Benchmarking and Improving Large Vision-Language Models for Fundamental Visual Graph Understanding and Reasoning

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Abstract

Large Vision-Language Models (LVLMs) have demonstrated remarkable performance across diverse tasks. Despite great success, recent studies show that LVLMs encounter substantial limitations when engaging with visual graphs. To study the reason behind these limitations, we propose VGCURE, a comprehensive benchmark covering 22 tasks for examining the fundamental graph understanding and reasoning capacities of LVLMs. Extensive evaluations conducted on 14 LVLMs reveal that LVLMs are weak in basic graph understanding and reasoning tasks, particularly those concerning relational or structurally complex information. Based on this observation, we propose a structure-aware fine-tuning framework to enhance LVLMs with structure learning abilities through 3 self-supervised learning tasks. Experiments validate the effectiveness of our method in improving LVLMs' zero-shot performance on fundamental graph learning tasks, as well as enhancing the robustness of LVLMs against complex visual graphs[1].

1 Introduction

Graphs serve as a fundamental data structure across a wide range of domains, including social network analysis (Schweimer et al., 2022), recommendation systems (Zhang et al., 2023), knowledge graphs (Zhang et al., 2024b), chemistry (Cao et al., 2024) and biomedical molecules (Liu et al., 2023). Existing methods have achieved great success in enhancing understanding and reasoning abilities in graph-based tasks (Kim et al., 2023a; Chen et al., 2024). However, these approaches typically focus on specific graph types or tasks, posing challenges in designing versatile systems that are suitable for various tasks and graphs across diverse domains.

Recently, Large Vision-Language Models (LVLMs) have exhibited outstanding performance across a diverse range of downstream tasks by unifying various inputs in the form of images and processing them with human-like understanding and reasoning abilities (Zhu et al., 2024; Zheng et al., 2024). This triggers an increasing interest in employing LVLMs for graph learning problems, given the vision modality offers a natural and intuitive way for comprehending structural information and facilitating general graph reasoning (Poklukar et al., 2022). Despite significant advancements, recent studies (Wei et al., 2024; Li et al., 2024d; Ai et al., 2024) reveal that LVLMs face significant challenges in addressing graph-based learning problems. Notably, LVLMs achieve less than 15% accuracy on mathematical graph reasoning tasks, markedly below their performance in image and text reasoning (Li et al., 2024d). Therefore, a natural challenge arises: *why do LVLMs fail in graph learning, and how to enhance LVLMs to process graphs like professionals?*

To address this challenge, we begin by identifying the research gap in existing evaluations

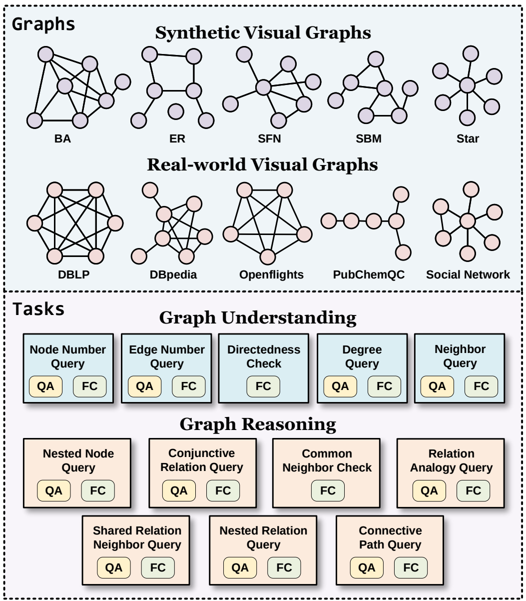


Figure 1: Overall of our VGCURE benchmark.

[1] Our dataset and code are available at https://anonymous.4open.science/r/VGCure-6C32.

Benchmark	Evaluation Topic	# Tasks	Graph Type	Anonymity	# Scale
VisionGraph	Graph Theory Problems	10	Synthetic	✓	3,000
Ai et al. (2024)	Multi-hop Reasoning	N/A	Real-world	✗	1,355
GVLQA	Graph Theory Problems	7	Synthetic	✓	157,896
our **VGCURE**	Fundamental Graph Understanding and Reasoning	22	Synthetic & Real-world	✓	223,646

Table 1: Comparisons among different visual graph analysis benchmarks for LVLMs, where *# Tasks* and *# Scale* represent the number of task types and test samples, respectively.

that limit our understanding of LVLMs. Current work primarily assesses LVLMs on graph theory problems or multi-hop reasoning tasks (Wei et al., 2024; Ai et al., 2024), which are inherently complex and necessitate a combination of diverse cognitive abilities. Thus it remains uncertain whether LVLMs have strong fundamental understanding and reasoning capabilities in processing visual graphs—such as recognizing the basic components of a graph and making basic logical inferences based on graph data—which is crucial for determining whether the limitations of LVLMs originate from a lack of fundamental abilities or other higher-order capabilities.

To this end, we present the **V**ision **G**raph **C**omprehensive **U**nderstanding and **RE**asoning benchmark, **VGCURE**, to thoroughly evaluate the fundamental understanding and reasoning capabilities of LVLMs concerning visual graphs. As shown in Figure 1, VGCURE evaluates the fundamental capabilities of LVLMs across a comprehensive set of tasks, including 9 graph understanding tasks and 13 graph reasoning tasks. Moreover, VGCURE encompasses 10 anonymized graph structures sourced from both synthetic and real-world sources, offering a robust testbed for assessing LVLMs' proficiency in handling diverse graphs. We conduct extensive experiments involving 14 representative LVLMs using VGCURE. Experiments show that 1) LVLMs exhibit subpar performance in most tasks, especially in capturing relational information, indicating their weak fundamental understanding and reasoning skills on visual graphs; 2) LVLMs are frequently confused when confronted with structurally complex visual graphs.

Motivated by the above observations, we further introduce a novel self-supervised, structure-aware fine-tuning framework MCDGRAPH to enhance the structure learning capabilities of LVLMs. In particular, MCDGRAPH comprises three tasks: 1) masked graph infilling, which guides LVLMs to infer missing local structural information; 2) contrastive graph discrimination, which guides LVLMs to distinguish structural differences between graphs; 3) graph description, which teaches LVLMs to summarize the global information inherent in graph structures. Experiments show that our self-supervised framework considerably enhances the graph understanding and reasoning abilities of two representative LVLMs, particularly in their performance on edge-related tasks. Further analysis demonstrates that our method improves LVLMs' robustness in handling more structurally complex visual graphs. The contributions of this work can be summarized as follows:

- We introduce VGCURE, a comprehensive benchmark to systematically evaluate LVLMs' fundamental understanding and reasoning abilities on visual graphs.
- Through extensive experiments on 14 LVLMs, we reveal LVLMs' limitations in fundamental graph understanding and reasoning, especially for tasks concerning relational or structural information. Besides, LVLMs' performance declines as graph complexity increases.
- We propose a self-supervised framework to enhance LVLMs' ability in capturing the structural information in visual graphs. Experiments validate the effectiveness of our approach across a wide range of tasks.

2 The VGCURE Benchmark

To evaluate LVLMs' capabilities in fundamental graph understanding and reasoning, we introduce VGCURE, a large-scale multimodal graph benchmark with 22 challenging tasks in two categories. VGCURE features 10 graph types, both synthetic and real-world, to assess LVLMs' effectiveness with diverse graphs. It anonymizes the graphs to minimize the impact of pre-existing LLM knowledge on core reasoning abilities, promoting *knowledge-free reasoning* (Hu et al., 2024). Table 1 offers a comparison between VGCURE and three recent benchmarks. It is evident that VGCURE excels in fundamental graph understanding and reasoning capabilities. Furthermore, VGCURE offers a comprehensive evaluation through more varied graph types, tasks, and test samples.

Task	QA sample	FC sample (Label)
NNu	Q: How many nodes are there in this graph? A: 12	There are 12 nodes in this graph. (True) There are 17 nodes in this graph. (False)
EN	Q: How many edges are there in this graph? A: 15	There are 15 edges in this graph. (True) There are 17 edges in this graph. (True)
DC	-	This graph is a directed graph. (True) This graph is an undirected graph. (True)
DQ	Q: What is the degree of E9 in this graph? A: 1	The degree of E9 in this graph is 1. (True) The degree of E9 in this graph is 2. (False)
NQ	Q: Which nodes are out-neighbors of E6 in this graph? A: [E3]	E3 is a out-neighbors of E6 in this graph. (True) E7 is a out-neighbors of E6 in this graph. (False)
NN	Q: Which entities are R6 of the entity that is R5 of E3? A: [E4, E7]	E4 is R6 of the entity that is R5 of E3. (True) E1 is R6 of the entity that is R5 of E3. (False)
CR	Q: Which entities are R4 of E9 as well as R8 of E1? A: [E2]	E2 is R4 of E9 as well as R8 of E1. (True) E1 is R4 of E9 as well as R8 of E1. (False)
CN	-	E8 and E1 share a common out-neighbor, i.e., common head entity. (True) E10 and E12 share a common out-neighbor, i.e., common head entity. (False)
RA	Q: Which entities are connected to E3 via the same relation from E3 to E1? A: [E2]	E2 is connected to E3 via the same relation from E3 to E1. (True) E6 is connected to E3 via the same relation from E3 to E1. (False)
SRN	Q: Which entities are both R2 of E10? A: [E4, E12]	E4 and E12 are both R2 of E10. (True) E4 and E3 are both R2 of E10. (False)
NR	Q: What is the relation from the entity that is R5 of E3 to E2? A: [R8]	E2 is R8 of the entity that is R5 of E3. (True) E2 is R4 of the entity that is R5 of E3. (False)
CP	Q: Is there a path from E3 to E4? A: Yes. The paths are [[E3, E1, E2, E4], [E3, E1, E4]]	There are 2 paths from E3 to E4. (True) There are 3 paths from E3 to E4. (False)

Table 2: Examples for each task in VGCURE. These samples all correspond to the graph shown in Figure 6(d).

2.1 Graph Structure Generation

We begin by collecting a wide variety of graph structures that we will then use to generate visual graphs and challenging tasks. Following Fatemi et al. (2024), we first leverage *NetworkX* library (Hagberg et al., 2008) for generating a diverse set of random synthetic structures, including Erdős-Rényi (ER) graphs (ERDdS and R&wi, 1959), scale-free networks (SFN) (Barabási and Albert, 1999), Barabási–Albert (BA) model (Albert and Barabási, 2002), stochastic block model (SBM) (Holland et al., 1983) and star graphs. In addition, we extract anonymized structures from real-world graphs in GraphArena benchmark (Tang et al., 2024), including DBLP, Social Network, DBpedia, Openflights and PubChemQC. All the entity and relation names in each graph are replaced with generic names to eliminate the impact of the model's internal knowledge on reasoning. After initializing the graph structure, we use the Graphviz library (Ellson et al., 2002) to generate concise *directed* and *undirected* visual graphs.

2.2 Tasks Design

To thoroughly assess the abilities of LVLMs in fundamental graph structure understanding and reasoning, the proposed VGCURE encompasses the following categories of tasks. Table 2 presents examples for each task.

Category 1: Graph Understanding. The graph understanding tasks involve analyzing and extracting structural, relational, and property-based information from the visual graph, which aims to gain insights into the composition and topology of the graph, including its nodes, edges, connectivity, and the relationships among its components.

- **Node Number Query (NNu)**: Calculate the total number of nodes in the graph.
- **Edge Number Query (EN)**: Determine the total number of edges in the graph.
- **Directedness Check (DC)**: Verify whether the graph is undirected or directed.
- **Degree Query (DQ)**: Calculate the degree of the given node, representing the number of edges connected to it.
- **Neighbor Query (NQ)**: Identify the nodes that are directly connected to the given node.

Category 2: Graph Reasoning. The reasoning tasks focus on exploring the *knowledge-free reasoning* ability of LVLMs on visual graphs. To differentiate from graph understanding tasks, we designed a series of 2-hop reasoning tasks.

- **Nested Node Query (NN)**: Identify the entities linked to the given entity through a composite chain involving the given relations.
- **Conjunctive Relation Query (CR)**: Retrieve the entities that simultaneously satisfied two independent relationship constraints with two distinct entities.
- **Common Neighbor Check (CN)**: Determine

whether two entities share at least one common neighbor in a 2-hop relational path.

- **Relation Analogy Query (RA)**: Find the entities linked to a target entity via a relation identical to that links a given entity pair.
- **Shared Relation Neighbor Query (SRN)**: Identify the set of entities that are connected to the given entity through the given relation.
- **Nested Relation Query (NR)**: Identify the relation between a target entity and an intermediate entity obtained by traversing a specific relation path from a given entity.
- **Connective Path Query (CP)**: Determine the existence of *directed* paths or *shortest undirected* paths between two given entities, and retrieve all possible paths if they exist.

For each task, we construct **one QA sample** and **two fact checking (FC) samples** (with labels of True and False, respectively) automatically based on the template, except for CN and DC which have only fact checking samples due to the strong similarity between the two samples. The total number of final samples is 223,646. More examples and detailed **statistics** about VGCURE can be found in Appendix A and Table 9.

3 Benchmarking LVLMs on VGCURE

3.1 Experimental Setup

We conduct evaluation on 13 open-source LVLMs, including InternLM-XComposer2.5-7B (Zhang et al., 2024a), InternVL2-8B, Llama3.2-11B-Vision-Instruct, LLaVA1.5-7B (Liu et al., 2024), LLaVA1.5-13B (Liu et al., 2024), LLaVA-NeXT-7B (Li et al., 2024b), LLaVA-OneVision-7B (Li et al., 2024a), MiniGPT-v2 (Chen et al., 2023), Monkey (Li et al., 2024e), mPLUG-Owl3-7B (Ye et al., 2024), Qwen-VL (Bai et al., 2023), Qwen2-VL-7B-Instruct (Wang et al., 2024) and SPHINX (Lin et al., 2023). Meanwhile, we also evaluate the performance of the GPT-4o-mini, which is a strong closed-source LVLM[2]. Due to the high cost of GPT-4o-mini, we randomly select 50 graphs from each graph structure for testing. For all methods, the **zero-shot** setting is adopted during evaluation. More details can be found in Appendix B.

3.2 Main Result

Graph Understanding Table 3 and Table 4 present the evaluation results in the forms of question answering (QA) and fact checking (FC), respectively. We report the averaged performance across various graph structures. In general, most LVLMs struggle to precisely understand the structural and relational information in visual graphs. In specific, (I) Among the graph understanding tasks, *Node Number Query (NNu)* and *Directedness Check (DC)* are the easiest for most LVLMs. This indicates that most LVLMs are able to accurately recognize the number of specific elements in the visual graph. (II) All LVLMs struggle with *Edge Number Query (EN)* and *Neighbor Query (NQ)* tasks, with the highest performance ratings remaining 16.28% accuracy and 30.81% F1 score, respectively. This indicates that current LVLMs are weak in understanding relational and structural information. (III) Even with a similar number of parameters, the graph understanding abilities of open-source LVLMs vary significantly, with Qwen2-VL and InternVL2 showing better performance in both QA and FC samples. (IV) For the same task, LVLMs perform differently on QA and FC samples, likely due to different ways in reasoning and understanding required by each task (Thorne et al., 2018). (V) The closed-source LVLM, GPT-4o-mini, offers no significant advantages and even underperforms open-source LVLMs, especially on FC tasks.

Graph Reasoning Based on graph reasoning results in Tables 3 and 4, it can be observed that, (I) Compared to graph understanding, the graph reasoning tasks are more challenging and the overall performance of LVLMs is worse on both QA and FC samples. This may be a knock-on effect due to deficiencies in visual graph understanding. (II) Among all open-source LVLMs, InternVL2 and Llama3.2-Vision achieve better performance and LLaVA1.5-7B perform the worst on graph reasoning tasks. (III) All the LVLMs perform poorly on *Nested Relation Query (NR)* for both QA and FC samples, which is similar to the observation in the graph understanding task. This suggests that LVLMs are deficient in recognizing edges and understanding structural information within visual graphs. (IV) On the QA samples, the performance of different LVLMs on *Connective Path Query (CP)* varies widely. SPHINX, Monkey and Qwen-VL demonstrate almost no ability to recognize paths between two specific nodes in the visual graph. (V) Similarly, GPT-4o-mini underperforms in most tasks compared to open-source LVLMs, except for the *Connective Path Query (CP)* task.

[2]We excluded GPT-4o as a baseline due to its high cost.

Models	Understanding					Reasoning											
	NNu	EN	DQ	NQ		NN		CR		RA		SRN		NR		CP	
	Acc	Acc	Acc	F1	Hits@1	F1	Hits@1	F1	Hits@1	F1	Hits@1	F1	Hits@1	F1	Hits@1	EM_F1	Label_Acc
SPHINX	21.03	11.38	15.45	12.84	29.45	6.05	9.81	7.28	16.44	14.62	21.69	11.62	26.93	1.54	4.99	0.68	**95.59**
Monkey	40.09	9.22	17.81	9.90	21.88	8.90	12.96	2.85	4.62	3.74	4.13	9.79	21.61	3.06	7.98	0.46	5.11
MiniGPT-v2	11.80	10.61	18.03	16.40	27.08	8.92	18.02	2.01	2.65	7.50	14.87	9.85	27.47	5.86	13.87	5.26	**95.59**
mPLUG-Owl3	28.38	8.84	6.86	20.32	51.16	8.68	11.39	5.42	11.81	11.07	14.81	6.48	18.06	2.03	0.33	10.87	74.97
LLaVA1.5-7B	14.53	7.56	30.14	11.43	21.25	1.80	0.21	2.22	0.13	6.36	9.37	5.38	7.73	0.84	2.23	2.63	78.64
LLaVA-NeXT	47.89	9.59	19.52	23.27	44.11	14.77	21.74	6.60	12.44	10.14	15.29	12.68	27.88	9.88	6.46	8.27	95.56
LLaVA-OV	23.47	3.08	23.80	15.00	39.12	10.74	19.87	7.50	16.61	9.85	19.30	10.21	30.99	1.04	1.36	9.69	94.83
LLaVA1.5-13B	17.08	7.62	26.33	15.68	32.66	6.08	7.83	4.31	13.23	6.52	10.80	7.48	12.86	4.21	6.21	5.91	82.41
InternLM-XC2.5	60.20	10.53	41.12	18.90	55.33	14.64	26.14	19.19	45.60	11.50	19.06	14.12	46.53	3.09	5.49	28.82	95.53
Llama3.2	77.31	9.39	35.56	18.79	42.34	**18.93**	29.43	21.90	55.00	**15.80**	27.51	20.79	61.30	**14.11**	**24.05**	20.80	94.70
Qwen-VL	42.45	9.66	20.56	10.95	21.25	11.44	15.51	7.93	18.30	12.48	17.36	11.11	22.79	5.43	4.01	0.00	4.48
Qwen2-VL	**97.80**	**16.38**	48.09	16.18	38.12	16.52	28.34	21.02	48.57	14.19	**27.96**	19.48	56.42	12.73	25.07	12.90	38.06
InternVL2	77.45	9.78	50.75	25.01	68.58	18.30	**30.82**	**24.87**	**59.31**	10.83	17.12	20.72	**59.99**	10.58	18.97	14.53	43.97
GPT-4o-mini*	89.20	15.40	**56.40**	**30.81**	**77.40**	17.01	29.98	22.33	53.15	15.47	24.81	**22.25**	59.48	8.62	13.48	**42.55**	92.40

Table 3: Model performance on QA samples across various tasks, where *EM_F1* is the macro F1 score calculated based on the exact match between the predicted path and the ground truth path, *Label_Acc* measures the accuracy of the model's prediction on whether a path exists or not. The best results are **bolded**.

Models	Understanding										Reasoning													
	NNu		EN		DC		DQ		NQ		NN		CR		CN		RA		SRN		NR		CP	
	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc	F1	Acc
SPHINX	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.84	51.16	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00
Monkey	40.31	53.23	51.38	55.58	64.25	65.24	50.01	55.62	44.04	53.29	50.54	50.76	37.37	51.08	48.85	49.71	38.32	50.13	33.52	49.78	40.29	48.05	51.44	**58.87**
MiniGPT-v2	34.37	50.38	34.28	50.39	33.92	50.18	33.69	49.91	44.29	50.99	49.68	50.03	47.94	53.19	45.66	51.80	36.71	49.48	43.08	43.22	36.68	50.07	51.68	52.39
mPLUG-Owl3	37.53	50.80	31.16	38.59	73.04	74.76	39.84	46.92	33.33	50.00	34.75	49.86	46.11	52.04	33.96	51.20	44.80	48.54	47.35	53.10	36.65	49.30	37.34	50.27
LLaVA1.5-7B	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.84	51.16	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00
LLaVA-NeXT	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00	33.84	51.16	33.33	50.00	33.33	50.00	33.33	50.00	33.33	50.00
LLaVA-OV	39.13	52.69	33.79	49.68	65.02	68.49	36.87	51.49	37.12	51.70	46.83	53.37	39.66	52.41	34.09	51.23	39.64	48.89	44.12	52.19	48.19	52.19	33.35	49.05
LLaVA1.5-13B	60.31	63.26	50.78	57.09	87.74	87.92	33.33	50.00	36.39	49.31	47.65	50.31	35.93	50.94	34.68	49.31	33.33	50.00	33.47	50.03	35.18	43.68	44.55	52.91
InternLM-XC2.5	37.19	51.79	40.00	51.05	65.76	66.72	43.07	49.16	64.46	65.40	50.81	54.05	58.72	61.66	39.34	50.05	35.54	50.47	49.36	51.98	49.12	53.08	52.12	52.76
Llama3.2	87.66	**87.66**	47.26	49.67	43.27	51.83	42.23	51.39	65.87	66.03	53.47	56.40	62.79	63.74	39.00	50.30	**59.89**	**61.20**	48.82	49.38	**58.59**	**60.36**	45.65	49.32
Qwen-VL	32.30	47.72	32.27	47.56	9.50	10.49	31.04	44.54	36.69	49.97	27.07	32.57	15.55	17.99	31.68	45.30	27.83	29.13	32.71	33.70	34.72	41.94	36.37	42.63
Qwen2-VL	**76.50**	77.67	**68.26**	**68.27**	**94.92**	**94.94**	**64.32**	**67.40**	67.34	68.76	44.17	53.77	74.28	75.24	38.52	51.10	35.28	50.55	**57.07**	**59.18**	42.08	52.95	42.25	53.38
InternVL2	68.63	71.18	36.82	50.23	93.17	93.18	63.28	63.84	**72.81**	**73.27**	**62.46**	**63.62**	**75.37**	**76.18**	47.12	50.40	33.70	50.14	56.98	57.42	55.94	58.42	**54.71**	54.71
GPT-4o-mini*	64.49	67.00	39.85	52.30	90.52	90.60	42.03	52.90	48.77	56.80	50.77	51.51	62.17	62.82	**53.03**	**55.05**	36.50	50.78	54.87	54.89	44.37	51.11	51.39	54.50

Table 4: Model performance on FC samples across various tasks. The best results are **bolded**.

3.3 Impact of Structures

Inspired by Fatemi et al. (2024), we investigate whether graph structure influences LVLMs' ability to understand and reason over visual graphs. Figure 2 compares the performance of the top five LVLMs on QA samples across various graph structures. It is evident that graph structure significantly affects the understanding and reasoning performance of LVLMs on most tasks. Specifically, all LVLMs obtain impressive results on *PCQC* and weaker performance on *BA*, possibly due to the simpler structure of PCQC with fewer nodes and edges (averaging 5.45 nodes and 4.76 edges), while BA contains the largest number of edges in VGCURE (averaging 11 nodes and 21.02 edges). Furthermore, on different tasks, the performance of LVLMs is affected differently by the graph structure. *Edge Number Query (EN)* and *Connective Path Query (CP)* show larger performance variations across graph structures, whereas *Node Number Query (NNu)* and *Nested Node Query (NN)* show smaller differences. As presented in Figure 9, the overall trend of FC is similar to that of QA.

3.4 Impact of Complexity

We further discuss the impact of graph complexity on the LVLMs' ability to understand and reason over the visual graph considering the number of edges, number of nodes, and average degree of the graph. Figure 3 shows the performance comparison of five LVLMs on QA samples across representative tasks and complexity levels. It can be observed that as graph complexity increases, the performance of LVLMs declines on most tasks, especially on *Edge Number Query*, where results vary greatly with complexity. Besides, some LVLMs achieve peak performance at intermediate complexity levels on some tasks, but struggle with more complex graphs. This reflects a balance between information richness and complexity of visual graphs, whereas higher complexity likely overwhelm the LVLMs' reasoning capacity, attention mechanisms, or ability to generalize due to training biases or compounded errors in large graphs. In addition, different complexity

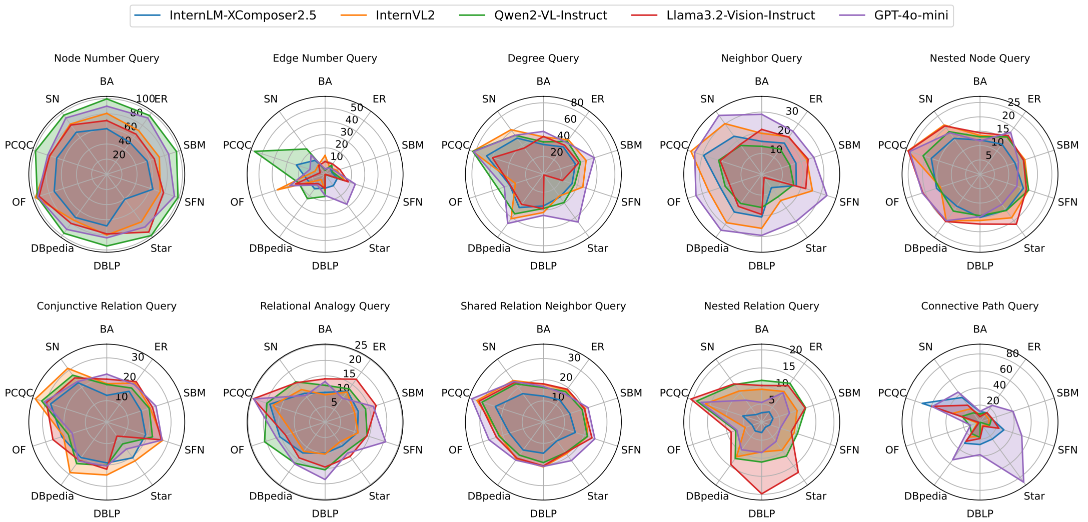
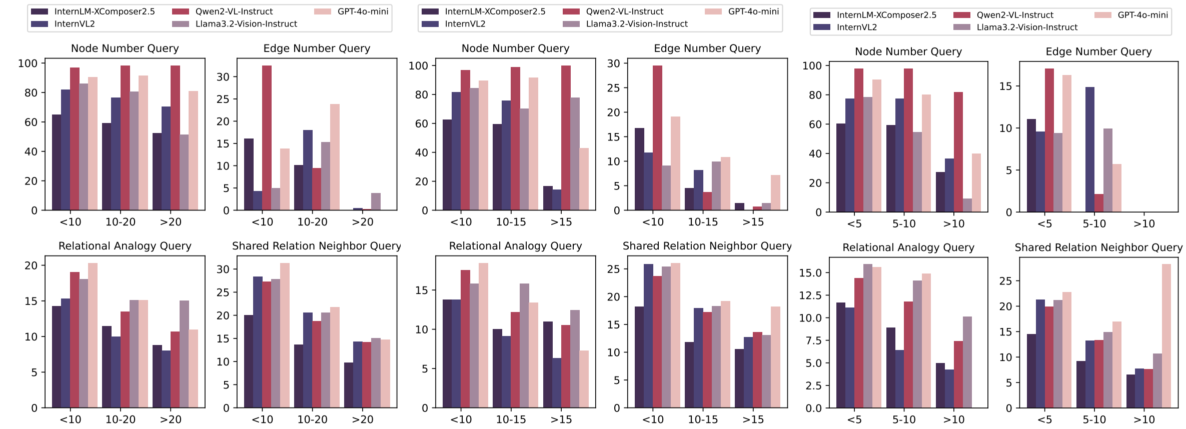


Figure 2: Model performance (F1/Acc) on QA samples across various graph structures and tasks , where OF, PCQC and SN denotes Openflights, PubChemQC and Social network, respectively.



(a) Number of Edges (b) Number of Nodes (c) Average Degree

Figure 3: Model performance (F1/Acc) comparison on QA samples across various dimensions of complexity.

dimensions have varying effects on the LVLMs performance on different tasks. For instance, on *Nodes Number Query*, LVLMs are minimally affected by the number of edges while strongly affected by the number of nodes and average degree. More results are shown in Figures 10-15 in the Appendix due to space limit, and the overall trend remains similar to the above findings.

4 The MCDGRAPH Framework

To enhance the ability of open-source LVLMs to understand and reason on visual graphs, we propose MCDGRAPH, a **self-supervised** fine-tuning framework designed to enhance LVLMs' ability to capture structural and relational information within visual graphs. As illustrated in Figure 4, MCDGRAPH comprises three key tasks: **M**asked Graph Infilling, **C**ontrastive Graph Discrimination, and Graph **D**escription.

4.1 Task1: Masked Graph Infilling

In Masked Graph Infilling, we randomly mask either nodes or edges in a visual graph and challenge the model to predict the masked element based on the partially observed graph and the corresponding text triples.

$$M = \text{LVLMs}(\hat{G}, I, T), \tag{1}$$

where M denotes the masked content in the graph, and $\hat{G}$, I, T denotes the masked graph, task instruction, and text triples of the original graph, respectively. This task encourages LVLMs to infer missing structure information, improving its ability to understand graph structure and the relationships between elements.

4.2 Task2: Contrastive Graph Discrimination

To further refine the LVLMs' understanding of graph structure, we introduce a contrastive learning

Models	Understanding					Reasoning						
	NNu	EN	DC	DQ	NQ	NN	CR	CN	RA	SRN	NR	CP
	QA Samples											
Qwen2-VL	97.80	16.38	-	48.09	16.18	16.52	21.02	-	14.19	19.48	12.73	12.90
w MCDGRAPH	98.34 $\uparrow$	25.92 $\uparrow$	-	60.94 $\uparrow$	25.44 $\uparrow$	13.32	26.14 $\uparrow$	-	13.14	20.74 $\uparrow$	14.44 $\uparrow$	11.95
InternVL2	77.45	9.78	-	50.75	25.01	18.30	24.87	-	10.83	20.72	10.58	14.53
w MCDGRAPH	95.68 $\uparrow$	40.45 $\uparrow$	-	54.78 $\uparrow$	28.80 $\uparrow$	19.43 $\uparrow$	28.53 $\uparrow$	-	11.67 $\uparrow$	22.34 $\uparrow$	16.50 $\uparrow$	12.76
	FC Samples											
Qwen2-VL	76.50	68.26	94.92	64.32	67.34	44.17	74.28	38.52	35.28	57.07	42.08	42.25
w MCDGRAPH	89.58 $\uparrow$	65.80	95.84 $\uparrow$	77.10 $\uparrow$	79.75 $\uparrow$	60.71 $\uparrow$	83.07 $\uparrow$	53.90 $\uparrow$	53.48 $\uparrow$	64.17 $\uparrow$	64.12 $\uparrow$	60.11 $\uparrow$
InternVL2	68.63	36.82	93.17	63.28	72.81	62.46	75.37	47.12	33.70	56.98	55.94	54.71
w MCDGRAPH	76.55 $\uparrow$	71.98 $\uparrow$	90.04	56.83	80.98 $\uparrow$	73.14 $\uparrow$	80.23 $\uparrow$	52.09 $\uparrow$	52.81 $\uparrow$	59.07 $\uparrow$	69.03 $\uparrow$	45.82

Table 5: Model performance (Acc/F1/EM_F1 for QA and F1 for FC) on various tasks. $\uparrow$ indicates an improvement compared to the original model. The complete experimental results are shown in Table 13 and 14.

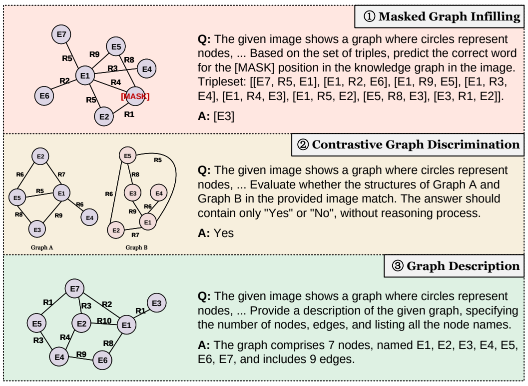


Figure 4: Overall illustration of MCDGRAPH.

task, which helps train the LVLMs to distinguish between two visual graphs that may either represent the *same graph with different layouts* or two *distinct graphs with similar layouts*.

$$Y = \text{LVLMs}(G_1, G_2, I), \quad (2)$$

where the answer $Y \in \{\textit{Yes, No}\}$, G_1, G_2 denotes two graphs, and I is the task instruction. By learning how to perform structural reasoning and graphical isomorphism detection, this task aims to improve LVLMs by recognizing subtle structural differences between two visual graphs.

4.3 Task3: Graph Description

Graph Description task requires LVLMs to generate a textual description of a given visual graph. The description should include the total number of nodes and edges, as well as the names of all the nodes in the graph,

$$D = \text{LVLMs}(G, I), \quad (3)$$

where D represents the description, and G, I denotes the input graph and task instruction, respectively. This task ensures that the LVLMs develop a clear understanding of the graph's composition, thereby enhancing their ability to interpret and summarize graph-based information.

5 Enhancing LVLMs with MCDGRAPH

5.1 Experimental Setup

We validate the effectiveness of MCDGRAPH on top two performing LVLMs on VGCURE, i.e., Qwen2-VL and InternVL2. We collect a new set of visual graphs **beyond VGCURE** with synthetic structures and automatically create 20k training samples for MCDGRAPH. To prevent catastrophic forgetting, we apply LoRA (Hu et al., 2022) to efficiently enhance the LVLMs' abilities while preserving their original performance. More details about training samples and implementation are available in Appendix C.

5.2 Results and Analysis

Main Results Table 5 compares the performance of Qwen2-VL and InternVL2 before and after applying MCDGRAPH on both visual graph understanding and reasoning tasks. It can be observed that MCDGRAPH improves the performance of LVLMs on almost all tasks, demonstrating the effectiveness of the proposed method. Notably, the improvement of LVLMs is particularly impressive on edge-related tasks, i.e., *Edge Number Query (EN)* and *Nested Relation Query (NR)*, that are relatively difficult for LVLMs. This suggests that MCDGRAPH enhances LVLMs' ability to understand the graph structures. In addition, although MDCGraph does not optimize for the tasks in VGCURE, MCDGRAPH shows obvious improvement in both QA and FC samples for most tasks in VGCURE. This demonstrates that the proposed method can improve the fundamental graph structure understanding of LVLMs, which leads to better performance on downstream tasks. We also present a case on *NR* to further understand the effectiveness of the proposed method, please refer to Figure 22 for detailed information.

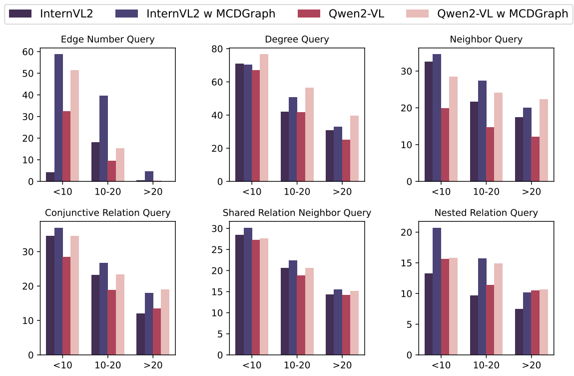


Figure 5: Model performance (F1/Acc) comparison on QA samples across representative tasks and edge ranges.

Performance on Varying Complexity Figure 5 illustrates the performance improvements of MCDGraph on LVLMs across varying graph complexities on six representative tasks in VGCure. For both models, fine-tuning with MCDGraph consistently improves performance across most tasks and complexity levels. This indicates that MCDGraph effectively enhances the LVLMs' ability to understand and reason over visual graphs. For simpler graphs, MCDGraph provides a smaller improvement where LVLMs already perform well. However, as graph complexity increases, the performance gap between fine-tuned and baseline models becomes more pronounced on most tasks, highlighting MCDGraph's importance in handling more complex visual graphs. Due to the space limit, only the results with the number of edges are presented here, and the findings are similar in the other dimensions. More results are exhibited in Figures 16-21 in the Appendix.

5.3 Evaluation on Downstream Tasks

To further demonstrate the scalability and applicability of our proposed method, we also conduct extra experiments on two graph-related downstream tasks.

Results on VisionGraph We first evaluate the performance of MCDGraph on three representative graph theory problems in VisionGraph (Li et al., 2024d), a multimodal benchmark designed to assess the graphical structure understanding and multistep reasoning capabilities of LVLMs. The results are shown in Table 6. We can observe that our method can generally improve the performance of LVLMs on graph theory problems, especially for the relatively difficult Maximum Flow task. This confirms the effectiveness as well as the scalability of our method.

Model	Connect	Cycle	Max. Flow
Qwen2-VL	55.8	52.88	1.72
w MCDGraph	53.37	52.88	**5.17**
InternVL2	46.9	52.88	6.9
w MCDGraph	**54.72**	52.88	**8.62**

Table 6: Model performance (Acc) on graph theory problems in VisionGraph.

Models	Accuracy	Precision	Recall	F1
Qwen2-VL	79.60	81.18	79.13	79.13
w MCDGraph	**80.15**	**81.71**	**79.69**	**79.71**
InternVL2	79.41	80.93	78.95	78.95
w MCDGraph	**79.78**	**81.34**	**79.32**	**79.33**

Table 7: Model performance on FactKG, where each model is fine-tuned on the training set for this task.

Results on FactKG We then evaluate our MCDGraph on FactKG dataset (Kim et al., 2023b), which is a knowledge graph-based fact verification dataset collected from real-world database, requiring the model to verify the veracity of claims against the given KG triples. We first generate the corresponding visual graphs based on the text triples provided by FactKG, and then input the visual graphs and corresponding claims to the model for training and testing. As the results shown in Table 7, it can be observed that our method is able to improve the performance of LVLMs on FactKG, suggesting that MCDGraph may also have a wide range of applications in real-world graph-related task scenarios. Meanwhile, this task requires not only fundamental visual graph understanding and reasoning abilities, but also relies on LVLMs' understanding of semantic and logical relationships between entities, the latter of which is not addressed by our method. Therefore, the performance improvement of LVLMs is not as significant as that of the graph theory problems.

5.4 Impact on Visual Style

In order to explore the impact of visual graph styles and the generalization of our method, we employ NetworkX and Matplotlib library to regenerate 50 visual graphs with different visual styles (different color of node, different font and different layout, as shown in Figure 7) from those in VGCure for each graph structure. Then, we evaluate the performance of our proposed MCDGraph on Qwen2-VL and InternVL2. As the results shown in Table 8, although LVLMs never encounter this style of visual graph when fine-tuned, our method is still

Models	Understanding					Reasoning						
	NNu	EN	DC	DQ	NQ	NN	CR	CN	RA	SRN	NR	CP
	QA Samples											
Qwen2-VL	98.20	18.10	-	50.70	18.64	15.66	22.66	-	14.83	20.45	16.95	11.04
w MCDGraph	99.40 ↑	40.20 ↑	-	56.80 ↑	28.44 ↑	14.64	27.02	-	13.69	22.22 ↑	14.73	11.99 ↑
InternVL2	73.70	8.60	-	48.40	26.33	18.26	26.19	-	9.85	21.75	11.20	1.60
w MCDGraph	95.80 ↑	35.70 ↑	-	52.90 ↑	28.89 ↑	19.90 ↑	29.24 ↑	-	11.73 ↑	23.23 ↑	18.04 ↑	↑ 14.49
	FC Samples											
Qwen2-VL	71.37	61.78	86.53	73.82	73.03	48.00	77.35	39.98	36.04	60.22	45.31	42.93
w MCDGraph	88.45 ↑	63.14 ↑	94.43 ↑	76.26 ↑	78.59 ↑	63.17 ↑	82.63 ↑	53.78 ↑	54.33 ↑	66.26 ↑	65.95 ↑	56.30 ↑
InternVL2	75.43	34.80	86.85	63.68	74.52	61.12	74.23	47.22	33.48	55.85	55.32	53.15
w MCDGraph	83.82 ↑	70.14 ↑	83.48	60.77	79.69 ↑	71.39 ↑	78.30 ↑	52.38 ↑	51.24 ↑	59.83 ↑	68.58 ↑	44.73

Table 8: Model performance (Acc/F1/EM_F1 for QA and F1 for FC) on various tasks with different visual styles.

able to enhance the performance of the LVLMs on almost all tasks. This demonstrates the ability of our method to enhance LVLMs' ability in capturing the structural information in visual graphs with excellent generalization. In addition, compared to Table 5, it can be noticed that the experimental results before and after the change of style are similar, which indicates that the style itself has no effect on the evaluation of LVLMs. More results are available in Appendix D

6 Related Work

Multimodal Benchmark for Graphs With the emergence of LVLMs, the evaluation of LVLMs for visual graph understanding and reasoning has gained increasing attention from researchers. Li et al. (2024d) and Wei et al. (2024) introduce VisionGraph and GVLQA based on existing NLGraph dataset (Li et al., 2024c), respectively, for evaluating the problem-solving capabilities of LVLMs in graph theory. Both of them contain a large number of synthetic visual graphs and the corresponding complex graph theory problems. Besides, Ai et al. (2024) propose a novel instruction-following benchmark for multimodal graph understanding and reasoning in both English and Chinese, which contains a number of real-world graph images with diverse structures across various domains. However, these benchmarks are proposed for challenging graph theory problems or multi-hop reasoning tasks where LVLMs achieve unsatisfactory results. The goal of our VGCure is to explore the fundamental understanding and reasoning abilities of LVLMs on visual graphs in order to explore the underlying reasons for the failure of LVLMs.

Boosting LVLMs for Visual Graph Reasoning Aware of the limitations of current LVLMs on visual graph reasoning tasks, several works propose novel methods to improve the performance of LVLMs on visual graphs. Li et al. (2024d) present a Description-Program-Reasoning (DPR) chain to improve the logical accuracy in reasoning processes via graphical structure description generation and algorithm-aware multi-step reasoning. Wei et al. (2024) propose an end-to-end framework, GITA, to systematically integrate visual information into instruction-based graph reasoning. Furthermore, Deng et al. (2024) introduce GraphVis, which uses a curriculum fine-tuning scheme to train LVLMs on basic graphical feature recognition, followed by reasoning on visual graph QA tasks. Different from current methods which focus on optimizing LVLMs for specific downstream tasks, the proposed MCDGraph is a general-purpose, self-supervised method that can integrally improve the fundamental understanding and reasoning of LVLMs on visual graphs, thereby can be flexibly applied to most downstream graph-learning tasks.

7 Conclusion

In this paper, we first introduce VGCure, a comprehensive benchmark comprising 22 tasks designed to evaluate LVLMs' fundamental understanding and reasoning capabilities on visual graphs. Experimental results on 14 LVLMs reveal prominent limitations of LVLMs on VGCure, particularly in capturing relational or structural information within graphs. Based on this observation, we further propose MCDGraph, a structure-aware self-supervised method designed to improve open-source LVLMs' structural understanding of visual graphs. Experiments validate the effectiveness of MCDGraph, confirming its potential to improve LVLMs' performance on fundamental visual graph learning tasks, as well as the robustness against complex graphs.

Limitations

- **Styles of Visual Graph.** Although we introduce a variety of graph structures from both synthetic and real-world sources, we use the same visualization style, e.g., the same node shapes, colors, and layouts, for the generation of visual graphs. Thus, the single graph style might lead to biased evaluation results.
- **Complexity of Visual Graphs.** Due to the limitations of current LVLMs' performance on visual graph tasks, we restrict the number of nodes in the synthetic graph structure to between 7 and 15, potentially limiting the exploration and improvement of the LVLMs' performance on more complex visual graphs.
- **Evaluation of MCDGRAPH.** We only evaluate MCDGRAPH on the LVLMs' fundamental visual graph understanding and reasoning abilities, lacking the validation in real-world scenarios, e.g., KGQA. In addition, due to resource limitations, we do not evaluate our method on more and larger LVLMs.

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A VGCure Construction

A.1 Graphs Generation

For synthetic graph structures, we use the NetworkX library for random generation and employ hyperparameters to control the expected macroscopic properties of each graph:

- **ER**: This structure takes an edge probablity parameter p, which we choose randomly from $\{0.2, 0.3, 0.4\}$ during generation.
- **BA**: This structure takes the parameter m, which denotes the number of edges to attach from a new node to existing nodes. We choose randomly from $\{2, 3\}$ during generation.
- **SFN**: For this structure, we use the default parameters provided by NetworkX except for the number of nodes during generation.
- **SBM**: This structure takes the sizes of blocks s and the density of edges going from the nodes of one group to nodes of another group p as parameters. During generation, we set s to $[n, m]$ and p to $[[p_1, p_2], [p_2, p_3]]$, where n and m are a random integer from $[3, 7]$ and $[4, 8]$, respectively, and p_1, p_2, p_3 are all randomly selected from $\{0.2, 0.3, 0.4\}$.
- **Star**: This structure requires no parameters other than the number of nodes.

For all the above structures except SBM, the number of nodes during generation is an arbitrary integer in the range $[7, 15]$. To anonymize the visual graph, we use the unique name Ex containing no information to name the nodes in the graph structure, where $x \in \{1, 2, \ldots, n\}$ and n is the number of nodes in the graph. For edges, we choose a random identify from {R1, R2, ... , R10} to name them. The name can be repeated for each edge. The examples of synthetic visual graph are shown in Figure 6.

A.2 Tasks Generation

To ensure the correctness of the generated samples, we first search for relevant paths in the given graph that satisfy the conditions of the task. Then the final QA samples and FC samples are generated based on the paths and corresponding templates. If no path exists, the generation of samples for the task is skipped. The final statistics of VGCure and the example samples with undirected graph for each task are shown in Table 9 and Table 10, respectively.

B Experimental Setup for Evaluation

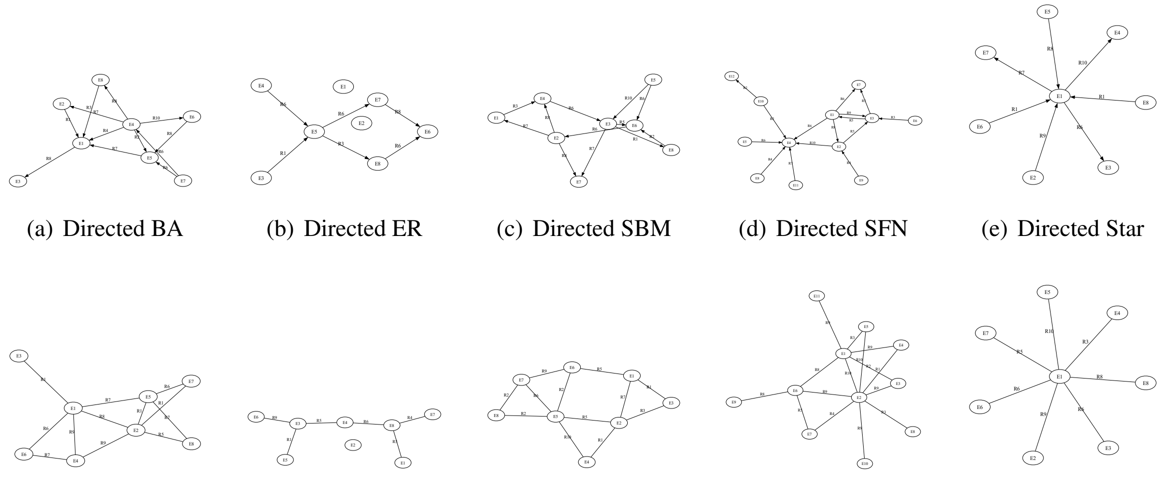
B.1 Prompts

To facilitate the LVLMs to understand the content in the visual graph, we take a **visual graph description** in addition to the input during test.

- **Directed Visual Graph Description**: The given image shows a graph where circles represent nodes, with the content inside indicating the node names. The arrowed lines connecting two nodes represent edges, and the content in the middle of the edges indicates the edge names.
- **Undirected Visual Graph Description**: The given image shows a graph where circles represent nodes, with the content inside being the node names. The lines connecting two nodes represent edges, and the content in the middle of the edges represents the edge names.

The complete prompt for QA samples are as follow:

- **NN, CR, RA, SRN, NQ**: [Visual Graph Description] Answer the given questions based on the graph in the image.\nQuestion: [question]\nPlease provide the answer directly without the reasoning process and present your answer in the LIST format: [Entity1, Entity2, ...].
- **NR**: [Visual Graph Description] Answer



(a) Directed BA (b) Directed ER (c) Directed SBM (d) Directed SFN (e) Directed Star

(f) Undirected BA (g) Undirected ER (h) Undirected SBM (i) Undirected SFN (j) Undirected Star

Figure 6: Examples of synthetic visual graphs.

the given questions based on the graph in the image.\nQuestion: [question]\nPlease provide the answer directly without the reasoning process and present your answer in the LIST format: [Relation1, Relation2, ...].

- **CP**: [Visual Graph Description] Answer the given questions based on the graph in the image.\nQuestion: [question]\nIf yes, please output all the shortest paths in the LIST Format and conclude your answer with "Yes. The shortest paths are [[Entity1, Entity2,...], [Entity3, Entity4,...], ...]". If no path exists, please answer "No".
- **NNu, EN, DQ**: [Visual Graph Description] Answer the given questions based on the graph in the image.\nQuestion: [question]\nPlease provide the answer directly without the reasoning process.

The complete prompt for FC samples are as follow:

- [Visual Graph Description] Verify the truth of the given claim against the graph in the image.\nClaim: [claim]\nThe answer should contain only "True" or "False", without reasoning process.

B.2 Evaluation Metrics

For the QA samples of NQ, NN, CR, RA, SRN, and NR tasks, we use (macro-averaged) F1 score and Hits@1 as in the previous QA benchmarks (Rajpurkar et al., 2016; Zhang et al., 2018). For the QA samples of CP task, we employ EM_F1, which iss the macro F1 score calculated based on the exact match between the predicted path and the ground truth path, and Label_Acc, which measures the accuracy of the model's prediction on whether a path exists or not. For the QA samples of NNu, EN and DQ tasks, we compute the accuracy between predicted answers and ground truth. For the FC samples of all tasks, following Si et al. (2024), we use macro F1 and accuracy as the metrics.

C Experimental Setup for Training

C.1 Training Samples

Graphs Generation For Masked Graph Infilling and Graph Description task, we use the same synthetic visual graph generation strategy as VGCure. As for the Contrastive Graph Discrimination, in order to reduce the difficulty, we limited the number of nodes per graph structure to $[4, 8]$ during generation.

Task Instruction To increase the diversity of samples, we designed various instructions with similar semantics for each task in the MCDGraph.

- **Masked Graph Infilling**
  - Using the given set of triples, predict the word that should fill the [MASK] position in the knowledge graph in the image.
  - Based on the provided triples, determine the correct word to complete the [MASK] position in the knowledge graph shown in the image.
  - Given the set of triples, predict the word

Structue Type		# Graphs	Number of QA Samples												Avg. Nodes	Avg. Edges
			NN	CR	CN	RA	SRN	NR	CP	NNu	EN	DC	DQ	NQ		
BA	Directed	400	400	400	400	370	324	400	400	400	400	400	400	400	10.98	20.99
	Undirected	400	400	400	400	400	400	400	400	400	400	400	400	400	11.02	21.04
ER	Directed	400	387	377	377	304	229	387	400	400	400	400	400	400	11.06	17.69
	Undirected	400	396	395	396	346	346	395	400	400	400	400	400	400	11.00	17.41
SBM	Directed	400	399	392	392	314	399	400	253	400	400	400	400	400	10.99	17.13
	Undirected	400	399	399	399	399	400	371	371	400	400	400	400	400	11.04	17.32
SFN	Directed	400	400	400	400	331	149	400	400	400	400	400	400	400	10.95	13.86
	Undirected	400	400	400	400	400	400	379	379	400	400	400	400	400	11.05	12.80
Star	Directed	400	396	388	388	350	288	396	400	400	400	400	400	400	12.05	11.05
	Undirected	400	400	400	400	393	393	400	400	400	400	400	400	400	12.11	11.11
DBLP	Directed	200	196	192	192	140	196	200	145	200	200	200	200	200	7.85	17.76
	Undirected	200	200	200	200	173	173	200	200	200	200	200	200	200	7.85	17.76
Dbpedia	Directed	200	186	185	185	93	186	200	101	200	200	200	200	200	8.13	11.36
	Undirected	200	200	200	200	155	155	200	200	200	200	200	200	200	8.13	11.36
Openflights	Directed	100	100	100	100	65	100	100	63	100	100	100	100	100	5.51	13.59
	Undirected	100	100	100	100	90	90	100	100	100	100	100	100	100	5.51	13.59
PubChemQC	Directed	400	400	138	400	400	119	119	37	400	400	400	400	400	5.45	4.76
	Undirected	400	400	398	400	398	400	151	151	400	400	400	400	400	5.45	4.76
Social Network	Directed	300	262	254	254	134	262	300	124	300	300	300	300	300	7.57	9.25
	Undirected	300	299	297	299	238	238	297	300	300	300	300	300	300	7.57	9.25
Total		6400	6320	6015	6282	5493	5247	5795	5224	6400	6400	6400	6400	6400	-	-

Table 9: Statistics of VGCURE benchmark, where *# Graphs* represents the number of visual graphs, *Avg.Nodes* and *Avg.Edges* denote the average number of nodes and edges in the graph, respectively. For each task, the number of QA samples is the values in the table, except for CN and DC, which have no QA samples, and the number of FC samples is **twice** the value in the table.

that should be placed in the [MASK] position within the knowledge graph in the image.

  - Use the given triples to predict the appropriate word for the [MASK] position in the knowledge graph depicted in the image.
  - Using the set of triples, identify the word that should fill the [MASK] position in the knowledge graph in the image.
  - Based on the set of triples, predict the correct word for the [MASK] position in the knowledge graph in the image.
  - Given the triples, predict the word that fits the [MASK] position in the knowledge graph present in the image.
  - Using the triples provided, determine the word that should be used to fill the [MASK] position in the knowledge graph in the image.
  - Predict the word that should occupy the [MASK] position in the knowledge graph in the image, based on the given triples.
  - Using the provided triples, identify the word that should complete the [MASK] position in the knowledge graph in the image.

- **Contrastive Graph Discrimination**
  - Determine whether Graph A and Graph B in the given image are identical.
  - Assess if Graph A and Graph B depicted in the image are equivalent.
  - Evaluate whether the structures of Graph A and Graph B in the provided image match.
  - Identify if there are any differences between Graph A and Graph B in the shown image.
  - Check if Graph A and Graph B illustrated in the image are the same.
  - Analyze the image to determine if Graph A is identical to Graph B.
  - Investigate whether Graph A and Graph B in the given image are congruent.
  - Examine the provided image to see if Graph A and Graph B are equivalent.

Task	QA sample	FC sample (Label)
NNu	Q: How many nodes are there in this graph? A: 11	There are 11 nodes in this graph. (True) There are 15 nodes in this graph. (False)
EN	Q: How many edges are there in this graph? A: 15	There are 15 edges in this graph. (True) There are 19 edges in this graph. (True)
DC	-	This graph is an undirected graph. (True) This graph is a directed graph. (True)
DQ	Q: What is the degree of E7 in this graph? A: 2	The degree of E7 in this graph is 2. (True) The degree of E7 in this graph is 7. (False)
NQ	Q: Which nodes are neighbors of E6 in this graph? A: [E1, E2, E7, E9]	E7 is a neighbors of E6 in this graph. (True) E10 is a neighbors of E6 in this graph. (False)
NN	Q: Which entities are connected to the entity that has R10 with E2 via R9? A: [E11, E4]	E4 is connected to the entity that has R10 with E2 via R9. (True) E3 is connected to the entity that has R10 with E2 via R9. (False)
CR	Q: Which entities are connected to E8 via R3 as well as connected E1 via R10? A: [E2]	E2 is connected to E8 via R3 as well as connected E1 via R10. (True) E3 is connected to E8 via R3 as well as connected E1 via R10. (False)
CN	-	E5 and E2 share a common neighbor. (True) E10 and E11 share a common neighbor. (False)
RA	Q: Which entities are connected to E1 via the same relation between E11 and E1? A: [E4]	E4 is connected to E1 via the same relation between E11 and E1. (True) E2 is connected to E1 via the same relation between E11 and E1. (False)
SRN	Q: Which entities are both connected to E2 via R10? A: [E1, E5]	E5 and E1 both connected to E2 via R10. (True) E5 and E3 are both connected to E2 via R10. (False)
NR	Q: What is the relation between E2 and the entity that is connected to E6 via R8? A: [R10]	The relation between E2 and the entity that is connected to E6 via R8 is R10. (True) The relation between E2 and the entity that is connected to E6 via R8 is R4. (False)
CP	Q: Is there a path between E5 and E3? A: Yes. The shortest paths are [[E5, E1, E3], [E5, E2, E3]]	[E5, E1, E3] is one of the shortest path between E5 and E3. (True) [E5, E11, E2, E3] is one of the shortest path between E5 and E3. (False)

Table 10: Examples with undirected graph for each task in VGCURE. These samples all correspond to the SFN graph shown in Figure 6(i).

Model	Lora_rank	Lora_ alpha	Global Batch Size	Learning rate	Epoch
Qwen2-VL	8	16	64	1e-4	5
InternVL2	64	128	64	4e-5	1

Table 11: Hyperparameters for training

  - Compare Graph A and Graph B in the image to establish their similarity.
  - Confirm if Graph A and Graph B presented in the image are indistinguishable.
- **Graph Description**
  - Describe the given graph, including the number of nodes, the number of edges, and the names of all the nodes.
  - Provide a description of the given graph, specifying the number of nodes, edges, and listing all the node names.
  - Analyze the given graph by stating the number of nodes, edges, and enumerating the names of all the nodes.
  - Summarize the graph by detailing the number of nodes, edges, and listing the names of each node.
  - Explain the graph, including the count of nodes and edges, and provide the names of all the nodes.
  - Describe the graph, indicating how many nodes and edges it contains, and listing all the node names.
  - Provide an overview of the graph, mentioning the number of nodes, edges, and the names of all nodes.
  - Characterize the given graph, noting the number of nodes, edges, and listing all the node names.
  - Detail the structure of the given graph, including node and edge counts, and providing a list of all node names.
  - Give a description of the graph, including the total number of nodes, edges, and the names of all the nodes.

Similar to VGCURE, we include a visual graph description in input as well. Thus, the complete **task instruction** I for each training sample in MCDGRAPH is "[Visual Graph Description] [Instruction]".

Number of Samples For Masked Graph Infilling task, we generate **10,000 samples**, with half of the samples masking nodes and the other half masking edges. For Contrastive Graph Discrimination tasks, **5,000 samples**, where each sample consists of two visual graphs, are generated automatically. Similarly, the Graph Description task also contains **5,000 samples**, each corresponding to a unique visual graphs.

C.2 Implementation Details

For Qwen2-VL, we employ the LoRA-based supervised fine-tuning scripts provided by LLaMA-

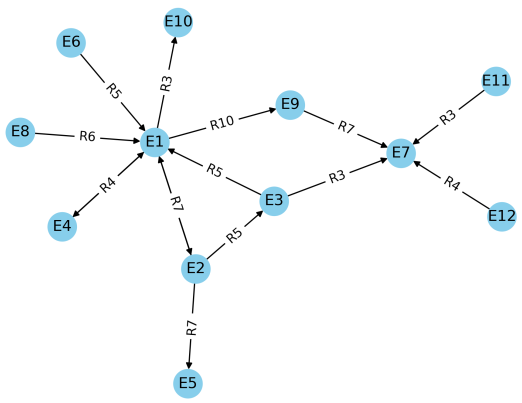


Figure 7: An example of visual graph with different style for the experimental results in Table 8

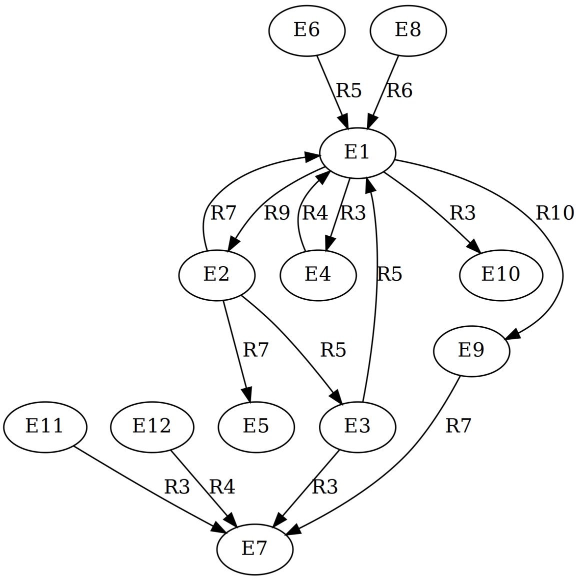


Figure 8: An example of visual graph with different style for the experimental results in Table 12

Factory[3]. For InternVL2, we perform LoRA-based fine-tuning based on the code and documentation provided officially[4]. The hyperparameters used for training are shown in Table 11. All the experiments are finished on 4 A100 GPUs with 80GB memory.

D Impact on Visual Styles

The examples of **the same** visual graph with different styles are illustrated in Figure 7 and Figure 8. The results of the visual style in Figure 8 are presented in Table 12.

[3] https://github.com/hiyouga/LLaMA-Factory

[4] https://github.com/OpenGVLab/InternVL

Models	Understanding					Reasoning						
	NNu	EN	DC	DQ	NQ	NN	CR	CN	RA	SRN	NR	CP
	QA Samples											
Qwen2-VL	95.30	20.80	-	40.00	13.95	8.73	19.04	-	11.73	14.89	13.16	3.17
w MCDGraph	98.80 ↑	17.30	-	50.50 ↑	22.33 ↑	11.56 ↑	21.92 ↑	-	11.05	17.84 ↑	11.60	0.12
InternVL2	85.20	17.90	-	39.60	24.21	19.99	22.26	-	8.06	19.46	12.03	2.25
w MCDGraph	97.20 ↑	35.70 ↑	-	43.00 ↑	26.46 ↑	19.12	23.54 ↑	-	11.00 ↑	20.45 ↑	14.80 ↑	12.11 ↑
	FC Samples											
Qwen2-VL	70.88	68.06	66.94	57.90	65.09	43.62	67.32	34.28	34.79	53.23	42.54	42.89
w MCDGraph	76.36 ↑	58.47	85.20 ↑	74.38 ↑	73.69 ↑	56.97 ↑	75.05 ↑	48.68 ↑	53.84 ↑	60.99 ↑	60.44 ↑	56.93 ↑
InternVL2	68.42	38.35	91.84	64.58	65.45	62.91	72.42	48.17	34.60	57.88	57.77	52.48
w MCDGraph	69.45 ↑	69.11 ↑	84.10	62.09	74.68 ↑	71.52 ↑	75.19 ↑	52.97 ↑	50.89 ↑	61.00 ↑	66.44 ↑	43.19

Table 12: Model performance (Acc/F1/EM_F1 for QA and F1 for FC) on various tasks with different visual styles.

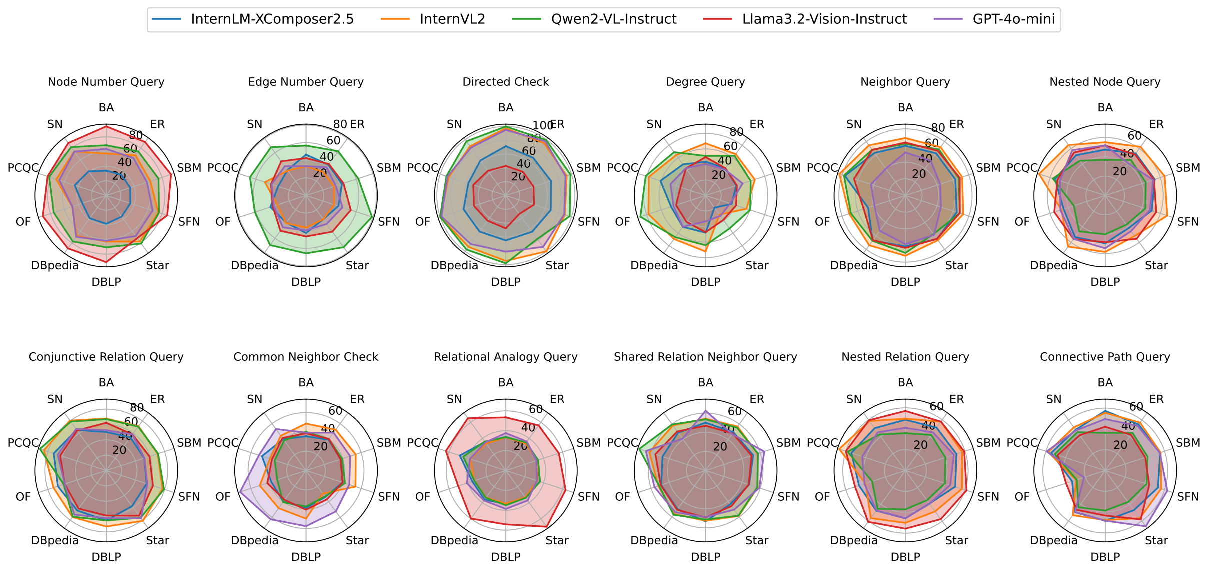


Figure 9: Model performance (F1) on FC samples across various graph structures and tasks. Each radar chart corresponds to a specific question type, showing comparative results on QA samples across all graph types, where OF, PCQC and SN denotes Openflights, PubChemQC and Social network, respectively.

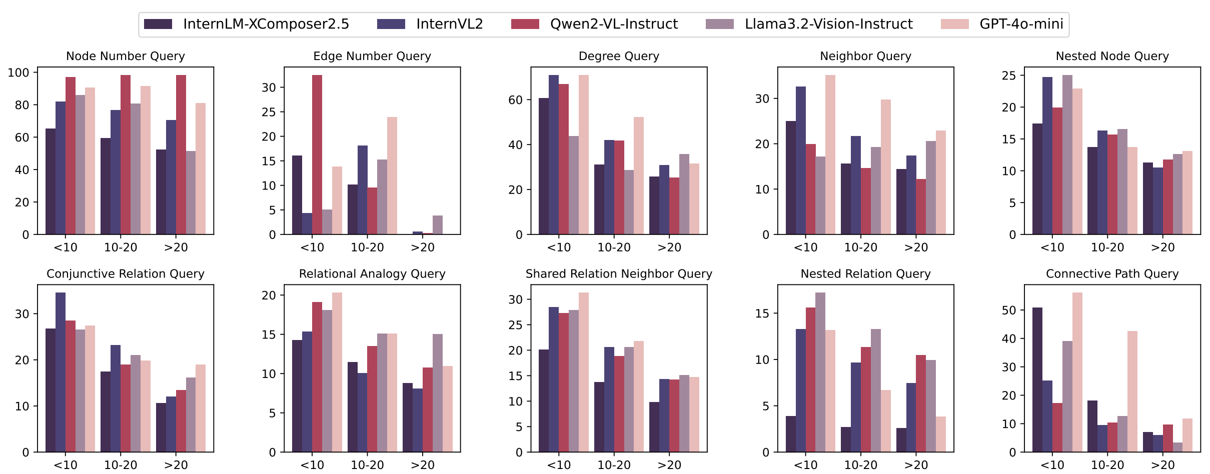


Figure 10: Model performance (F1/Acc) comparison on QA samples across various tasks and **edge** ranges.

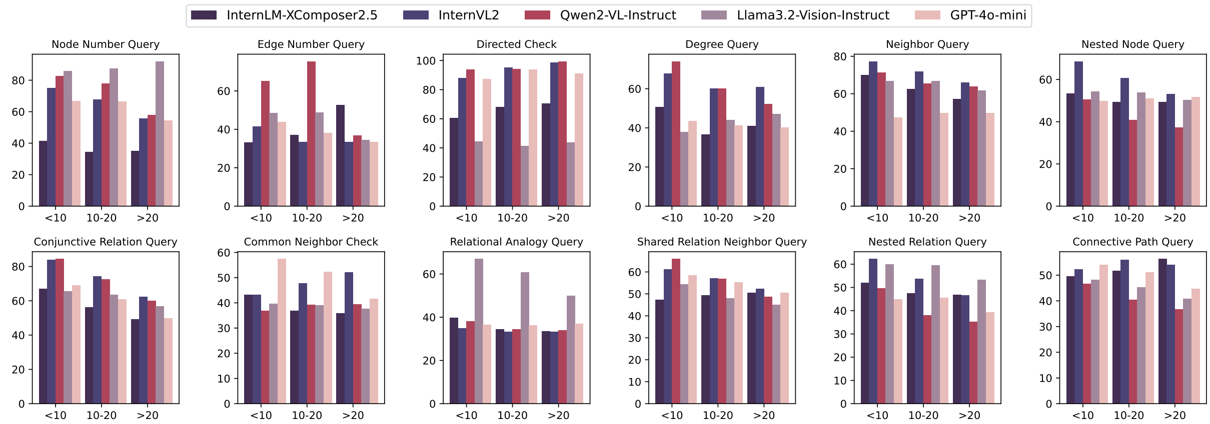


Figure 11: Model performance (F1) comparison on FC samples across various tasks and **edge** ranges.

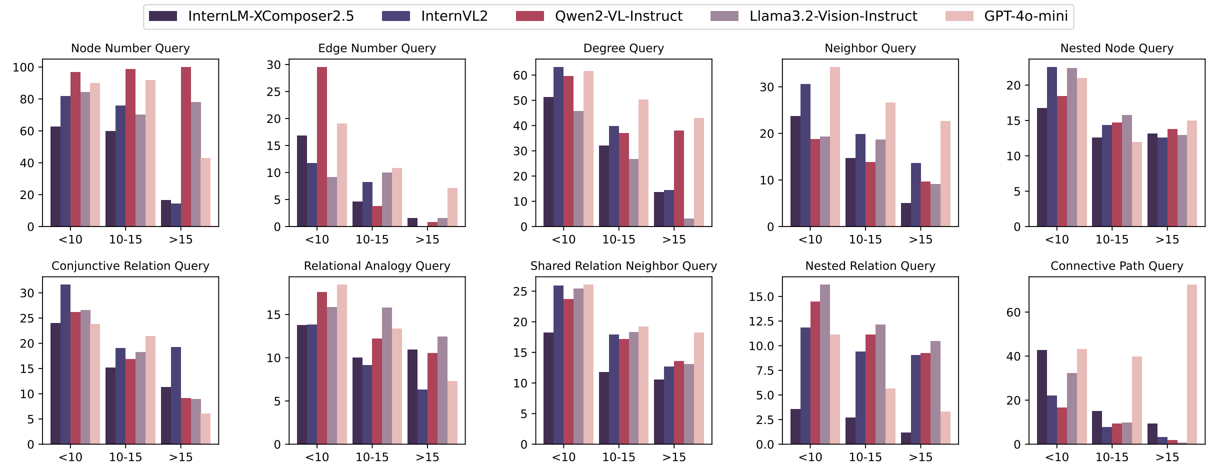


Figure 12: Model performance (F1/Acc) comparison on QA samples across various tasks and **node** ranges.

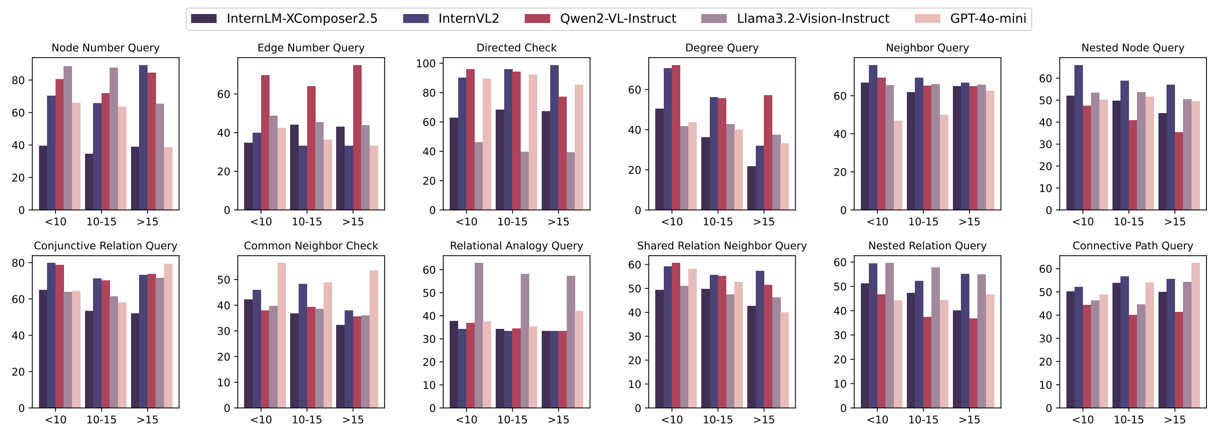


Figure 13: Model performance (F1) comparison on FC samples across various tasks and **node** ranges.

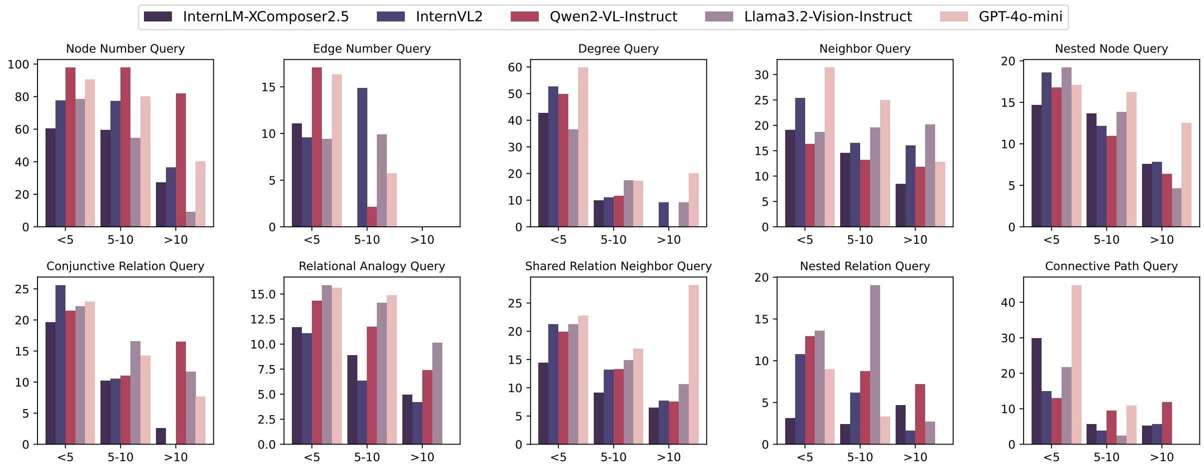


Figure 14: Model performance (F1/Acc) comparison on QA samples across various tasks and **average degree**.

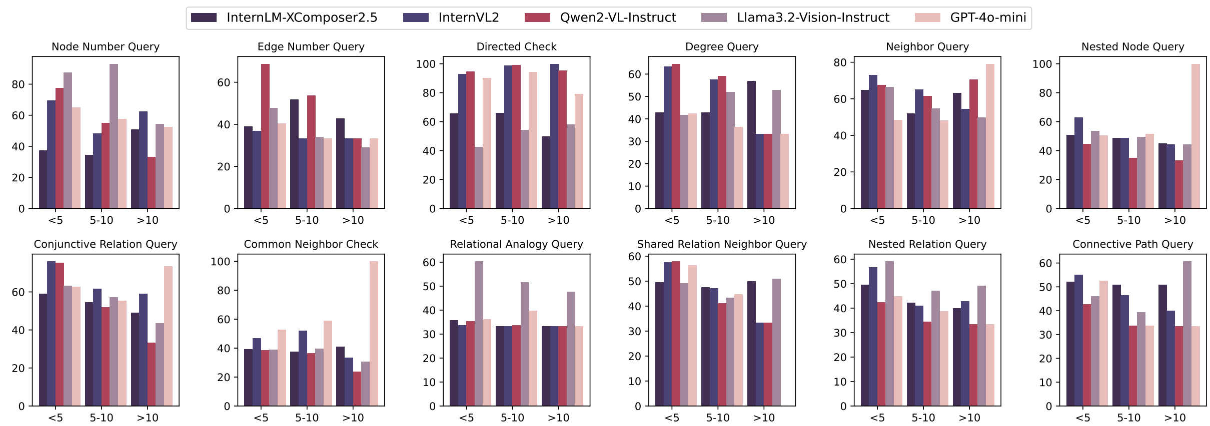


Figure 15: Model performance (F1) comparison on FC samples across various tasks and **average degree**.

QA Samples																	
Models	**Understanding**					**Reasoning**											
	NNu	**EN**	**DQ**	**NQ**		**NN**		**CR**		**RA**		**SRN**		**NR**		**CP**	
	Acc	**Acc**	**Acc**	**F1**	**Hits@1**	**F1**	**Hits@1**	**F1**	**Hits@1**	**F1**	**Hits@1**	**F1**	**Hits@1**	**F1**	**Hits@1**	**EM_F1**	**Label_Acc**
Qwen2-VL	97.80	16.38	48.09	16.18	38.12	16.52	28.34	21.02	48.57	14.19	27.96	19.48	56.42	12.73	25.07	12.90	38.06
w MCDGraph	98.34 ↑	25.92 ↑	60.94 ↑	25.44 ↑	63.44 ↑	13.32	28.97 ↑	26.14 ↑	63.84 ↑	13.14	28.42 ↑	20.74 ↑	62.21 ↑	14.44 ↑	23.71 ↑	11.95	63.98 ↑
InternVL2	77.45	9.78	50.75	25.01	68.58	18.30	30.82	24.87	59.31	10.83	17.12	20.72	59.99	10.58	18.97	14.53	43.97
w MCDGraph	95.68 ↑	40.45 ↑	54.78 ↑	28.80 ↑	72.72 ↑	19.43 ↑	27.86	28.53 ↑	67.61 ↑	11.67 ↑	19.81 ↑	22.34 ↑	61.67 ↑	16.50 ↑	40.21 ↑	12.76	25.23

Table 13: Performance Improvement of MCDGraph on QA samples across various tasks. ↑ indicates an improvement compared to the original model.

FC Samples																							
Models	**Understanding**										**Reasoning**													
	NNu		**EN**		**DC**		**DQ**		**NQ**		**NN**		**CR**		**CN**		**RA**		**SRN**		**NR**		**CP**	
	F1	**Acc**	**F1**	**Acc**	**F1**	**Acc**	**F1**	**Acc**	**F1**	**Acc**	**F1**	**Acc**	**F1**	**Acc**	**F1**	**Acc**	**F1**	**Acc**	**F1**	**Acc**	**F1**	**Acc**	**F1**	**Acc**
Qwen2-VL	76.50	77.67	68.26	68.27	94.92	94.94	64.32	67.40	67.34	68.76	44.17	53.77	74.28	75.24	38.52	51.10	35.28	50.55	57.07	59.18	42.08	52.95	42.25	53.38
w MCDGraph	89.58 ↑	89.69 ↑	65.80	68.64 ↑	95.84 ↑	95.84 ↑	77.10 ↑	77.23 ↑	79.75 ↑	80.03 ↑	60.71 ↑	63.35 ↑	83.07 ↑	83.08 ↑	53.90 ↑	54.12 ↑	53.48 ↑	53.69 ↑	64.17 ↑	64.21 ↑	64.12 ↑	65.51 ↑	60.11 ↑	60.17 ↑
InternVL2	68.63	71.18	36.82	50.23	93.17	93.18	63.28	63.84	72.81	73.27	62.46	63.62	75.37	76.18	47.12	50.40	33.70	50.14	56.98	57.42	55.94	58.42	54.71	54.71
w MCDGraph	76.55 ↑	77.71 ↑	71.98 ↑	72.02 ↑	90.04	90.50	56.83	58.53	80.98 ↑	81.89 ↑	73.14 ↑	73.98 ↑	80.23 ↑	80.69 ↑	52.09 ↑	52.99 ↑	52.81 ↑	57.08 ↑	59.07 ↑	60.07 ↑	69.03 ↑	70.24 ↑	45.82	49.27

Table 14: Performance Improvement of MCDGraph on FC samples across various tasks. ↑ indicates an improvement compared to the original model.

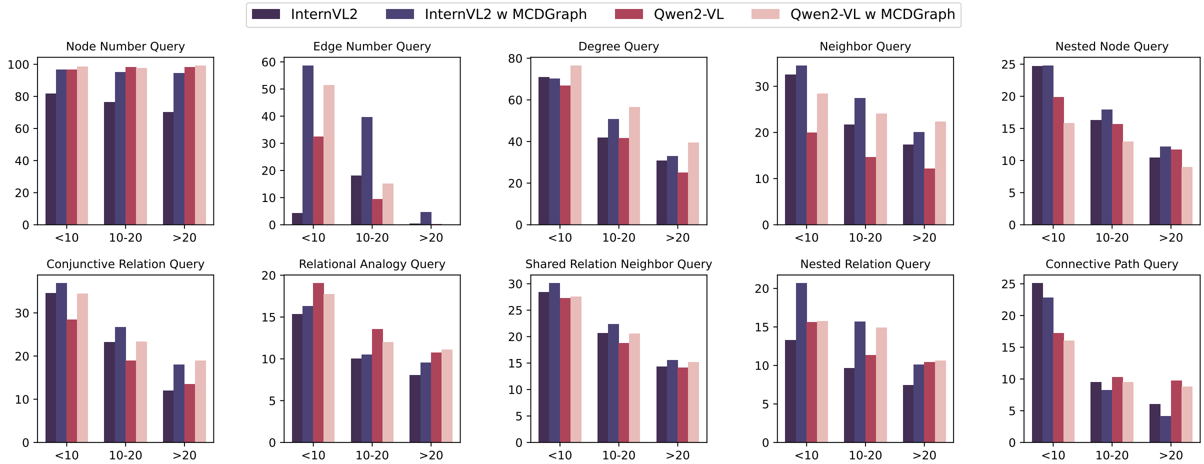


Figure 16: Performance Improvement of MCDGRAPH (F1/Acc) on QA samples across various tasks and **edge** ranges.

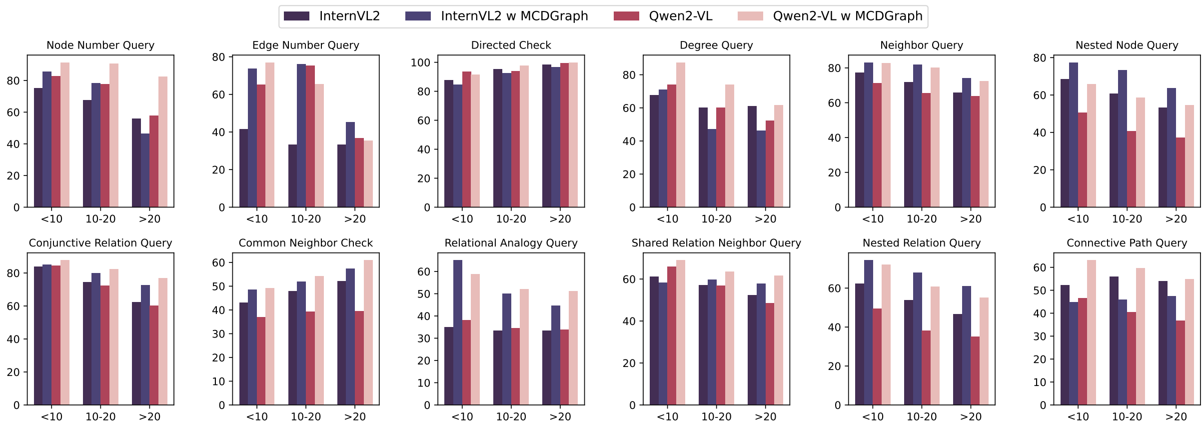


Figure 17: Performance Improvement of MCDGRAPH (F1) comparison on FC samples across various tasks and **edge** ranges.

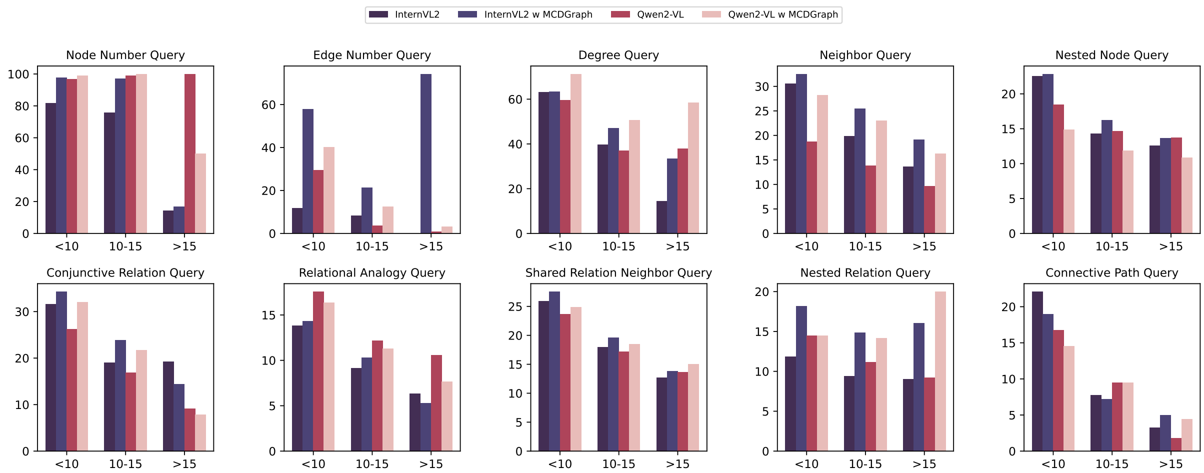


Figure 18: Performance Improvement of MCDGRAPH (F1/Acc) on QA samples across various tasks and **node** ranges.

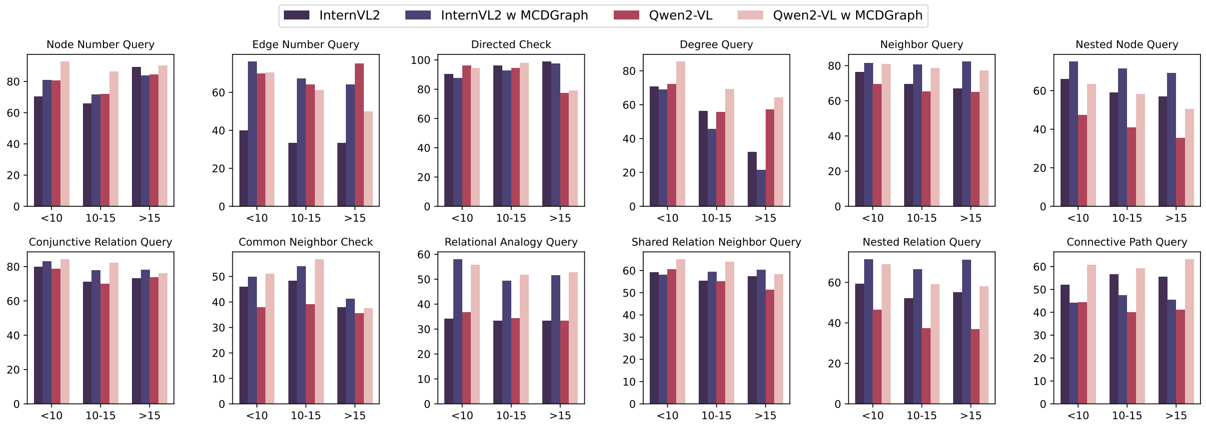


Figure 19: Performance Improvement of MCDGRAPH (F1) comparison on FC samples across various tasks and **node** ranges.

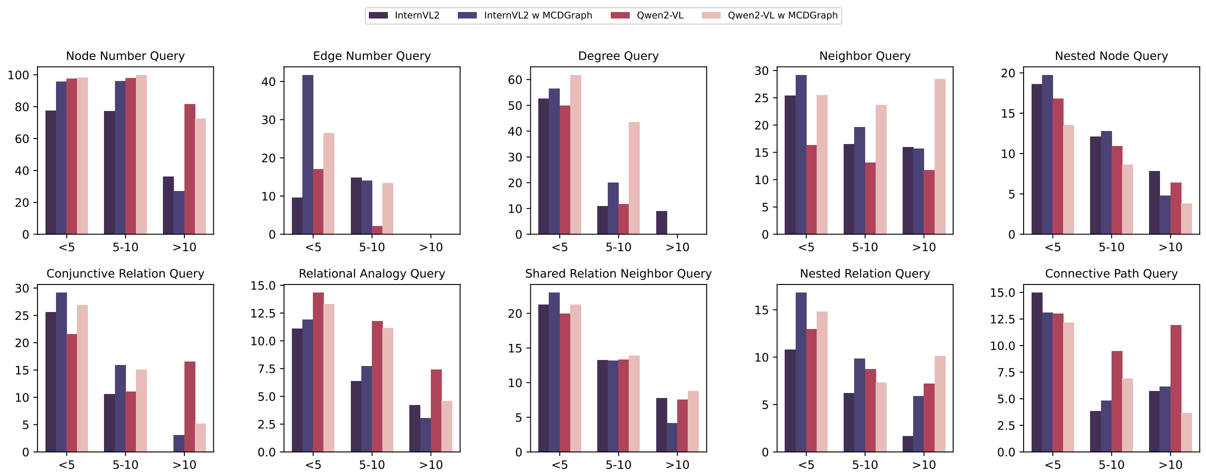


Figure 20: Performance Improvement of MCDGRAPH (F1/Acc) on QA samples across various tasks and **average degree**.

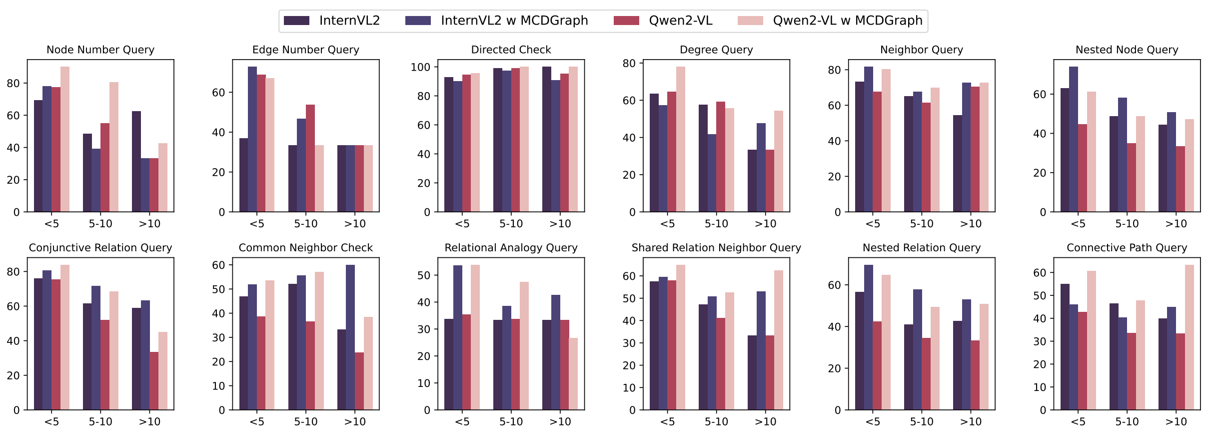


Figure 21: Performance Improvement of MCDGRAPH (F1) comparison on FC samples across various tasks and **average degree**.

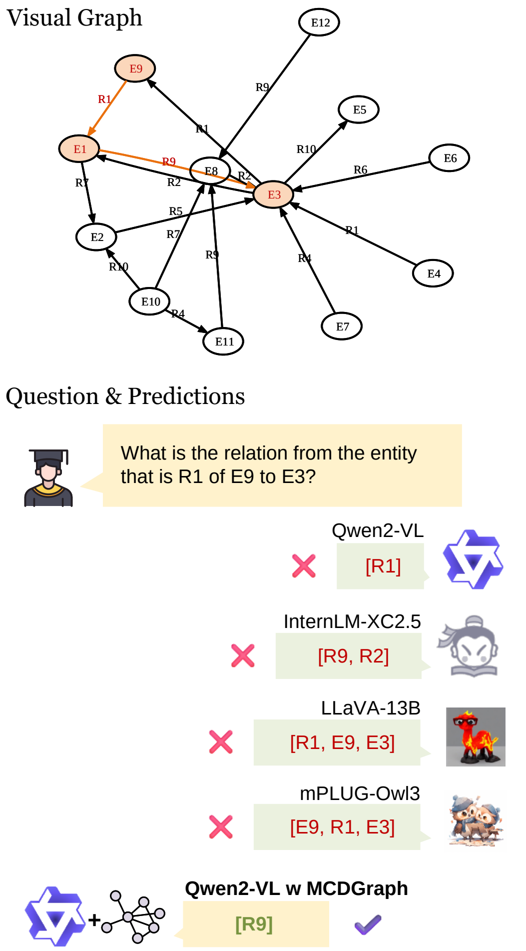


Figure 22: A case of Nested Relation Query task.