequential order, a common practice in graph descriptions, may enhance LLM performance. This suggests that LLMs could leverage some form of memory recognition to predict connectivity more effectively and thus achieve higher performance.

E Knowledge graph

E.1 Dataset

We used WN18RR (Shang et al., 2019) as the base dataset, which provides both ID names and Entity names. The ID names consist of strings of random numbers, and Entity names are used as specific and meaningful identifiers. From its training set, we randomly selected 150 subgraphs based on ego graphs with a depth of 3. Within each subgraph, we identified two nodes with the longest paths and segmented the paths into k'-hops. This strategy allowed us to generate k' question-answer pairs, ranging from 1-hop to k'-hop.

Table 10 contains information about knowledge graph dataset, Including number of samples, average number of nodes, average number of edges in all connectivity types.

F K-hops influence on the connectivity task

In Section 4, we have demonstrated that performance in the graph connectivity task is closely related to the number of nodes and k-hops in a graph. However, it is important to note that smaller graphs inherently support shorter paths. To fairly assess the impact of k-hops on different graph sizes, we further evaluate the relations between k-hop and graph density.

We create a subset with 100 undirected graphs where the graph node number is 16 - 36 and the density is in the range of (0.2,0.4) and evaluate them by Node and Edge List descriptions. The results are shown in Figure 7.

The results indicate that 1-hop cases maintain a very high accuracy regardless of graph density, while 2-hop and 3-hop cases show a slight accuracy decrease. In contrast, 4-hop and 5-hop cases exhibit high accuracy only in sparse graphs but significantly decline when graph density approaches 0.38. This suggests that LLMs become confused as the graph complexity increases.

Comparing the Node List and Edge List descriptions, it is observed that the Node List exhibits a smaller reduction in performance compared to the Edge List. This suggests that the Node List may be more effective in describing complex graphs.

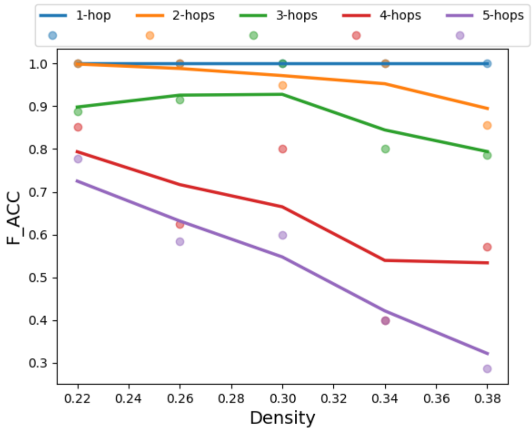


Figure 7: Accuracy of K-hops across varying graph densities (Node List)

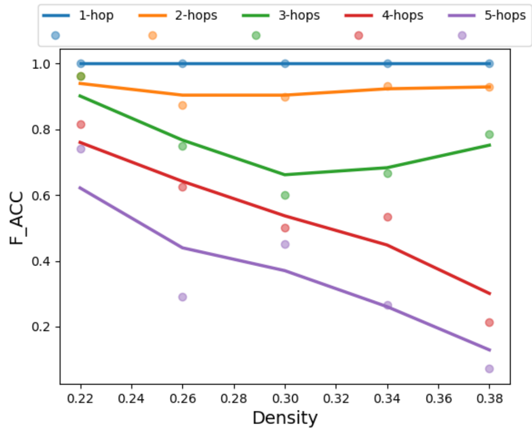


Figure 8: Accuracy of K-hops across varying graph densities (Edge List)

G The explanations for the reasoning ability of LLMs in K-hops

G.1 Traing on GPT-2

We adopt the transformer reasoning framework proposed in (Wang et al., 2024b) to train a k-hop-specific reasoning model. Specifically, we simplify the edge list and node list by converting them into node symbols, as shown in Table 14.

We select different scales of the GPT-2 model, as shown in Table 15. During training, we sequentially predict the nodes on the shortest path using cross-entropy loss, following the approach outlined in (Wang et al., 2024b). The models were trained for 20,000 epochs on a single H100 GPU, starting with a learning rate of 1e-4, which is reduced to 1e-5 after 20,000 epochs. We apply a dropout rate of 0.2 and saved the best-performing model based on the validation set. During testing, we evaluate the loss across all predicted tokens.

G.2 Finetune on LLama

Furthermore, we evaluate the impact of data on fine-tuning. The fine-tuning data is derived from a specifically designed dataset with standard graph descriptions, as illustrated in Figure 2. The test data aligns with the dataset described in 11. We use Llama3.2-3B as the backbone model and apply LoRA for fine-tuning to enhance shortest-path reasoning. The results are presented in Figure 9.

We find that only a little finetuning data can make the model have better performance. Although we are limited by the computation resource, we believe more data can drive model perform well, which is align with our observation on the training setting.

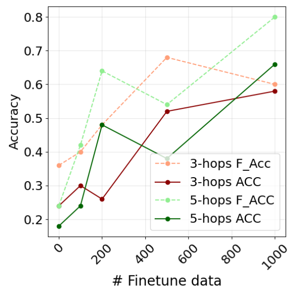


Figure 9: The effect of fine-tuning on the LLama.

H Reasoning process

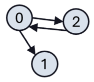
We drew inspiration from syntax analysis in language models (Jawahar et al., 2019) to the reasoning analysis. In the graph description, <S> and <T> are designated as the source and target nodes, highlighted in green. <PATH>$_i$ in gray, denotes the i-th node on the path from the source node to the target node, while <O_N> represents other nodes, shown in yellow. In the question, the source and target nodes are labeled as <SQ> and <TQ> in blue, respectively. When the models predict the $i+1$-th nodes, they require previous information, denoted as <PRED$_i$> in red.

Figure 10 and Figure 11 provides more detail information when the GPT-2 do the reasoning with different graph descriptions.

I Failed cases

In this section, we will list some failed cases. We mark the added edges in Red and ignored edges in Green.

Table 14: The simplified description forms of graphs

Graph	Node list	Edge list
	<START_Q>0: 1, 2; 2: 0 between 2, 1 <END_Q>2, 0, 1 <END>	<START_Q> 0 1 | 0 2 | 2 0 between 2, 1 <END_Q>2, 0, 1 <END>

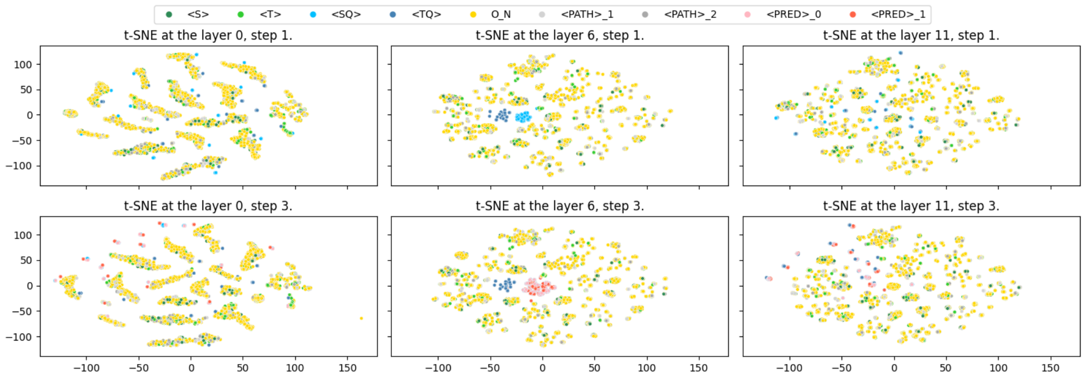


Figure 10: The t-SNE results on the Node List.

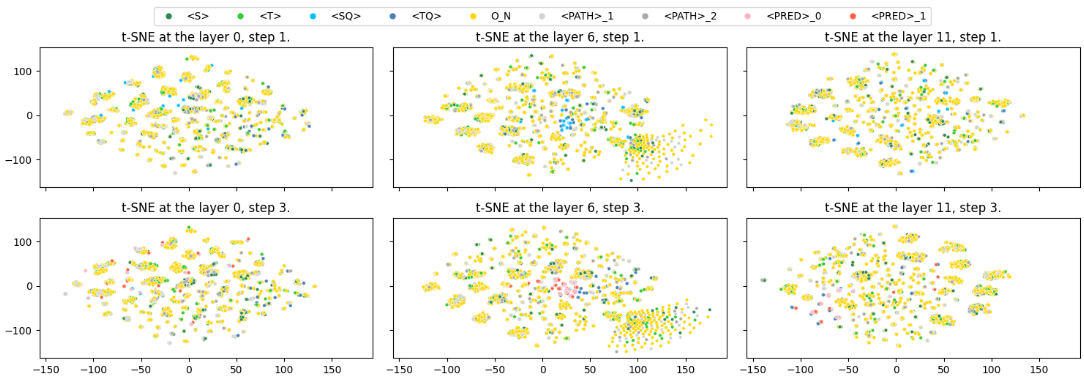


Figure 11: The t-SNE results on the Edge List.

Table 15: The version of GPT-2 models

	# Params	# head	# layer	# emb
Baby-GPT2	80M	6	6	384
Small-GPT2	124M	12	12	768
Medium-GPT2	350M	24	16	1024

I.1 Translation for Edge List to Node List

Question: Your task is giving the neighbors of each node.G describes an undirected graph among node 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, and 12.

Node 0 is connected to Node 1. Node 0 is connected to Node 5. Node 0 is connected to Node 9. Node 0 is connected to Node 12. Node 0 is connected to Node 3. Node 0 is connected to Node 10. Node 0 is connected to Node 8. Node 0 is connected to Node 11. Node 0 is connected to Node 7.

Node 1 is connected to Node 2. Node 1 is connected to Node 4. Node 1 is connected to Node 3. Node 1 is connected to Node 12. Node 1 is connected to Node 9. Node 1 is connected to Node 11. Node 1 is connected to Node 10. Node 1 is connected to Node 5. Node 1 is connected to Node 6.

Node 2 is connected to Node 3. Node 2 is connected to Node 4. Node 2 is connected to Node 6. Node 2 is connected to Node 10. Node 2 is connected to Node 9. Node 2 is connected to Node 12. Node 2 is connected to Node 7. Node 2 is connected to Node 11.

Node 3 is connected to Node 4. Node 3 is connected to Node 11. Node 3 is connected to Node 5. Node 3 is connected to Node 10. Node 3 is connected to Node 12. Node 3 is connected to Node 8.

Node 4 is connected to Node 5. Node 4 is connected to Node 9. Node 4 is connected to Node 8. Node 4 is connected to Node 10. Node 4 is connected to Node 6. Node 4 is connected to Node 11. Node 4 is connected to Node 7.

Node 5 is connected to Node 6. Node 5 is connected to Node 9. Node 5 is connected to Node 10. Node 5 is connected to Node 7. Node 5 is connected to Node 8.

Node 6 is connected to Node 7. Node 6 is connected to Node 9. Node 6 is connected to Node 12. Node 6 is connected to Node 8.

Node 7 is connected to Node 8. Node 7 is connected to Node 10. Node 7 is connected to Node 9. Node 7 is connected to Node 12.

Node 8 is connected to Node 9. Node 8 is connected to Node 12. Node 8 is connected to Node 10. Node 8 is connected to Node 11.

Node 9 is connected to Node 10. Node 9 is connected to Node 11. Node 9 is connected to Node 12.

Node 10 is connected to Node 11. Node 10 is connected to Node 12. Node 11 is connected to Node 12. For each node, the neighboring nodes are listed as follows: "Node #1: [] Node #2: []"

Answer: Given the connections in the undirected graph, the neighbors of each node can be summarized as follows:

- Node 0: [1, 5, 9, 12, 3, 10, 8, 11, 7] - Node 1: [0, 2, 4, 3, 12, 9, 11, 10, 5, 6] - Node 2: [1, 3, 4, 6, 10, 9, 12, 7, 11] - Node 3: [0, 1, 2, 4, 11, 5, 10, 12, 8] - Node 4: [1, 2, 3, 5, 9, 8, 10, 6, 11, 7] - Node 5: [0, 1, 3, 4, 6, 9, 10, 7, 8] - Node 6: [1, 2, 4, 5, 7, 9, 12, 8] - Node 7: [0, 2, 4, 5, 6, 8, 10, 9, 12] - Node 8: [0, 3, 4, 5, 6, 7, 9, 12, 10, 11] - Node 9: [0, 1, 2, 4, 5, 6, 7, 8, 10, 11, 12] - Node 10: [0, 1, 2, 3, 4, 5, 7, 8, 9, 11, 12] - Node 11: [0, 1, 2, 3, 4, 8, 9, 10, 12] - Node 12: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]

I.2 Translation for Node List to Edge List

Question: Your task is to identify all the edges in a graph and represent them in sparse form.G describes an undirected graph among 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, and 13. In this graph:

Node 0 is connected to nodes 1, 11, 2.

Node 1 is connected to nodes 0, 2, 3, 4, 9, 11, 7.

Node 2 is connected to nodes 0, 1, 3, 9, 8, 10.

Node 3 is connected to nodes 1, 2, 4, 8, 6, 13, 12.

Node 4 is connected to nodes 1, 3, 5, 10, 9.

Node 5 is connected to nodes 4, 6, 9, 7.

Node 6 is connected to nodes 3, 5, 7.

Node 7 is connected to nodes 1, 5, 6, 8, 12, 9, 11.

Node 8 is connected to nodes 2, 3, 7, 9, 12, 10.

Node 9 is connected to nodes 1, 2, 4, 5, 7, 8, 10.

Node 10 is connected to nodes 2, 4, 8, 9, 11.

Node 11 is connected to nodes 0, 1, 7, 10, 12.

Node 12 is connected to nodes 3, 7, 8, 11, 13.

Node 13 is connected to nodes 3, 12.

The edges should be list as: (Node #1, Node #2), ...

Answer: To represent the edges of the given undirected graph in sparse form, we'll list each connection between nodes as a tuple '(Node #1, Node #2)'. Since the graph is undirected, each edge is bidirectional, meaning if '(Node A, Node B)' is listed, '(Node B, Node A)' is not listed again to avoid redundancy. We'll go through each node's connections as provided, ensuring to list each edge only once.

Here are the edges in sparse form:

''' (0, 1), (0, 11), (0, 2), (1, 2), (1, 3), (1, 4), (1, 9), (1, 7), (2, 3), (2, 9), (2, 8), (2, 10), (3, 4), (3, 8), (3, 6), (3, 13), (3, 12), (4, 5), (4, 10), (5, 6), (5, 9), (5, 7), (6, 7), (7, 8), (7, 12), (7, 9), (7, 11), (8, 9), (8, 12), (8, 10), (9, 10), (10, 11), (11, 12), (12, 13) '''

This list includes all unique edges in the graph, ensuring that each connection is represented once, respecting the undirected nature of the graph.