Evaluating and Enhancing the Vulnerability Reasoning Capabilities of Large Language Models

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Abstract

Large Language Models (LLMs) have demonstrated remarkable proficiency in vulnerability detection. However, a critical reliability gap persists: models frequently yield correct detection verdicts based on hallucinated logic or superficial patterns that deviate from the actual root cause. This misalignment remains largely obscured because contemporary benchmarks predominantly prioritize coarse-grained classification metrics, lacking the granular ground truth required to evaluate the underlying reasoning process. To bridge this gap, we first construct a benchmark consisting of two datasets: (1) real-world vulnerabilities with expert-curated causal reasoning as ground truth, and (2) semantically equivalent code perturbations for assessing reasoning robustness. Our large-scale empirical study reveals that even state-of-the-art models struggle to maintain logical consistency during semantic code comprehension, exhibiting 12 systematic failure patterns. Addressing these limitations, we propose DAGVUL, a novel framework that models vulnerability reasoning as a Directed Acyclic Graph (DAG) generation task. Unlike linear chain-of-thought (CoT), our approach explicitly maps causal dependencies to enforce structural consistency. By further introducing Reinforcement Learning with Verifiable Rewards (RLVR), we align model reasoning trace with program-intrinsic logic. Experimental results demonstrate that our framework improves the reasoning F1-score by an average of 18.9% over all the baselines. Remarkably, our 8B-parameter implementation not only outperforms existing models of comparable scale but also surpasses specialized large-scale reasoning models, including Qwen3-30B-Reasoning and GPT-OSS-20B-High. It is even competitive with state-of-the-art models like Claude-Sonnet-4.5 (75.47% vs. 76.11%), establishing new efficiency in vulnerability reasoning across model scales.

1 Introduction

Automated vulnerability detection has long been dominated by the rigid rule-based paradigms of Static (SAST) and Dynamic (DAST) Application Security Testing [1–3]. Despite their widespread adoption, these traditional tools are increasingly constrained by escalating modern software complexity, often suffering from high false-positive rates, prohibitive scanning overheads, and an intrinsic inability to capture context-dependent logic flaws [4, 5].

The advent of Large Language Models (LLMs) represents a significant paradigm shift from rigid syntactic pattern matching to deep semantic comprehension [6–8]. By learning from vast code corpora, LLMs can identify complex dependencies and even autonomously exploit zero-day vulnerabilities [9, 10] that elude rule-based systems. Preliminary evaluations show that LLMs can achieve detection performance competitive with state-of-the-art (SOTA) SAST tools in binary classification tasks [11]. However, for LLM-based security auditing systems, **the reliability of the underlying reasoning, specifically the ability to correctly articulate the causal chain of a vulnerability, is far more important than the binary verdict itself**. Flawed reasoning in an automated auditor not only undermines trust but can lead to catastrophic failures in downstream tasks like automated vulnerability repair [12].

Despite its importance, the advancement of LLM vulnerability reasoning is fundamentally hindered by two major gaps. First, on the evaluation side, current benchmarks often lack the structured, expert-curated ground truth required to verify the logical fidelity of reasoning traces [13, 14]. **This obscures whether LLMs arrive at correct answers through rigorous logical reasoning or merely through lucky guesses based on superficial patterns.** Second, on the enhancement side, there is a severe lack of high-quality, vulnerability-related reasoning data [15], which limits our ability to effectively train and align models toward logical consistency.

In this paper, we address this gap through a large-scale empirical study examining the reasoning fidelity of SOTA LLMs. We first introduce a dual-component benchmark comprising (1) real-world vulnerabilities annotated with ground-truth reasoning, and (2) synthetically perturbed code variants with semantic-preserving transformations for robustness evaluation. Our study reveals a concerning **"Flawed Reasoning, Correct Answer"** phenomenon, where **36.4%** of correct

binary verdicts stem from hallucinatory or irrelevant logic, rather than sound reasoning. Through systematic qualitative analysis, we taxonomize 12 distinct failure modes observed across LLM reasoning trace.

Motivated by these findings, we propose DAGVUL, a novel framework that models vulnerability reasoning as a Directed Acyclic Graph (DAG) generation task to enforce structural consistency in causal inference. Unlike linear chain-of-thought approaches that may propagate errors sequentially, our DAG formulation explicitly captures the dependency relationships among reasoning steps, ensuring logical coherence throughout the detection process. To further align model reasoning with program-intrinsic causal logic, we introduce Reinforcement Learning with Verifiable Rewards (RLVR), which leverages program semantics to guide the learning process. Experimental results demonstrate substantial improvements in reasoning quality: our framework achieves significant gains in both precision and F1-score over strong baselines including Retrieval-Augmented Generation (RAG) and Supervised Fine-Tuning (SFT). Notably, despite being built upon 8B-parameter models, DAGVUL surpasses specialized large-scale reasoning models such as Qwen3-30B-Reasoning and GPT-OSS-20B-High, and even approaches SOTA models like Claude-Sonnet-4.5 [16], demonstrating that **structured reasoning mechanisms can be more effective than simply scaling model size for complex program analysis tasks**.

In summary, our contributions are as follows:

1. We conduct the first large-scale empirical study focused specifically on the vulnerability **reasoning capabilities** of 10 LLMs, uncovering the widespread "Flawed Reasoning, Correct Answer" issue. Through extensive manual open coding of 200 erroneous reasoning traces, we establish a taxonomy of 12 systematic reasoning failure modes.

2. We construct a **high-quality benchmark for reasoning evaluation**, comprising: (1) a real-world dataset of 5,078 CVEs across 149 CWE types, featuring fine-grained ground truths; and (2) a robustness dataset featuring 26 semantic-preserving transformations, where 100 critical samples are manually annotated by authors to ensure the vulnerability characteristics remain unchanged.

3. We propose DAGVUL, a framework that models vulnerability reasoning as DAG generation. By integrating RLVR, we align model reasoning trace with program-intrinsic logic, achieving an average 18.9% F1-score improvement and outperforming specialized reasoning models.

2 Definition and Background

2.1 Vulnerability Reasoning Task

Traditionally, automated vulnerability detection is modeled as a **binary classification task**. Formally, given a code snippet C, the goal is to learn a mapping $f : C \rightarrow Y$, where $Y \in \{0, 1\}$ denotes the absence or presence of a vulnerability. Current evaluations typically focus on maximizing the probability of the label $P(Y|C)$, measuring performance via coarse-grained metrics like F1 score [17–23]. However, this paradigm inherently ignores the intermediate logic, making it impossible to distinguish whether a model genuinely understands the vulnerability or merely "guesses" through surface pattern matching.

To address this limitation, we redefine the task as **Vulnerability Reasoning**. Instead of predicting a solitary label, the model must generate a tuple (Y, R). Here, Y remains the classification verdict, while R represents the *reasoning trace*, which explicitly identifies the root cause and triggering logic. The optimization objective thus shifts from maximizing $P(Y|C)$ to maximizing the joint probability $P(Y, R|C)$. Consequently, successful evaluation requires a more rigorous standard than simple detection accuracy. We define **Reasoning Success** as satisfying two conditions: the verdict must be correct ($\hat{Y} = Y$), AND the reasoning trace must be verified against the ground truth ($\text{Verify}(\hat{R}, R_{gt}) = \text{True}$).

Table 1: Comparison of benchmarks for vulnerability reasoning. (✓ = Supported, ✗ = Not Supported, ● = Partially Supported).

Study	Real-World Dataset	Label Accuracy	Comprehensive Context	Fine-grained Ground Truth	Perturb Method	Open Coding
SecLLMHolmes [24]	✗	✓	✗	●	✓	✗
CORRECT [25]	✓	✓	✓	●	✗	✗
R2Vul [11]	✓	✓	✗	✗	✗	●
SECVULEVAL [26]	✓	✓	✓	✗	✗	●
ReVD [27]	✓	●	✗	✗	✗	✗
SV-TrustEval-C [28]	✗	✓	✗	✓	✓	✗
VulnLLM-R [15]	✓	✓	●	✗	✗	✗

As shown in Table 1, while recent years have seen the emergence of new benchmarks [11, 15, 24–28] shifting focus from binary classification to vulnerability reasoning, most existing works suffer from limitations that undermine the validity of reasoning evaluation. First, regarding **comprehensive context**, although recent datasets have improved label accuracy via techniques like patch untangling, they predominantly rely on isolated functions or files. This isolation strips away critical cross-file dependencies, rendering the evaluation of complex reasoning unreliable. Second, concerning **fine-grained ground truth**, most benchmarks lack definitive explanations for the vulnerability's root cause. They either resort to non-scalable manual sampling to audit reasoning quality or simply utilize unreliable CVE descriptions or coarse-grained CWE categories as the ground truth. Third, few studies incorporate **perturbation methods** to evaluate the robustness of reasoning against semantic-preserving code transformations. Finally, there is a notable absence of **open coding** methodologies [29, 30]; most works focus solely on quantitative metrics, neglecting the systematic qualitative analysis required to categorize and understand specific reasoning failure modes.
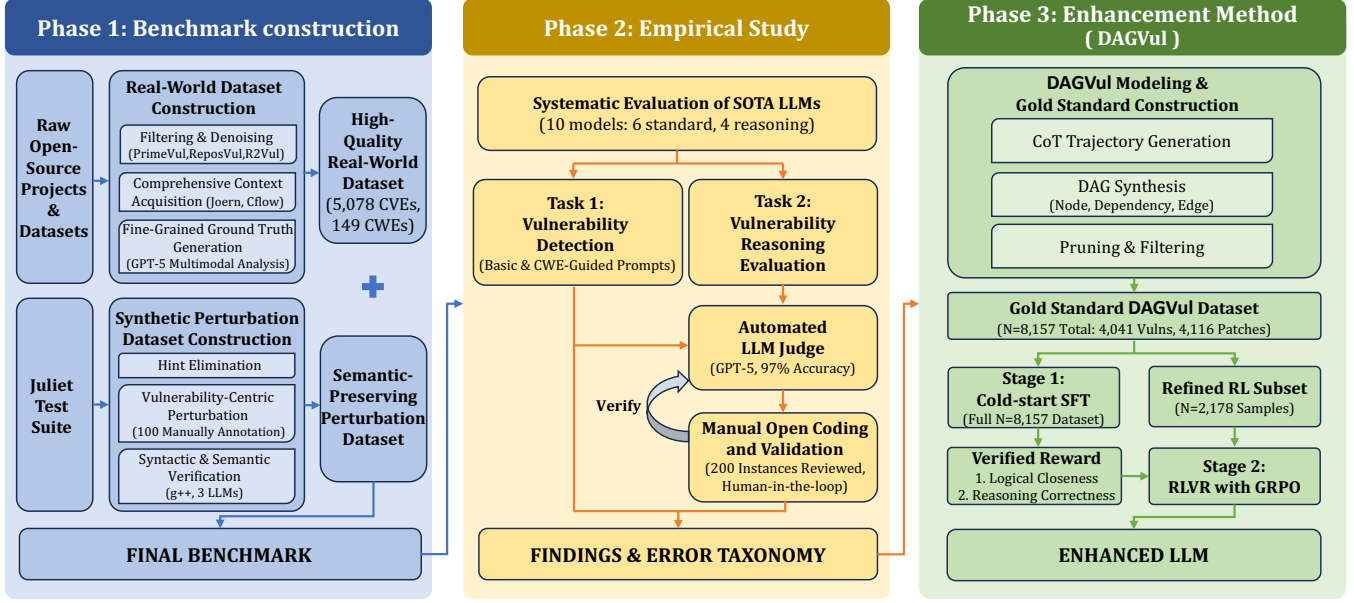
Figure 1: Overview of our systematic framework, spanning from benchmark construction and empirical study to the proposed DAGVUL reasoning enhancement method.

2.2 Reasoning Enhancement Techniques

Recent advancements in LLMs have driven the exploration of reasoning enhancement methods tailored for vulnerability detection tasks. These approaches aim to transition models from superficial pattern matching to deep semantic analysis by optimizing either the input context or the model's internal representations. We categorize existing techniques into three primary paradigms:

RAG-enhanced Vulnerability Detection: RAG [31, 32] enhances the accuracy of LLM responses by retrieving relevant external knowledge and augmenting input prompts with this information. In the context of vulnerability detection, RAG typically retrieves code snippets with known vulnerabilities or patches that are semantically similar to the target code [33, 34]. While this approach addresses domain-specific knowledge gaps and mitigates hallucinations by grounding responses in retrieved evidence, it relies solely on semantic similarity to determine which external knowledge to incorporate. Consequently, it fails to guarantee that the retrieved logic shares the same vulnerability root cause as the target, potentially introducing noise into the reasoning process [35].

SFT-enhanced Vulnerability Detection: SFT [36, 37] aims to internalize reasoning patterns directly into the model parameters by training on domain-specific datasets. Unlike standard instruction tuning, reasoning-focused SFT for vulnerability detection often leverages Chain-of-Thought (CoT) [38] data, where the model is trained on step-by-step reasoning traces rather than just final labels [39]. This method effectively teaches the model to follow structured analysis formats

and mimic expert reasoning paths. However, SFT fundamentally operates as "behavior cloning" [40]. As a result, models trained solely via SFT tend to imitate the style of training data but often struggle to generalize to out-of-distribution vulnerabilities or correct logical errors during the analysis.

RL-enhanced Vulnerability Detection: Reinforcement Learning (RL) [41–43] represents a more advanced paradigm that encourages models to explore and optimize their reasoning policies beyond simple imitation. Approaches are generally categorized into Offline and Online RL. Offline algorithms, such as DPO [44] and ORPO [45], serve as cost-effective alternatives by learning from static datasets of chosen/rejected pairs. Conversely, Online algorithms, such as PPO [46] and the recently prominent GRPO [47], optimize models by interacting with a reward model or environment in real-time, offering a higher upper bound for performance. A significant emerging trend is the shift from traditional Reinforcement Learning from Human Feedback (RLHF) to RLVR [48, 49], which utilizes objective signals to guide reasoning. While prior works have applied RAG, SFT, or Offline RL to vulnerability tasks, the potential of Online RL and RLVR (especially for enforcing logical correctness in vulnerability reasoning) remains largely unexplored.

3 Methodology

Our methodology is structured in three phases designed to first rigorously define and measure the problem of vulnerability reasoning in LLMs, and then to develop and evaluate a novel method for its enhancement. As illustrated in Figure 1,

we first construct a high-quality benchmark specifically designed to assess **fine-grained reasoning capabilities**. Second, we conduct a comprehensive empirical study to evaluate the performance of state-of-the-art LLMs, moving beyond simple detection accuracy to the quality of the reasoning process itself. Finally, based on the findings, we introduce a novel framework that aligns model reasoning with causal program logic through DAGVUL to enforce structural consistency and logical closeness.

3.1 Benchmark Construction for Reasoning Evaluation

A primary limitation of existing research is the reliance on datasets with coarse-grained labels (e.g., binary vulnerability flags), which lack the granularity required to evaluate reasoning fidelity. To address this gap, we developed a benchmark comprising two distinct datasets: a curated collection of real-world cases paired with detailed causal annotations, and a systematically generated set of code perturbations preserving semantic equivalence for robustness testing.

3.1.1 Real-World Vulnerability Dataset

We curate this dataset from open-source projects via a three-step process ensuring annotation quality:

Filtering & De-noising: Legacy commit-based datasets (e.g., BigVul [50], CVEFixes [20], and DiverseVul [17]) often suffer from significant label noise due to tangled patches [51], where security-irrelevant modifications (e.g., refactoring) are mixed with vulnerability fixes. To mitigate this, we construct our dataset foundation by integrating three high-quality datasets: PrimeVul [22], ReposVul [52], and R2Vul [11]. These datasets employ rigorous vulnerability untangling strategies, including: (1) the *single-function principle*, retaining only commits that modify a solitary function to ensure atomicity; (2) *NVD-based verification*, cross-referencing function names and file paths with official CVE descriptions; (3) *LLM-assisted filtration*, utilizing LLMs for relevance scoring followed by human sampling validation; and (4) *static analysis filtering*, leveraging tools (e.g., Infer [53]) combined with commit tracing to verify vulnerability presence.

Building upon this foundation, we applied three additional standard filtering procedures to further purify the data: (1) *Scope Filtering*: We excluded non-source files (e.g., documentation, configurations) and test files to focus solely on production code vulnerabilities. (2) *Length Constraints*: We filtered out functions exceeding typical LLM context windows of 8,192 tokens and those that were overly concise (e.g., empty wrappers) to ensure meaningful reasoning. (3) *Strict De-duplication*: Following established practices [24, 26], we normalized code snippets by removing whitespace and comments, then performed MD5 hash matching to eliminate semantically identical duplicates within and across data splits.

The resulting high-quality dataset comprises 5,078 CVEs covering 149 CWE types.

Comprehensive Context Acquisition: Real-world C/C++ vulnerabilities often stem from complex interprocedural interactions. While prior benchmarks explore external context, their acquisition methods remain limited: static-analysis-based approaches [25, 52] often provide insufficient contextual richness (e.g., missing caller info or incomplete types), while LLM-driven or summary-based methods [26, 54] are hindered by the unreliability of model-generated content or the incompleteness of API summaries. To address these gaps, we utilize Joern [55] and Cflow [56] to implement an enhanced pipeline featuring three key refinements: (1) *Bidirectional Call Graph Analysis*: Beyond simple callee-oriented approaches, we extract direct caller methods with a recursion depth of 3 to reveal a multi-layered impact scope. (2) *Recursive Type Resolution*: We trace *typedef* aliases to their original *struct/union/enum* definitions, resolving the issue of having only forward declarations in previous studies. (3) *Global State Tracking*: We capture global variables modified or accessed by relevant callers and callees, ensuring a comprehensive view of the global state often overlooked by local analysis. Finally, this process aggregates `calleeMethods`, `callerMethods`, `globalVars`, `importLibs`, `typeDefs`, and `vulnerableMethods_before/after` into a comprehensive context that facilitates deep semantic reasoning while maintaining a manageable token footprint.

Fine-grained Ground Truth Annotation: This is the cornerstone of our dataset. Current benchmarks predominantly rely on concise NVD descriptions [57], neglecting the forensic depth in unstructured references (e.g., GitHub issues and PRs) where experts provide detailed vulnerability diagnostics. Notably, vulnerability reports are not plain text but embed critical screenshots and code snippets; for instance, a screenshot demonstrating a launched calculator provides empirical proof of remote code execution. To capture this complexity, we utilize the multimodal GPT-5 to aggregate evidence across four structured dimensions: (1) *Report Analysis*: We synthesize core reports by summarizing CVE descriptions, CWE ID, and interpreting visual proofs alongside GitHub issues and project READMEs to reconstruct the vulnerability background. (2) *Code-Level Evidence*: We correlate the commit message and the code diff obtained from the commit to understand code-level changes. (3) *Contextual Information*: We extract community insights from pull request discussions, capturing details like dispute resolutions or impact clarifications not present in the initial report. (4) *Conflict Resolution*: We adjudicate discrepancies between information sources to generate comprehensive reports that include definitive root causes, fixing patterns, and a binary label (Resolved/Unresolved) indicating whether the model successfully resolves the conflict. To ensure the credibility of the report, we implemented a confidence-based verification process. For each synthetic report, GPT-5 needs to provide a confidence score

of 1-5 based on the consistency of the evidence. Two authors manually annotate all sample scoring below 4 or exhibiting irreconcilable conflicts. This human-in-the-loop process ultimately produced 4,998 fine-grained ground truths.

3.1.2 Semantic-Preserving Perturbation Dataset

To evaluate the semantic robustness of LLM reasoning and mitigate potential data leakage [58], we construct a semantic-preserving perturbation dataset. While real-world datasets are representative, they often lack sufficient compilability for iterative verification and are too complex to isolate specific reasoning failures. In contrast, we utilize the Juliet Test Suite [59] due to its clear CWE classifications and manageable dependency structures (e.g., resolvable via include flags), allowing for rigorous syntactic and semantic validation during perturbation.

Inspired by CodeMorph [60], we adopt 26 types of semantic-preserving transformations and further enhance the pipeline in three key dimensions: (1) **Hint Elimination**: We first apply regex-based filtering to remove suggestive comments (e.g., /* FLAW */) and diagnostic `printf` statements that might leak vulnerability information. (2) **Vulnerability-Centric Perturbation**: Unlike standard code augmentation, we manually annotated 100 samples across five representative CWEs (CWE-78, 190, 400, 416, 476, with 20 samples per CWE) to identify lines critical to the vulnerability's root cause. These lines are kept invariant during the perturbation process. This ensures that any change in the model's prediction can be strictly attributed to interference from vulnerability-irrelevant code features. (3) **Syntactic & Semantic Verification**: Each perturbed instance undergoes a dual-gate validation: successful compilation using the g++ compiler to ensure syntactic correctness, followed by a semantic equivalence check through a majority vote of three LLMs (GPT-5, Claude-4, and DeepSeek-R1). **This dataset enables rigorous assessment of reasoning robustness to semantically-neutral transformations.** We provide a comprehensive taxonomy of these perturbation strategies in Table 7 in the appendix, and detail the representative cases in Appendix A.

3.2 Empirical Study

Using the newly constructed benchmark, we conducted a large-scale empirical study to systematically quantify the vulnerability detection and reasoning capabilities of state-of-the-art LLMs, which include 6 standard models and 4 reasoning models as shown in Table 2. Our evaluation consists of two stages: vulnerability detection followed by reasoning quality assessment.

Detection Stage: We prompt models to determine whether a given code snippet contains a vulnerability and provide reasoning for their conclusion. We employ two prompting strategies: (1) *Basic Prompt* provides only the code and its

Table 2: SOTA LLMs selected for evaluation. Our study includes 10 models accessed through both local deployment and remote APIs, with diverse parameter scales, maximum input token limits, and knowledge cut-off dates.

Model API	Parameters	Max. Tokens	Type	Knowledge Cut-off
Standard Models				
qwen2.5:7b	7B	32,768	Local	06/2023
llama3.1:8b	8B	131,072	Local	12/2023
llama3.2:3b	3B	131,072	Local	12/2023
gpt-3.5	—	16,385	Remote	09/2021
deepseek-v3	671B	131,072	Remote	07/2024
claude-4-sonnet	—	200,000	Remote	01/2025
Reasoning Models				
qwq-32b	32B	131,072	Local	12/2024
deepseek-r1	671B	131,072	Remote	07/2024
gemini-2.5-pro	—	1,048,576	Remote	01/2025
grok-4	—	256,000	Remote	12/2024

context, and (2) *CWE-Guided Prompt* additionally specifies the CWE type and asks whether a vulnerability of that type exists. This dual-strategy design allows us to assess both zero-shot detection capability and performance under focused vulnerability type guidance.

Reasoning Evaluation Stage: We assess the generated reasoning through automated and manual analysis. For automated evaluation, we employ GPT-5 as an LLM judge to compare generated reasoning against ground truth. The ground truth protocol is dataset-specific: for real-world cases, we use our curated vulnerability reports detailing root causes and fixing patterns; for perturbed cases, we synthesize ground truth from Juliet suite comments combined with human-annotated vulnerability-related code lines. The judge outputs MATCH if reasoning is semantically consistent with ground truth, and MISMATCH otherwise.

Manual Open Coding and Validation: To ensure the reliability of our automated metrics and gain deep qualitative insights, we conducted a rigorous manual analysis following the open coding methodology [29, 30]. Two authors with expertise in software security performed the annotation using a custom-developed WebApp. The process followed an iterative workflow: independent labeling, conflict negotiation, and category merging until consensus was reached. Critically, this phase served as a *human-in-the-loop* validation mechanism where annotators manually reviewed and corrected the verdicts given by the automated LLM judge. Specifically, we focused on samples flagged as MISMATCH by the judge LLM and randomly selected 200 instances (20 per model), accounting for 10.9% of the total error cases. After manual audit and rectification, we observed that the automated evaluator's error rate was merely 3%, with discrepancies primarily stemming from ambiguities in the ground truth descriptions. This low error rate confirms the high efficacy and reliability of our LLM-based evaluator. Finally, this systematic analysis culminated in the maintenance of a standardized *codebook* that documents distinct vulnerability reasoning error patterns.

3.3 Enhancement Method

Building upon the findings from our empirical study (detailed in § 4.4), we identified that the primary bottlenecks restricting LLMs in vulnerability detection are code comprehension and logical reasoning. While the CoT paradigm can effectively guide LLMs to analyze code step-by-step, we argue that the traditional linear CoT is insufficient to constrain complex logical errors, such as a lack of evidence, self-contradiction, and excessive extrapolation. To address these limitations, we introduce DAGVUL. Drawing on recent advances that model mathematical reasoning as Directed Acyclic Graphs (DAGs) [61, 62], we propose to reformulate vulnerability reasoning as a DAG generation task. The DAG structure explicitly captures dependencies between reasoning steps and enforces logical consistency constraints, addressing the structural limitations of linear CoT. By imposing this architectural rigor on the reasoning process, we aim to reduce logical errors and improve overall reasoning correctness.

3.3.1 Modeling the DAGVUL

We build upon the graph-based reasoning formalization established in prior literature [61], focusing specifically on its specialization for vulnerability detection while omitting redundant theoretical proofs. We formalize the vulnerability reasoning process as a DAG, denoted as $G(x_{in}) = (V(x_{in}), E(x_{in}))$, where x_{in} represents the input code snippet. The node set $V(x_{in})$ encodes the discrete steps of the security analysis, while the edge set $E(x_{in})$ captures the causal inferential dependencies between these steps. In the context of vulnerability reasoning, nodes $V(x_{in})$ are categorized into three distinct classes based on their role in the analysis pipeline:

- **Source Nodes (V_{in}):** These nodes represent the security-relevant "ground facts" extracted directly from the source code, such as buffer capacities, API definitions, or entry points. For instance, in Figure 2, v_1 to v_5 serve as source nodes that identify critical buffer declarations and control-flow checkpoints. Crucially, source nodes must contain only literal code facts without any derived inference.

- **Intermediate Nodes (V_{inter}):** These nodes represent the logical inferences derived from preceding steps, encompassing operations such as taint tracking, pointer analysis, and constraint solving. As illustrated by v_6 to v_{10} in Figure 2, these nodes lift raw code facts into semantic abstractions.

- **Sink Nodes (V_{out}):** Unlike traditional reasoning tasks, vulnerability auditing necessitates a dual-terminal structure to represent the final audit verdict. We define two types of sink nodes: the *verified_sink* (v_{11}), which concludes a confirmed vulnerability and summarizes the exploit path, and the *sanitized_sink* (v_{12}), which formally asserts the safety of a path by proving the efficacy of sanitization or checks. In modern

security auditing, proving safety is considered as critical as identifying flaws.

The edges $E(x_{in})$ are governed by two fundamental principles to ensure structural rigor: (1) *Program Analysis Principle*, which requires each edge to explicitly state the underlying primitive used (e.g., Taint Propagation, Data Flow Analysis, or Constraint Solving); and (2) *Citation Rule*, which mandates that the reasoning justification must explicitly reference prior antecedents using the exact tag "Step X".

We define the node-level transition rule. Let $v_{1:t-1}$ be the sequence of reasoning steps generated up to time $t-1$. The set of admissible nodes for the next step t is defined as:

$$\mathcal{V}(v_{1:t-1}|x_{in}) := \{v \in V(x_{in}) : pa(v) \subseteq \{v_{1:t-1}\}, \\ v \notin \{v_{1:t-1}\}\} \tag{1}$$

This rule enforces a strict logical order; a node can only be visited once all its parent dependencies have been established in the preceding context. As shown in our illustrative example in Figure 2, after the model has collected $\{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$, the only logically admissible next step is the state inference node v_8. Nodes v_9 through v_{12} remain inaccessible until the dependency v_8 is resolved.

To rigorously evaluate the fidelity of vulnerability reasoning, we define two primary metrics within the DAGVUL:

- **Logical Closeness:** We define a reasoning as closed if every path originating from the source nodes (V_{in}) terminates at a defined terminal sink (V_{out}). This ensures that no intermediate assertions are left "dangling" and that the final verdict is the exhaustive culmination of all preceding logic.

- **Reasoning Correctness:** This metric assesses the alignment between the generated sink nodes and the ground truth. Specifically, the presence of a *verified_sink* indicates the discovery of a flaw, while a trajectory consisting solely of *sanitized_sinks* represents a confirmation of code safety.

3.3.2 Gold Standard DAGVUL Dataset

Constructing perfect DAGVUL structures directly from source code is inherently challenging. We therefore first generate CoT trajectories aligned with vulnerability ground truth to serve as a scaffold for a three-stage DAG synthesis process. We utilize the ground truth as an anchor to prompt DeepSeek-R1 for step-by-step analysis from the original code, encompassing code comprehension and control-data flow tracing. To ensure reasoning faithfulness and prevent the model from replicating ground-truth text rather than deriving it from the code, we implement a rigorous filtering pipeline. This includes regular expression matching for explicit ground-truth terminology and semantic similarity analysis using the *all-MiniLM-L6-v2* Sentence-BERT model. Responses exceeding a 0.8 similarity threshold or containing explicit "ground truth"
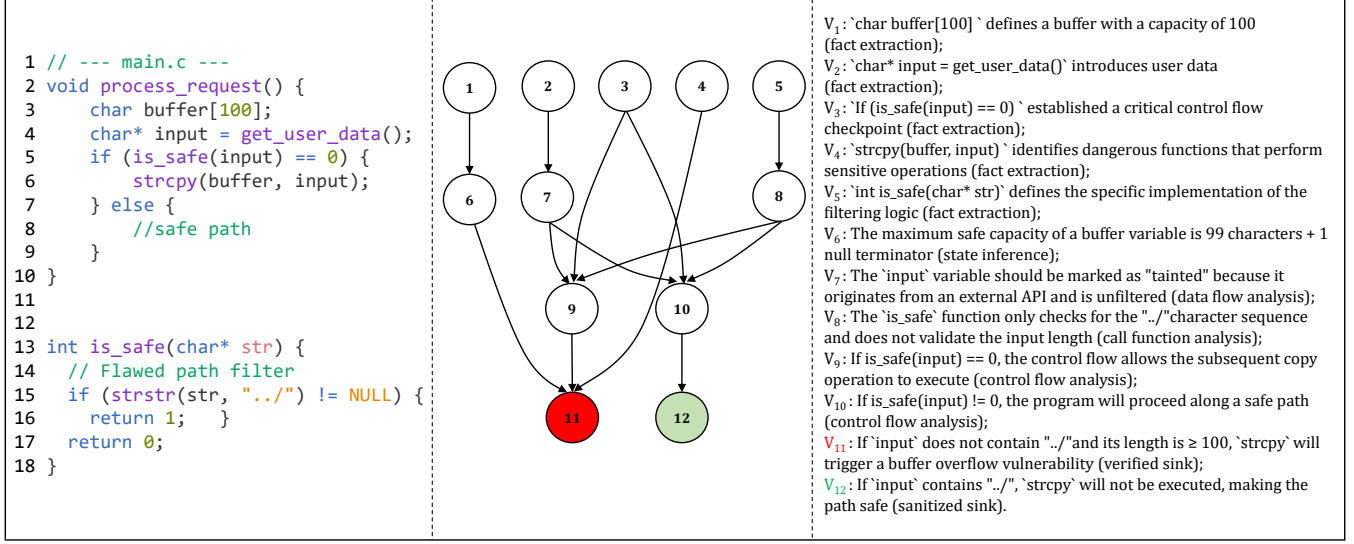
6

Figure 2: Illustrative example of the DAGVUL. The left panel presents a simplified C code snippet with a flawed check; the middle panel visualizes the DAG topology; and the right panel provides the semantic descriptions of nodes v_1–v_{12}.

are rejected. We allow a maximum of three resampling attempts before a sample is discarded. For example, the right panel of Figure 2 displays a CoT trajectory generated by DeepSeek-R1, while the example DAG topology was manually curated by the authors, they can also be elicited from LLMs through specialized prompting.

Subsequently, we synthesize the DAG through three stages: (1) **Node Identification**, (2) **Dependency Assignment**, and (3) **Edge Generation**. The detailed prompts for these stages are provided in Appendix B. Following initial construction, we apply pruning and filtering algorithms to refine the graph structure. We prune all dangling nodes ($v \in V_{inter} \cup V_{in}$) that do not contribute to any path reaching a terminal sink. Furthermore, we discard any sample where an intermediate node ($v \in V_{inter}$) leading to a *verified_sink* lacks parent dependencies, as this signifies a conclusion drawn without sufficient evidentiary support. After executing these quality control measures, the final Gold Standard DAGVUL Dataset comprises 4,041 vulnerability samples and 4,116 patch samples (see Appendix C for detailed topological statistics). Notably, the high-quality CoT trajectories generated during this procedure are also preserved to serve as a specialized training corpus for establishing a reasoning baseline in our experiments.

3.3.3 Two-Stage Training Approach

To internalize the structured reasoning capabilities defined by DAGVUL, we employ a two-stage training paradigm: Cold-start SFT followed by RLVR.

Stage 1: Cold-start SFT. We initialize the training process by performing SFT on the complete Gold Standard DAGVUL Dataset ($N = 8,157$). This stage aims to provide the model

with a strong prior over the DAGVUL format and the underlying program analysis semantics. The model is trained for 3 epochs to ensure a stable "cold start" for the subsequent reinforcement learning phase.

Stage 2: RLVR with GRPO. Building upon the SFT model, we implement RLVR to align the reasoning process with structural integrity and causal correctness. We utilize GRPO [47] with a rollout size of 16 to optimize the reasoning policy. To balance semantic fidelity with structural rigor, we define a hybrid reward function R_{total} for each generated trajectory G_{gen} as follows:

$$R_{total} = \omega_1 \cdot \delta_{close}(G_{gen}) + \omega_2 \cdot \delta_{final}(G_{gen}) \quad (2)$$

where δ_{close} is a rule-based indicator verifying the logical closeness of the graph structure, and δ_{final} is a model-based indicator. Specifically, δ_{final} is evaluated by DeepSeek-R1, which serves as a judge to determine whether the generated sink node aligns with the ground truth.

Due to the significant computational overhead associated with RLVR, we further filter the Gold Standard dataset using a 4,096-token context window to ensure efficiency. This results in a refined RL subset comprising 2,178 high-quality samples. The RLVR stage is conducted for 2 epochs, focusing the model's optimization on navigating the logical dependencies rather than simple textual imitation.

4 Results

We present our evaluation results organized by four research questions (RQs). We first analyze baseline LLM performance to uncover systematic reasoning failures (§ 4.2 through § 4.4),

and subsequently evaluate the effectiveness of our proposed enhancement methodology (§ 4.5).

- **RQ1 (Real-World Performance):** To what extent can SOTA LLMs correctly reason about vulnerabilities?

- **RQ2 (Semantic Robustness):** How robust are LLMs' vulnerability reasoning capabilities against semantic-preserving code perturbations?

- **RQ3 (Failure Taxonomy):** What are the prevalent failure patterns in the reasoning traces generated by LLMs?

- **RQ4 (Enhancement Efficacy):** Can we effectively enhance LLMs' reasoning through DAGVUL?

4.1 Experiment Setup

Models. For the empirical analysis in RQ1 and RQ2, we evaluate the 10 representative models detailed in Table 2. For the comparative evaluations in RQ4, we utilize two SOTA sub-8B models, Qwen3-8B and Llama3.1-Nemo-8B, alongside their respective reasoning versions.

Datasets. RQ1 utilizes 114 samples from our real-world dataset, each accompanied by a comprehensive expert-curated ground truth, including GitHub issues and PR discussions. RQ2 evaluates robustness using 100 perturbed pairs from the semantic-preserving perturbation dataset. To ensure cross-domain representativeness in RQ4, we utilize the SVEN [21], which remains a real-world dataset despite its more concise context lengths. It covers 9 prevalent CWEs with generic vulnerability patterns. We strictly exclude samples sharing the same commit URLs as our training set, resulting in 114 entirely unseen test instances with ground truth constructed via the methodology in § 3.1.1.

Baselines. Our evaluation for RQ4 encompasses *simple* and *CoT* inference strategies. We implement strong baselines including RAG, SFT, and ORPO. Specifically, the RAG corpus is constructed using the SVEN training set with a retrieval method following Vul-RAG [33], while rejected responses for ORPO are generated by providing incorrect labels following R2Vul [11]. The training methods are applied exclusively to standard models to avoid the fixed inference patterns (e.g., `<think>` tags) inherent in reasoning models. We also include Qwen3-30B and GPT-OSS-20B as representative large-parameter baselines for performance comparison.

Evaluation Metrics. We define two complementary metric sets to evaluate model performance:

Detection Correctness: Standard binary classification metrics (Accuracy, Precision, Recall, F1-score) assess **binary predictions** without considering reasoning quality.

Reasoning Correctness: We introduce reasoning-aware metrics based on the triplet (G, P, R), where $G \in \{0, 1\}$ denotes ground truth (0: patched, 1: vulnerable), $P \in \{0, 1\}$ denotes prediction, and $R \in \{\texttt{MATCH}, \texttt{MISMATCH}\}$ indicates whether the reasoning aligns with ground truth vulnerability logic. As shown in Table 3, our classification scheme applies asymmetric criteria:

- **Strict evaluation for vulnerable code ($G = 1$):** We require both correct prediction and sound reasoning. Only the triplet (1, 1, MATCH) qualifies as a True Positive. Critically, (1, 1, MISMATCH) counts as a False Negative despite a correct prediction, since the model fails to identify the actual vulnerability mechanism.

- **Lenient evaluation for patched code ($G = 0$):** Standard True Negatives include (0, 0, –). However, we reclassify (0, 1, MATCH) as True Negative rather than False Positive. This reflects a key insight: when the model might identify alternative concerns or correctly analyze the efficacy of the patch, represent a sophisticated understanding of the code rather than a false alarm regarding the target vulnerability.

Using this reasoning-adjusted confusion matrix, we compute **Reasoning Accuracy** (R_{Acc}), **Reasoning Precision** (R_P), **Reasoning Recall** (R_R), and **Reasoning F1-score** (R_{F1}).

Table 3: Reasoning-aware evaluation outcomes based on triplet (G, P, R).

Ground Truth (G)	LLM Prediction (P)	Reasoning Correctness (R)	Outcome Category
1 (Vul.)	1 (Vul.)	MATCH	TP
1 (Vul.)	1 (Vul.)	MISMATCH	FN
1 (Vul.)	0 (Pat.)	–	FN
0 (Pat.)	0 (Pat.)	–	TN
0 (Pat.)	1 (Vul.)	MISMATCH	FP
0 (Pat.)	1 (Vul.)	MATCH	TN*

*[*]**Reclassified as TN: reasoning omits the rectified vulnerability or identifies the fixing pattern within the code.**

Execution Environment. All model training and local inference are conducted on a server equipped with eight NVIDIA A800 (40GB) GPUs.

4.2 RQ1: Real-World Performance

To address RQ1, we evaluate 10 SOTA LLMs on our real-world benchmark. As illustrated in Figure 3, a comparison between traditional detection and our reasoning metrics reveals that binary classification evaluation is profoundly unreliable. Even for premier models such as Grok-4, Gemini-2.5-Pro, and DeepSeek-R1, R_{F1} plummets from over 60% in detection to under 50% when reasoning is verified. This disparity is even more critical in smaller models like Llama-3.1-8B, where R_{F1} drop below 10%, indicating that previous coarse-grained evaluations largely masked instances where models simply guessed the correct answer. **This substantial gap provides compelling quantitative evidence for the widespread**
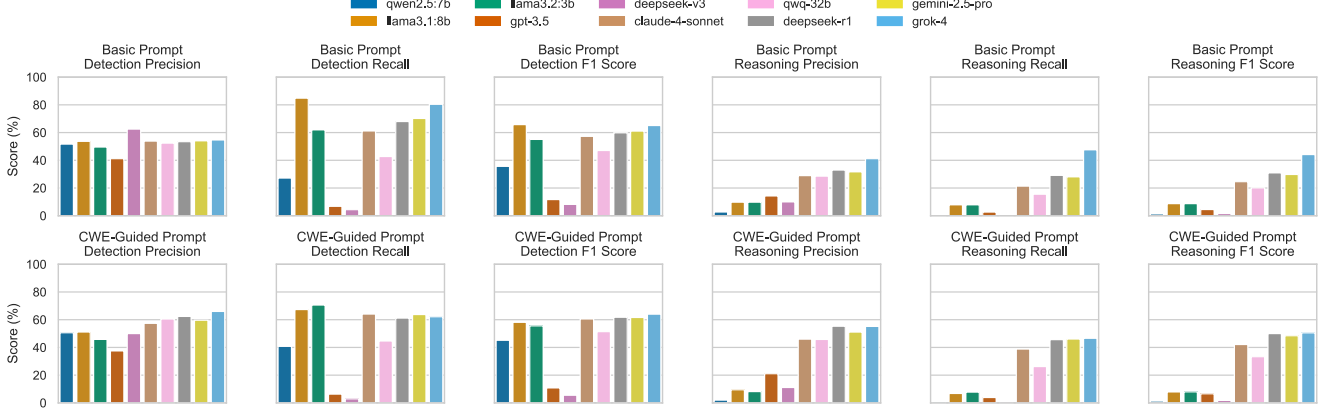
Figure 3: Performance of SOTA LLMs on vulnerability detection and reasoning. The 12 subplots compare Detection and Reasoning (R_P, R_R, R_{F1}) metrics across Basic Prompt and CWE General Prompt strategies.

"Flawed Reasoning, Correct Answer" phenomenon, with our statistical analysis showing that 36.4% of correct binary verdicts stem from incorrect reasoning.

To further investigate inferential consistency, we conduct a pair-wise analysis (Figure 4) by treating each vulnerable snippet and its corresponding patch as a coupled pair. A robust LLM must simultaneously identify the root cause in the vulnerable version and confirm the safety of the patched version based on valid fix logic. However, the proportion of (MATCH, MATCH) outcomes is remarkably low across all evaluated models; even for top-tier reasoners like Grok-4 and DeepSeek-R1, this consistent success rate remains below 30%. Such results indicate that LLMs struggle to distinguish the precise semantic boundaries of security logic. The results of both subfigures demonstrate that providing CWE-specific hints consistently improves reasoning accuracy. This suggests that the transition from generic detection to CWE-targeted analysis is a promising path to enhance the practical efficacy of LLM-based vulnerability auditing.

> *Finding 1: SOTA LLMs exhibit a significant gap between high vulnerability detection accuracy and low reasoning accuracy. Furthermore, pair-wise analysis further reveals a lack of semantic stability across vulnerable and patched code, though providing targeted CWE context can partially mitigate these reasoning deficiencies.*

4.3 RQ2: Semantic Robustness

To evaluate the stability of the vulnerability reasoning process, we tested the LLMs on our semantic-preserving perturbation dataset. The motivation for this dataset is that a robust LLM should maintain consistent reasoning regardless of coding style variations, as long as the underlying program semantics and the vulnerability's root cause remain invariant.
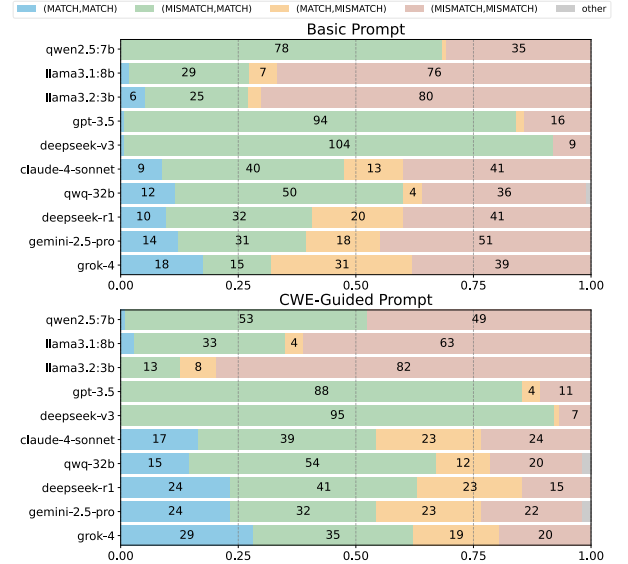

Figure 4: Distribution of pair-wise vulnerability reasoning outcomes. A "pair" consists of a vulnerability and its corresponding patch. (MATCH, MATCH) indicates the model reasoned correctly for both versions.

As shown in Table 4, even the most advanced models exhibit a significant performance drop when subjected to these perturbations. This indicates that the vulnerability reasoning capabilities of LLMs face severe challenges in terms of robustness. Quantitatively, our analysis shows that in the basic prompt setting, the reasoning R_{F1} plummets by an average of 26.7% across all evaluated models. Notably, this degradation is significantly mitigated under the CWE-guided prompts, where the average R_{F1} drop is reduced to 14.5%. This improvement suggests that explicit CWE prompts help focus the model's attention on relevant vulnerability-related features,

partially shielding the reasoning process from being distracted by irrelevant syntactic noise.

Table 4: Reasoning Performance (R_P, R_R, R_{F1}) Across Prompts and Datasets. Arrows in Rephrased Dataset columns indicate performance shifts relative to the Original Dataset ($\downarrow$ for decline, $\uparrow$ for improvement).

Model	Original Dataset			Rephrased Dataset		
	R_P	R_R	R_{F1}	R_P	R_R	R_{F1}
Panel A: Basic Prompt						
qwen2.5:7b	20.83	20.00	20.41	15.56$\downarrow$	13.46$\downarrow$	14.43$\downarrow$
llama3.1:8b	34.21	52.00	41.27	17.74$\downarrow$	21.15$\downarrow$	19.30$\downarrow$
llama3.2:3b	25.40	32.00	28.32	9.09$\downarrow$	9.62$\downarrow$	9.35$\downarrow$
gpt-3.5	49.06	52.00	50.49	12.24$\downarrow$	11.54$\downarrow$	11.88$\downarrow$
deepseek-v3	46.77	58.00	51.79	12.50$\downarrow$	11.54$\downarrow$	12.00$\downarrow$
claude-4-sonnet	36.67	44.00	40.00	21.88$\downarrow$	26.92$\downarrow$	24.14$\downarrow$
qwq-32b	95.35	83.67	89.13	88.57$\downarrow$	60.78$\downarrow$	72.09$\downarrow$
deepseek-r1	78.26	72.00	75.00	77.42$\downarrow$	46.15$\downarrow$	57.83$\downarrow$
gemini-2.5-pro	63.33	76.00	69.09	22.64$\downarrow$	23.08$\downarrow$	22.86$\downarrow$
grok-4	64.91	74.00	69.16	22.41$\downarrow$	25.00$\downarrow$	23.64$\downarrow$
Panel B: CWE-Guided Prompt						
qwen2.5:7b	6.45	4.00	4.94	3.03$\downarrow$	1.92$\downarrow$	2.35$\downarrow$
llama3.1:8b	35.90	56.00	43.75	20.63$\downarrow$	25.00$\downarrow$	22.61$\downarrow$
llama3.2:3b	18.03	22.00	19.82	11.86$\downarrow$	13.46$\downarrow$	12.61$\downarrow$
gpt-3.5	63.16	72.00	67.29	48.00$\downarrow$	46.15$\downarrow$	47.06$\downarrow$
deepseek-v3	59.42	82.00	68.91	44.23$\downarrow$	44.23$\downarrow$	44.23$\downarrow$
claude-4-sonnet	50.98	52.00	51.49	45.56$\downarrow$	78.85$\uparrow$	57.75$\uparrow$
qwq-32b	91.49	86.00	88.66	78.38$\downarrow$	55.77$\downarrow$	65.17$\downarrow$
deepseek-r1	95.12	79.59	86.67	84.21$\downarrow$	61.54$\downarrow$	71.11$\downarrow$
gemini-2.5-pro	96.00	96.00	96.00	88.37$\downarrow$	73.08$\downarrow$	80.00$\downarrow$
grok-4	95.74	90.00	92.78	74.00$\downarrow$	71.15$\downarrow$	72.55$\downarrow$

> *Finding 2: LLM vulnerability reasoning is highly susceptible to semantic-preserving syntactic perturbations, with an average performance drop of 26.7% with basic prompts. While providing CWE context can focus model attention and halve this degradation, the overall inconsistency underscores that current LLMs lack the robustness required for stable semantic-based security auditing.*

4.4 RQ3: Prevalent Failure Patterns

We conduct a manual open coding on 200 erroneous reasoning traces to establish a taxonomy of failure modes. As detailed in Table 5, we identify 12 distinct error patterns categorized into four high-level dimensions: (1) Analytical Focus Errors, representing failures in identifying the critical security-relevant code segments; (2) Code Comprehension Errors, reflecting failures during the "perception" stage where the model misinterprets program semantics; (3) Logical Analysis and Reasoning Errors, representing failures in the "processing" stage where the model fails to derive valid conclusions from its understanding; and (4) Generative Bias, representing deviations introduced during the "expression" stage due to the probabilistic nature of autoregressive generation.

Notably, these failure modes are rarely isolated. We observe frequent cascading effects where a single reasoning trace exhibits multiple co-occurring errors. For instance, a failure in control-flow analysis (CS2) often leads to insufficient evidentiary support (AR1) in subsequent steps. Similarly, a lack of deep semantic understanding (CS3) frequently forces the model to revert to superficial pattern matching (AR2).
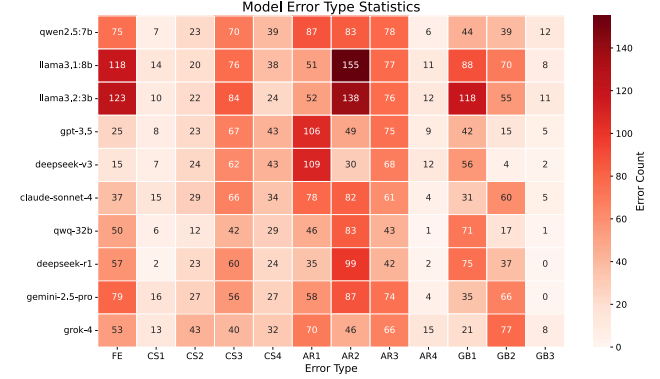

Figure 5: Distribution of error types across 10 SOTA LLMs. The heatmap shows the frequency of each error type (see Table 5) committed by different models during vulnerability reasoning.

To analyze the distribution of these errors at scale, we utilize GPT-5 as an automated classifier (limited to the top 4 most relevant labels per sample) to categorize the errors identified in our large-scale evaluation according to the established codebook. The resulting heatmap Figure 5 reveals that across all evaluated models, failure modes are heavily concentrated in the **CS** and **AR** categories. Specifically, even for SOTA models, errors in taint tracking and constraint solving are pervasive, suggesting that the fundamental bottleneck in LLM vulnerability reasoning lies in the model's inability to maintain logical consistency during the complex process of semantic code comprehension.

> *Finding 3: LLM reasoning failures are primarily driven by deficits in code comprehension and logical derivation, rather than sporadic hallucinations. The high density of these errors indicates that even SOTA models struggle to maintain logical consistency when navigating the complex causal dependencies of real-world vulnerabilities.*

4.5 RQ4: Enhancement Efficacy

As summarized in Table 6, our proposed DAGVUL consistently achieves the highest reasoning performance across almost all tested configurations. On Qwen3-8B, DAGVUL reaches an R_{F1} of 70.97% with basic prompts, significantly outperforming the Simple baseline (53.91%) and other optimization methods like SFT (63.37%) and ORPO (62.25%).

Table 5: Taxonomy of vulnerability reasoning failure modes identified through manual open-coding. The errors are classified into four high-level categories based on the stage of the analysis process where the failure occurs.

High-Level Category	Abbr.	Error Type Name	Description / Definition
Analysis Focus	FE	Analysis Focus Identification Error	The model fails to locate the analysis starting point or primary focus on the code snippet relevant to the vulnerability.
Code Comprehension Error	CS1	Data Flow Misunderstanding	Failure to accurately track data paths across variables, function calls, and object attributes. This includes missing data transformations (e.g., sanitization) or misjudging the data's final state.
	CS2	Control Flow Misunderstanding	Failure to accurately understand execution paths and conditions, including incorrect judgments on code block reachability, loop termination conditions, or branching logic.
	CS3	Intra-procedural Semantic Error	Misunderstanding logic within a single function or block (e.g., atomic operations, local calculations) without involving cross-function calls.
	CS4	Inter-procedural Semantic Error	Misunderstanding semantics across function calls, module boundaries, or interactions with external systems (e.g., threads, files, memory heap).
Logic Analysis & Reasoning Error	AR1	Fallacy of Incomplete Evidence	Creating an argument using only supporting evidence while systematically ignoring key counter-evidence (e.g., existing checks or context) that would refute the conclusion.
	AR2	Spurious Causality Fallacy	Incorrectly identifying a superficial feature (correlation) of the code as the root cause (causality) of a vulnerability.
	AR3	Flawed Premise Fallacy	Making incorrect assumptions about the execution environment, trust boundaries, API behaviors, or data sources.
	AR4	Contradiction Fallacy	Deriving two or more logically conflicting conclusions or statements within the same reasoning chain.
Generative Bias	GB1	Hallucination Bias	Generating information completely inconsistent with the code facts, such as fabricating non-existent variable names, function calls, dependencies.
	GB2	Over-inference Bias	Making disproportionate extrapolations based on weak clues, constructing extremely complex or practically impossible attack chains.
	GB3	Redundancy Bias	Generating excessive repetitive, templated, or common-sense information unrelated to the core argument.

Furthermore, R_{Acc} mirrors this improvement, reaching 76.11% and 67.54% on Qwen3-8B and Llama3.1-Nemo-8B respectively, which underscores the overall reasoning reliability. Ablation analysis confirms the superiority of RLVR, yielding a 7.6% absolute R_{F1} gain over the SFT-based DAG variant on Qwen3-8B (70.97% vs. 63.37%). Similarly, in Llama3.1-Nemo-8B, DAGVUL achieves the highest R_{F1} of 61.05% and 72.90% across the two prompting strategies, respectively. The R_P metrics for our method exhibit a universal and significant improvement, reaching 91.67% on Qwen3-8B, which we attribute to the structural constraints of the DAG format that compel the model to generate specific, verifiable causal nodes rather than relying on vague or hallucinated descriptions.

Our framework on a standard base model outperforms the specialized reasoning variant (e.g., Qwen3-8B-Reasoning's best R_{F1} of 67.23% vs. our 70.97%). Remarkably, this performance even exceeds that of larger models under their best configurations, such as GPT-OSS-20B (67.96% R_{F1} via RAG) and Qwen3-30B-Reasoning (69.39% R_{F1} via DAG). Furthermore, while the DAG baseline does not always surpass the CoT baseline, our method allows the DAG-based approach to reach the best performance. In contrast, RAG exhibits notable instability, with its R_{F1} on Qwen3-8B (61.42%) falling below the baseline, suggesting that external context often introduces distracting noise. Notably, under CWE-guided prompting, DAGVUL on Qwen3-8B achieves an R_{F1} of 75.47%, **nearly matching the best configuration of Claude-Sonnet-4.5** [16] (76.11%) despite using a significantly smaller model.

> *Finding 4:* DAGVUL *achieving an average improvement of 18.9% in reasoning F1-score over all the baselines and even surpassing specialized reasoning models. The results confirm that our method effectively mitigates reasoning failures by promoting superior logical consistency compared to linear or unstructured baselines.*

5 Discussion

5.1 Insights of DAGVUL

Logical closeness rate. We measured the percentage of instances achieving logical closeness (as defined in § 3.3.1). This metric exhibits significant improvement through DAGVUL. Specifically, Qwen3-8B increased from 32.90% to 73.25%, while Llama-Nemo-8B rose from 44.74% to 67.99%. These results demonstrate that structural constraints effectively guide models to complete the causal chain from the entry point to the vulnerability sink.

Mitigating reward hacking. To prevent reward hacking, we implement a balanced mechanism addressing the asymmetric difficulty between benign and vulnerable code analysis. Since vulnerable instances require complex root cause identification, we assign rewards for both identifying verified sinks and maintaining reasoning veracity. This approach discourages models from exploiting simpler benign classifications to maximize rewards.

Table 6: Performance of Qwen3, GPT-OSS, Llama3.1-Nemotron, and Claude Sonnet 4.5 across different scales. We evaluate Reasoning metrics under Basic and CWE-Guided prompts. (best , second-best R_{F1} within each model group).

Base Model	Inference Strategy	Optimization Method	Basic Prompt				CWE-Guided Prompt			
			R_{Acc}	R_P	R_R	$R_{F1}^{\dagger}$	R_{Acc}	R_P	R_R	$R_{F1}^{\dagger}$
Qwen3-8B	Simple*	Baseline	53.51	53.45	54.39	53.91	69.91	92.31	42.86	58.54
	CoT	Baseline	59.65	57.14	77.19	65.67	61.06	59.09	69.64	63.93
	CoT	RAG	57.02	55.71	68.42	61.42	64.60	62.32	75.44	68.25
	CoT	SFT	52.63	51.58	85.96	64.47	64.04	61.11	77.19	68.22
	CoT	ORPO	50.00	50.00	82.46	62.25	64.91	61.97	77.19	68.75
	DAG	Baseline	62.83	65.31	56.14	60.38	60.18	57.32	82.46	67.63
	DAG	SFT (for ablation analysis)	67.54	72.73	56.14	63.37	73.68	81.40	61.40	70.00
	DAG	**DAGVUL (Our Method)**	76.11	91.67	57.89	70.97	77.19	81.63	70.18	75.47
Qwen3-8B-Reasoning	Simple*	Baseline	64.91	66.67	59.65	62.96	71.05	76.09	61.40	67.96
	CoT	Baseline	65.79	64.52	70.18	67.23	71.05	74.00	64.91	69.16
	CoT	RAG	57.89	55.84	75.44	64.18	70.18	71.70	66.67	69.09
	DAG	Baseline	66.07	67.27	64.91	66.07	68.14	67.24	69.64	68.42
Llama3.1-Nemo-8B	Simple*	Baseline	33.33	35.82	42.11	38.71	50.00	50.00	57.89	53.66
	CoT	Baseline	48.67	47.50	33.93	39.58	49.12	49.21	54.39	51.67
	CoT	RAG	56.14	55.93	57.89	56.90	50.00	50.00	57.89	53.66
	CoT	SFT	54.39	54.72	50.88	52.73	58.77	56.58	75.44	64.66
	CoT	ORPO	52.63	52.94	47.37	50.00	59.65	57.33	75.44	65.15
	DAG	Baseline	53.27	53.85	26.92	35.90	41.51	44.00	62.26	51.56
	DAG	SFT (for ablation analysis)	60.53	63.04	50.88	56.31	69.30	70.37	66.67	68.47
	DAG	**DAGVUL (Our Method)**	67.54	76.32	50.88	61.05	74.34	78.00	68.42	72.90
Llama3.1-Nemo-8B-Reasoning	Simple*	Baseline	34.21	37.14	45.61	40.94	49.12	49.25	57.89	53.23
	CoT	Baseline	46.49	45.45	35.09	39.60	49.56	49.21	55.36	52.10
	CoT	RAG	56.14	55.74	59.65	57.63	50.00	50.00	59.65	54.40
	DAG	Baseline	51.40	51.16	41.51	45.83	48.04	48.53	64.71	55.46
Qwen3-30B-Reasoning	Simple*	Baseline	57.94	57.78	50.00	53.61	71.03	78.05	59.26	67.37
	CoT	Baseline	54.08	54.29	39.58	45.78	72.63	84.38	56.25	67.50
	CoT	RAG	72.73	87.88	55.77	68.24	76.92	87.18	64.15	73.91
	DAG	Baseline	75.00	94.44	54.84	69.39	71.23	76.92	57.14	65.57
GPT-OSS-20B-High	Simple*	Baseline	63.16	62.86	59.46	61.11	69.33	66.67	51.61	58.18
	CoT	Baseline	58.04	60.98	44.64	51.55	61.61	63.27	55.36	59.05
	CoT	RAG	70.54	74.47	62.50	67.96	70.54	73.47	64.29	68.57
	DAG	Baseline	75.71	80.00	55.17	65.31	67.16	71.43	58.82	64.52
Claude-Sonnet-4.5	Simple*	Baseline	69.30	68.97	70.18	69.57	70.18	74.47	61.40	67.31
	CoT	Baseline	70.18	69.49	71.93	70.69	69.03	66.15	76.79	71.07
	CoT	RAG	74.56	78.00	68.42	72.90	76.32	76.79	75.44	76.11
	DAG	Baseline	73.68	72.13	77.19	74.58	67.54	66.67	70.18	68.38

*Simple prompting: directly ask the model to identify vulnerabilities, e.g., "identify if the code is vulnerable and explain the reasoning". $^{\dagger}R_{F1}$ is the most important metric as it balances precision and recall in vulnerability reasoning.

Structural advantages. DAGVUL provides several structural benefits over linear CoT. Acyclicity prevents circular dependencies, while node atomicity mandates that logical leaps remain verifiable through single assertion steps. Additionally, the closure requirement eliminates irrelevant exploratory paths and mandates evidence-based grounding. These constraints effectively distinguish genuine causal derivation from superficial features found in unstructured baselines.

5.2 Future Work

Adversarial training. Due to the high cost associated with generating high-quality synthetic data, we have not yet utilized the semantic-preserving perturbation dataset for model training. Future work will explore adversarial training using these semantic-preserving transformations.

Formal verification. Our framework currently relies on reward models to judge reasoning quality. Future work could explore automated verification via formal languages like Datalog [63] or Lean [64] for increased reliability, though the dependency on manually written programs and the subsequent constraints on generalization remain open challenges.

Evidence extraction. While DAGVUL primarily mitigates CS and AR errors, focus errors (FE) in long-context scenarios remain a challenge. We plan to improve the identification of source nodes in the DAG by developing targeted training for evidence extraction, enabling the model to better prioritize vulnerability-relevant segments within extensive codebases.

5.3 Limitations

Language scope. Our evaluation focuses primarily on C/C++ vulnerabilities. While the DAGVUL framework is designed to be language-agnostic, its reasoning efficacy on other languages such as Java or Python has not yet been extensively tested. Expanding the benchmark to ensure cross-language applicability remains a critical objective for future research.

Judge reliability. We utilize GPT-5 as an automated judge to ensure scalability. Manual validation of 200 samples identified only 6 misclassifications, yielding a 3% error rate that confirms the high reliability of the approach. Nonetheless, LLM-as-a-Judge may still introduce subtle subjective biases compared to traditional human expert reviews.

Model generalization. While our methodology significantly improves performance on the current test set, its ability to generalize to out-of-distribution (OOD) CWE types remains an open question. Further studies are required to assess whether the learned causal logic can be effectively maintained when the model encounters unseen vulnerability categories.

6 Related Work

6.1 LLMs for Vulnerability Detection

LLMs are emerging as a promising new paradigm in software vulnerability detection, aiming to overcome the limitations of traditional Static Analysis and Dynamic Analysis tools, such as high false-positive rates and lack of contextual understanding [65–71]. To apply LLMs for vulnerability detection, researchers have explored various methods.

Integration with Static Analysis. Li et al. [3] proposed LLIFT, a framework that synergizes static analysis with LLMs through post-constraint guided path. Wen et al. [72] proposed SCALE, which integrates LLM-generated natural language comments into Abstract Syntax Trees to better capture both code semantics and execution sequences. Liu et al. [73] employed lightweight static analysis to detect Remote Code Execution vulnerabilities in LLM-integrated frameworks by constructing cross-library call chains.

Integration with Dynamic Analysis. Li et al. [74] proposed CHATAFL, which enhances protocol fuzzing by leveraging LLMs to generate and mutate structured messages for deeper state-space exploration. Wang et al. [75] developed HITS, a framework that improves the coverage of LLM-based unit test generation by employing method slicing to simplify complex methods into manageable code segments. Sen et al. [76] presented SELLM, a tool that utilizes symbolic execution to identify vulnerability-prone paths and extracts variable constraints to structure optimized prompts for LLM-based smart contract analysis.

LLM agent approach. Wen et al. [77] proposed a multi-agent framework that utilizes collaborative agents with distinct roles to overcome context window limitations and identify complex inter-procedural vulnerabilities at the repository level. Gao et al. [78] developed Mono, a multi-agent system that orchestrates a Leader for task decomposition and coordination, a Code Analyst for deep semantic investigation of patches, and a Security Reviewer for rigorous cross-verification, collectively simulating a human-expert collaborative auditing process.

Our work diverges from these streams by positing that these reliability issues are symptomatic of a deeper, unaddressed problem: the models' core reasoning process is flawed. **Instead of building complex systems on an unreliable foundation, our research first focuses on rigorously evaluating and then directly enhancing this core reasoning capability.**

6.2 Trustworthiness in AI-assisted Security

The application of LLMs to software security has led to an increased focus on the trustworthiness of AI-generated results. This trend emphasizes the need for transparent reasoning to make AI-assisted auditing practically viable in real-world environments. Recent research investigates various methodologies for ensuring such reliability. Sistla et al. [63] proposed a method to enhance the trustworthiness of LLM-based code reasoning by extracting formal representations of the model's reasoning steps and employing formal verification tools to automatically validate their correctness. Zhang et al. [79] introduced the Computational Thinking Model, which enhances the trustworthiness of LLM reasoning by integrating computational paradigms such as decomposition and abstraction with live code execution to mitigate logical inconsistencies and hallucinations. Our framework, DAGVUL, aligns with this emerging paradigm of trustworthy AI by bridging the gap between statistical probability and program-intrinsic logic. Continued investment in such verifiable reasoning frameworks is essential to ensure that AI remains a reliable asset rather than a liability in software security.

7 Conclusion

This paper systematically evaluates and enhances the vulnerability reasoning capabilities of LLMs. We construct a high-quality benchmark that incorporates expert-curated causal reasoning as ground truth and semantic-preserving perturbations. Our empirical study uncovers a pervasive reliability gap between binary detection and logical reasoning, formalizing a taxonomy of 12 systematic failure patterns. To address these limitations, we introduce DAGVUL, which integrates DAG modeling with RLVR, aligning model reasoning trace with the underlying causal logic of program vulnerabilities. Our approach effectively bridges the reliability gap between detection and reasoning.

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A Perturbation Methods

To comprehensively evaluate the robustness of vulnerability reasoning against adversarial but semantic-preserving modifications, we adopt 26 code transformation methods. As detailed in Table 7, these methods are organized into six categories: *Basic*, *Condition*, *Loop*, *Logic*, *Decomposition*, and *Arithmetic*. The *Basic* category introduces syntactic noise (e.g., renaming, dead code insertion) to test resilience against superficial pattern changes. *Condition*, *Loop*, and *Logic* methods alter control flow structures without modifying execution paths, challenging the model's ability to track program states. Finally, *Decomposition* and *Arithmetic* methods restructure code blocks and expressions to verify if the reasoning logic holds across structurally diverse but semantically equivalent implementations.

The example below contrasts the original and perturbed versions of a code snippet, which remain semantically equivalent. Despite the significant structural variations, the two snippets preserve the identical Use-After-Free (UAF) vulnerability pattern and maintain invariant memory operations. Specifically, both versions allocate a buffer of exactly 100 long integers, perform complete initialization of the allocated memory, release the memory at the same logical juncture, and subsequently access the dangling pointer. This transformation leverages several perturbation methods, including *Basic* (identifier renaming and junk function insertion), *Arithmetic* (equivalent expression replacement), and *Loop* (loop decomposition and for-to-while transformation).

While most models accurately identify the UAF mechanism in the original code, they frequently exhibit reasoning failures when evaluating the perturbed version. For instance, Llama-3.1-8B incorrectly predicts a potential buffer overflow, reasoning that the `math_func1` wrapper could return a large or negative value that leads to an unsafe allocation size for the `data_block` array. Similarly, DeepSeek-v3 yields a false negative by asserting that the code contains no obvious vulnerabilities, specifically claiming that all mathematical operations are well-defined and that the memory is properly allocated and deallocated without unsafe accesses. These errors highlight that the models are susceptible to interference from vulnerability-irrelevant features within the perturbed

Table 7: Perturbation methods and their corresponding categories.

Category	Methods	Description
Basic Methods	Add exception	Add exception handling blocks
	Change statement order	Change order of adjacent statements that share no variables
	Check arguments	Check if the arguments are none
	Insert junk function	Insert junk functions that won't be called
	Insert junk loop	Insert junk loops that won't be executed
	Insert variables	Insert variables that won't be used
	Move assignments	Move assignments if a variable is assigned directly
	Statement wrapping	Wrap the statements with if or for statement
	Function rename	Change the function name
	Variables rename	Change the variables name
Condition Methods	Add condition	Improve condition statements by adding else clauses
	Div if else	Divide the if else-if else into if else if else
	Div composed if	Divide the composed if statement into single
	If-continue to if-else	Transform if-continue statement to if-else statement
	If to switch/match	Transform if statement to switch/match statement
	Switch/match to if	Transform switch/match statement to if statement
Loop Methods	Div loop	Divide a loop into several loops
	For/while transformation	Transform for/while loop to while/for loop
Logic Methods	Equi boolean logic	Transform boolean logic equivalently
	Swap boolean expression	Swap the sides of the boolean expression
Decomposition Methods	Extract if	Extract method from if statements
	Extract arithmetic	Extract method from arithmetic statements
Arithmetic Methods	Equi arithmetic expression	Change arithmetic computation or assignment equivalently
	Expression div	Divide the long expression to several small expressions
	Modify operations	Modify compound assignment operations (e.g., a += b to a = a + b)

code, while failing to consider the underlying causal logic of the vulnerability.

CWE-416 (new_delete_class_13_unsafe)

```cpp
void func1() {
    long* data;
    data = NULL;
    if (1) {
        data = new long[100];
        {
            size_t i;
            for (i = 0; i < 100; i++) {
                data[i] = 5L;
            }
        }
        delete[] data;
    }
    if (1) {
        printLongLine(data[0]);
    }
}
```

Semantic-Preserving Perturbation

```cpp
int math_func1(int a, int b, int c) {
    int var3 = 99;
    if (true) {
        int var1 = 42;
        int temp1 = b - c;
        return a + temp1;
    }
}

int math_func2(int a, int b, int c) {
    long var4 = 987654321;
    for (int i = 0; i < 1 / 2; ++i) {
        long var2 = 123456789;
        int temp2 = b - c;
        return a + temp2;
    }
}

int math_func3(int a, int b) {
    int var5 = 111;
    if (true) {
        return a + b;
    }
}

void process_data() {
    long* data_block;
    data_block = NULL;
    if (math_func1(1, 2, 2)) {
        data_block = new long[math_func1
            (100, 4, 4)];
        {
            size_t i = math_func1(0, 5, 5);
            while (i < 50 / 2) {
                data_block[i] = math_func3
                    (5L, 6);
                ++i;
            }
            while (i < 100 / 2) {
                data_block[i] = math_func3
                    (5L, 6);
                ++i;
            }
            while (i < 100) {
                data_block[i] = math_func3
                    (5L, 6);
                ++i;
            }
        }
        delete[] data_block;
    }
    if (math_func2(1, 7, 7)) {
        printLongLine(data_block[0]);
    }
}
```

B Prompt for Gold DAGVUL Dataset

We outline the three-stage pipeline employed to synthesize the gold-standard DAGVUL dataset for vulnerability reasoning.

Stage 1: Node Identification. We utilize DeepSeek-R1 to extract a discrete node set by parsing previously generated CoT trajectories. Reasoning granularity is normalized by constraining each node to a solitary sentence containing a single primitive security assertion or atomic analysis step. This process ensures that every node represents either an immutable code fact or a solitary logical inference derived from the provided context.

Stage 2: Dependency Assignment. Conditioned on the identified node set, the model is prompted to assign the minimal collection of direct ancestors required for each logical derivation. We implement structural constraints to ensure acyclicity and require that all inferential paths remain logically connected to the terminal sink node. This connectivity ensures that every intermediate assertion contributes to a definitive and exhaustive audit verdict.

Stage 3: Edge Generation. Based on the verified parent-child pairs, DeepSeek-R1 produces edge justifications explaining the inferential leap between steps. These justifications are constrained to standard program analysis principles, such as taint propagation or control-flow tracing, without introducing external facts. Finally, these validated triplets are aggregated into a structured DAGVUL formatted trajectory in forward chronological order.

B.1 Prompt for Stage 1

Simplified System Prompt Node Identification

Role: Program Analysis and Code Security Expert.
Objective: Decompose source code and vulnerability reports into atomic logical nodes for Directed Acyclic Graph (DAG) construction.
Node Definitions:
- **SOURCE NODE (V_{in}):** Literal facts extracted directly from code (e.g., declarations, API usage). *Constraint:* No inference allowed.
- **INTERMEDIATE NODE (V_{inter}):** Derived logical reasoning (e.g., taint tracking, flow analysis).
- **SINK NODES (V_{out}):** *verified_sink* for confirmed vulnerabilities; *sanitized_sink* for proven safe paths.

Operational Constraints:
- **Atomicity:** Each node must be exactly one sentence containing a single atomic assertion (program state, data flow, or control flow).
- **Comprehensive Analysis:** Capture all potential paths. Output multiple sinks if the analysis describes both vulnerable and sanitized trajectories.

Input:
Core Code: `{core_code}`; Context: `{callee/caller_-methods}`, `{type_defs}`, `{global_vars}`;
Original Analysis: `{original_analysis}`.
Output: Generate a strictly structured JSON response containing the array of atomic nodes.

B.2 Prompt for Stage 2

Simplified System Prompt for Dependency Assignment

Role: Program Analysis and Code Security Expert.
Objective: Annotate each security analysis node with its minimal set of direct dependencies to establish a valid causal graph.
Dependency Logic:
- **Source Nodes (V_{in}):** Assign `null`, as these premises are extracted directly from code facts.
- **Inferential Nodes (V_{inter}, V_{out}):** List the minimal, directly required prior `step_id` values. This list must not be empty.

Structural Rules:
- **Acyclicity and Validity:** Every dependency must reference a prior `step_id` that exists in the input set.
- **Minimality:** Exclude transitive dependencies. If node A relies on B, and B relies on C, A should only cite B unless C is independently required.
- **Logical Closure:** Every V_{in} and V_{inter} node must be utilized by at least one subsequent step to support the final conclusion.

Refinement Strategy (Self-Correction):
- **Prune:** Remove nodes containing security-irrelevant information that does not contribute to the final audit verdict.
- **Connect:** If a relevant node is currently unreferenced, identify the appropriate downstream step and add the missing dependency link to resolve dangling logic.

Input: `{stage_1_output_json}`
Output: Return a strictly structured JSON array where each node is annotated with its `direct_dependent_steps`.

B.3 Prompt for Stage 3

Simplified System Prompt for Edge Generation

Role: Program Analysis and Code Security Expert.
Objective: For each node in the structured analysis, generate a concise justification paragraph (edge) clarifying its logical progression.
Content Requirements:
- **Conciseness:** Limit each output to 1–2 sentences. Avoid narrative storytelling; focus on direct causal links.
- **Dependency Citation:** Explicitly cite parent node IDs (e.g., "From Step X...") to justify how the current node is derived.
- **Analysis Principles:** State the specific program analysis methodology used, such as *Taint Propagation*, *Constraint Solving*, or *Reachability Analysis*.
- **Base Facts:** For Source Nodes (V_{in}) with null dependencies, simply state that the information is a fact extracted directly from the code context.
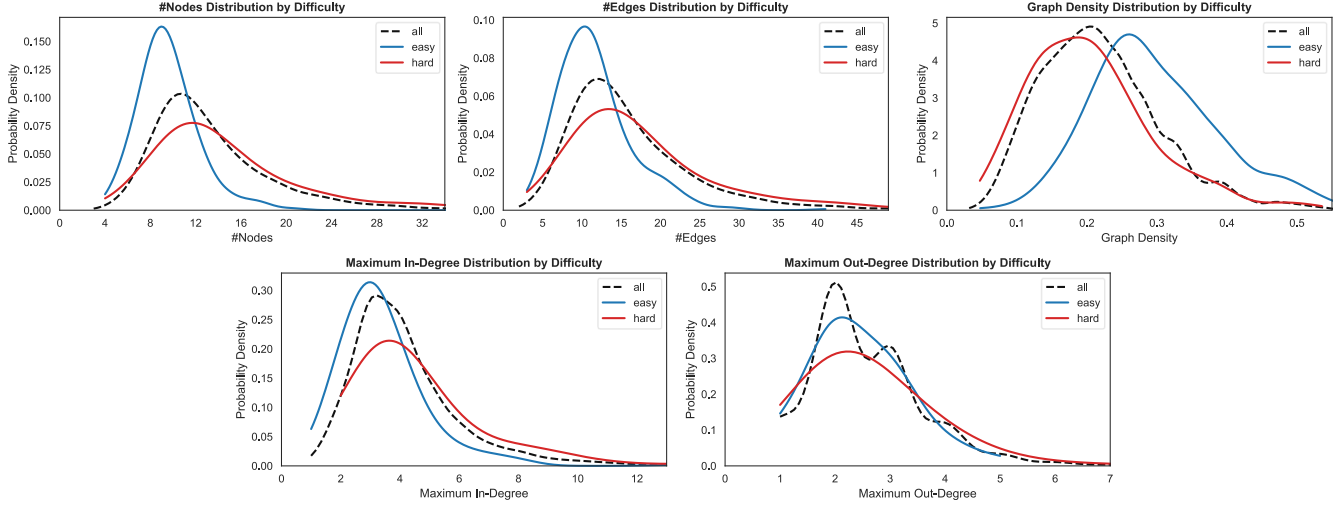
Few-shot Logic Patterns:

Figure 6: Topological statistics of reasoning graphs in the Gold DAGVUL dataset. The probability density plots illustrate the distribution of node counts, edge counts, graph density, and maximum degree constraints, categorized by analysis difficulty (all, easy, and hard).

- **Fact Extraction:** This statement is directly extracted from the code definition to establish the buffer's initial capacity.
- **Taint Propagation:** Since Step 1 introduces taint and Step 2 assigns it to the input variable, we infer the input is now tainted.
- **Semantic Analysis:** Analyzing the implementation in Step 5 reveals a lack of length checks, leading to the inference in Step 8.
- **Constraint Solving:** Based on the control flow check in Step 3 and the logic in Step 8, the branch is taken strictly when the input lacks validation.

Input: `{stage_2_output_json}`

Output: Return a JSON object with a `thinking` array, containing the `step_id` and the concise justification string.

C Topological Statistics of Gold DAGVUL

To investigate the impact of code complexity on reasoning topologies, we categorize the Gold DAGVUL samples based on a composite difficulty metric. As defined in Equation 3, this metric integrates the cyclomatic complexity of the vulnerable function (CC_{vuln}), the cumulative complexity of the aggregated context ($CC_{context}$), and the total token count (N_{tokens}). We empirically set the weights to $w_1 = 1$, $w_2 = 0.3$, and $w_3 = 0.005$ to balance the structural and textual influences on analysis difficulty.

$$Difficulty = w_1 \cdot CC_{vuln} + w_2 \cdot CC_{context} + w_3 \cdot N_{tokens} \quad (3)$$

To enhance the discriminability of our statistical results, we specifically select the samples within the top 10% of the difficulty distribution to represent Hard instances and those in the bottom 10% to represent Easy instances. We contrast the polar subsets of easy and hard instances against the aggregate statistics for the all 8,157 samples. Our analysis focuses on five graph-level statistics: (1) total number of nodes ($|V|$); (2) total number of edges ($|E|$); (3) graph density, defined as $\frac{2|E|}{|V|(|V|-1)}$; (4) maximum in-degree (d_{in}^{max}); and (5) maximum out-degree (d_{out}^{max}).

As illustrated in Figure 6, the topological profile of the reasoning graphs shifts significantly with increasing code difficulty. The distributions for $|V|$ and $|E|$ exhibit a pronounced rightward shift for Hard samples, confirming that sophisticated vulnerabilities necessitate more granular reasoning steps and additional causal links. Conversely, the graph structure becomes noticeably sparser as difficulty rises. This decrease in density suggests that harder reasoning tasks produce broader and less connected structures, reflecting a modular decomposition where semi-independent logical chains are eventually integrated to reach the terminal sink.

Furthermore, topological analysis reveals that logical complexity is reflected in the concurrent expansion of both maximum in-degree and out-degree distributions. For hard samples, both metrics exhibit a noticeable rightward shift and broadening compared to the easy samples. This observation implies that logical complexity in vulnerability auditing scales through both deeper prerequisite requirements and increased branching logic, where sophisticated vulnerabilities necessitate more complex inferential dependencies and broader analytical impacts across the reasoning graph.