# DAG-Math: Graph-Guided Mathematical Reasoning in LLMs

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Code: https://github.com/YuanheZ/DAG-MATH

## Abstract

Large Language Models (LLMs) achieve strong results on mathematical reasoning tasks with Chain-of-Thought (CoT), yet it remains unclear whether this reflects genuine rule-based reasoning or heuristic search. We propose a framework that models CoT as a stochastic process over directed acyclic graphs (DAGs), where nodes denote intermediate states and edges represent rule applications. Within this setting, we introduce **logical closeness**, a metric that measures how closely an LLM's derivation trajectory adheres to the DAG structure, extending evaluation beyond final-answer accuracy (PASS@$k$). To operationalize this, we design the *DAG-MATH* CoT format and construct a benchmark that elicits trajectories in this form, enabling structured evaluation of reasoning. Evaluation on mathematical reasoning datasets reveal statistically significant differences in reasoning fidelity across LLM families-even when final-answer accuracy is comparable-highlighting gaps between final-answer accuracy and rule-consistent inference. Our approach bridges free-form CoT with structured systems and provides actionable diagnostics for evaluating the quality of LLM reasoning.

## 1 Introduction

Large Language Models (LLMs) have demonstrated promising mathematical reasoning abilities on answer/proof-based problems by the Chain-of-Thought (CoT) (Nye et al., 2021; Wei et al., 2022; Kojima et al., 2022; Zhang et al., 2022), e.g., Gemini-2.5 (Gemini Team, 2025) and GPT-5 (OpenAI, 2025), DeepSeek-R1 (DeepSeek Team, 2025). The black-box nature of CoT in LLMs raises a key challenge: how to rigorously model and evaluate LLMs' mathematical reasoning abilities. Intuitively, LLM reasoning needs to identify all required premises (e.g., facts, constraints), and conduct correct logical inference from premises to reach the conclusion.[3] These operations must be exact, in line with the exact learning requirements in György et al. (2025). To test whether LLMs achieve this through CoT, two elements are crucial: (1) **a rigorous framework** to characterizes the mechanisms by which CoT operates in mathematical problem solving; (2) **an appropriate evaluation metric** to assess whether model outputs reflect authentic reasoning processes rather than the application of heuristic or search-based strategies[4].

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[3]Accurate calculation and symbolic execution are also required, see the discussion in Section A.1.

[4]Search-based strategies may yield irrelevant information, undermining solution's consistency. LLMs should be able to summarize the searched/thinking results to ensure the final output logic coherence.

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Existing approaches remain limited in both framework and evaluation. On the **framework** side, prior work (Dziri et al., 2023; Kim et al., 2025; Shalev-Shwartz & Shashua, 2025; Wang et al., 2023; Yin & Wang, 2025) casts CoT as Boolean-circuit analyses, $k$-parity models, or graph abstractions, leaving them unable to capture long-range and cross-branch dependencies or the goal-directed, absorbing-state nature of CoT. On the **evaluation** side, most studies (Dziri et al., 2023; Joshi et al., 2025; Kim et al., 2025; Xu & Sato, 2025) prioritize final-answer metrics like PASS@$k$, making it unclear whether success reflects logical inference or search. LEAN-based formal verification (De Moura et al., 2015; Moura & Ullrich, 2021; Google DeepMind, 2024; Ren et al., 2025; Wang et al., 2025; Lin et al., 2025) is promising but presupposes problems are already encoded in proof-oriented form, which typically demands substantial expert effort.

We address these limitations by formalizing CoT as a rule-based stochastic process on directed acyclic graphs (DAGs) in Section 2 and introducing the notion of *logical closeness* in Section 3, which evaluates whether an LLM solves a problem by searching over possible choices or by applying rigorous logical inference. This yields a new evaluation metric called the *perfect reasoning rate (PRR)* for ranking. In Section 4, we propose the *DAG-MATH* format to make CoT's structure explicit via DAG then employ few-shot prompting to guide LLMs to produce formatted CoT to evaluate on proposed metrics.

**Notations:** We denote a random variable by a capital letter (e.g., $V$) and its realization by the corresponding lowercase letter (e.g., $v$). For shorthand, we write $v_{1:t} = (v_1, v_2, \dots, v_t)$ for $t \geq 1$. We denote a DAG by $\mathcal{G} = (\mathcal{E}, \mathcal{V})$, where $\mathcal{V}$ is the node set and $\mathcal{E}$ is the edge set. For a node $v$, we write $\mathrm{pa}(v)$ as its parent set. Finally, we denote the input prompt by $\boldsymbol{X}_{\mathtt{in}} \in \mathcal{P}$, where $\mathcal{P}$ is the power set of the vocabulary.

## 2 A DAG Framework for Step-Level CoT

Motivated by empirical observations in Bogdan et al. (2025), we study CoT at the **step** level, rather than the token level. This step-level perspective has been widely considered in recent theoretical analyses (Dziri et al., 2023; Hu et al., 2024; Kim et al., 2025; Shalev-Shwartz & Shashua, 2025). We model step-level CoT in a two-phase workflow as below.

### 2.1 Phase 1: Task-specific DAG for Step-Level CoT

**Edges and Nodes in Step-Level CoT:** For math problems, a CoT step is a natural-language derivation of a new conclusion from prior information. Each step has two components: *Edge (Justification)*: This captures the inference that leads to the step's conclusion. *Node (Conclusion)*: The node represents the step's conclusion. Hence, a single CoT step can be viewed as node/edge decomposition, see an example in Section A.2. Consequently, prior work (Dziri et al., 2023; Hu et al., 2024; Kim et al., 2025; Shalev-Shwartz & Shashua, 2025; Bogdan et al., 2025) has typically defined steps heuristically. As a first attempt, we present an abstract mathe formulation, with the technical details deferred to Section A.3 (not essential for understanding the main text).

**Task-Specific DAG:** Empirical studies (Ye et al., 2025) demonstrate the existence of a latent directed dependency graph within LLMs, present as soon as a question/prompt is posted, before any output is generated. Formally, given a prompt $\boldsymbol{x}_{\mathtt{in}}$, we define the directed graph as

$$\mathcal{G}(\boldsymbol{x}_{\mathtt{in}}) := (\mathcal{V}(\boldsymbol{x}_{\mathtt{in}}), \mathcal{E}(\boldsymbol{x}_{\mathtt{in}})), \quad \text{where } \mathcal{E}(\boldsymbol{x}_{\mathtt{in}}) \subseteq \mathcal{V}(\boldsymbol{x}_{\mathtt{in}}) \times \mathcal{V}(\boldsymbol{x}_{\mathtt{in}}),$$

where $\mathcal{E}(\boldsymbol{x}_{\mathtt{in}})$ is the set of directed edges and $\mathcal{V}(\boldsymbol{x}_{\mathtt{in}})$ is the set of nodes divided into three classes:

- $\mathcal{V}_{\mathtt{in}}(\boldsymbol{x}_{\mathtt{in}})$ denotes the set of *source* nodes, i.e., nodes formulated solely from the input prompt.
- $\mathcal{V}_{\mathtt{out}}(\boldsymbol{x}_{\mathtt{in}})$ denotes the set of *sink* nodes, i.e., nodes with only incoming edges and no outgoing edges, corresponding to the final answer(s). The **correct** sink node represents the terminal object that matches the ground-truth answer.
- $\mathcal{V}_{\mathtt{inter}}(\boldsymbol{x}_{\mathtt{in}}) := \mathcal{V}(\boldsymbol{x}_{\mathtt{in}}) \setminus \big(\mathcal{V}_{\mathtt{in}}(\boldsymbol{x}_{\mathtt{in}}) \cup \mathcal{V}_{\mathtt{out}}(\boldsymbol{x}_{\mathtt{in}})\big)$ denotes the set of intermediate nodes.

We make the following assumption on the acyclic structure of the graph for the absence of circular dependencies, ensuring that no CoT step depends on its own output either directly or indirectly.

**Assumption 1.** *For any input prompt $\boldsymbol{x}_{\mathtt{in}}$, the task-specific directed graph $\mathcal{G}(\boldsymbol{x}_{\mathtt{in}})$ is acyclic.*

This assumption covers the answer-based math problems which have tractable computation graphs such as AIME (Art of Problem Solving, 2025a,b). Note that, if the correct sink node is included in $\mathcal{G}(\boldsymbol{x}_{\mathtt{in}})$, the task-specific DAG can be always **constructed by backtracking** through its ancestors.

### 2.2 Phase 2: Stochastic Process on Logic Dependence

Based on the task-specific DAG, the LLM generates CoT trajectories over this DAG as the final output via a certain sampling strategy. Given $\mathcal{G}(\boldsymbol{x}_{\texttt{in}})$ from Phase 1, we denote the node-level autoregressive distribution of an LLM as $\mathbb{P}$. A node-level CoT trajectory $\{V_i\}_{i=1}^{L}$ with length-$L$, given the input prompt $\boldsymbol{X}_{\texttt{in}}$, sequentially generates $V_t \in \mathcal{V}$ $(1 \le t \le L)$, ultimately leading to the final answer $V_L := V_{\texttt{out}}$. Specifically, the trajectory $\{V_i\}_{i=1}^{L}$ follows the stochastic process:

$$V_1 \sim \mathbb{P}(\cdot \mid \boldsymbol{X}_{\texttt{in}}), \cdots, V_t \sim \mathbb{P}(\cdot \mid V_{t-1}, \ldots, V_1, \boldsymbol{X}_{\texttt{in}}), \cdots, V_{\texttt{out}} \sim \mathbb{P}(\cdot \mid V_{L-1}, \cdots, V_1, \boldsymbol{X}_{\texttt{in}}).$$

Next, we define a stochastic transition rule to generate the node-level trajectory over $\mathcal{V}(\boldsymbol{x}_{\texttt{in}})$. We begin with the initial step, where $\mathbb{P}(V_1 = v \mid \boldsymbol{X}_{\texttt{in}} = \boldsymbol{x}_{\texttt{in}})$ is nonzero only for $v \in \mathcal{V}_{\texttt{in}}(\boldsymbol{x}_{\texttt{in}})$ and zero for all other nodes. Given $\mathcal{G}(\boldsymbol{x}_{\texttt{in}})$ and the previous $(t-1)$ steps $V_{1:t-1} = v_{1:t-1}$, the transition probability for the next step is not based on all previous nodes but depends on certain nodes, i.e.

$$\begin{aligned} &\mathbb{P}(V_t = v \mid V_{1:t-1} = v_{1:t-1}, \boldsymbol{X}_{\texttt{in}} = \boldsymbol{x}_{\texttt{in}}), \forall v \in \mathcal{V}(v_{1:t-1} \mid \boldsymbol{x}_{\texttt{in}}), \\ &\text{with } \mathcal{V}(v_{1:t-1} \mid \boldsymbol{x}_{\texttt{in}}) := \Big\{ v \in \mathcal{V}(\boldsymbol{x}_{\texttt{in}}) : \mathrm{pa}(v) \subseteq \{v_{1:t-1}\}, v \notin \{v_{1:t-1}\} \Big\}, \end{aligned} \tag{1}$$

and zero probability for $\forall v \notin \mathcal{V}(v_{1:t-1} \mid \boldsymbol{x}_{\texttt{in}})$. The sampling process is absorbing upon reaching any node $v \in \mathcal{V}_{\texttt{out}}(\boldsymbol{x}_{\texttt{in}})$, indicating that a final answer has been obtained. For better illustration, we provide a representative example to understand two phases in Section A.4.

**Remark:** For **non-thinking LLMs**, the model directly outputs such types of CoT for the given problem. For **thinking LLMs**, e.g. DeepSeek-R1 (DeepSeek Team, 2025), the thinking process can be viewed as an exploration of the task-specific DAG with self-correction or backtracking, but its final output shown to the users (excluding thinking tokens) is still consistent with our transition rule.

## 3 Formal Definition of Mathematical Reasoning Ability

Based on our DAG framework, we now present a formal definition of mathematical reasoning ability. Given an input prompt $\boldsymbol{x}_{\texttt{in}}$, we independently draw $N$ CoT trajectories $\{\boldsymbol{v}^{(i)}\}_{i=1}^{N}$ under the proposed sampling mechanism in Eq. (1). For each trajectory $\boldsymbol{v}^{(i)}$, we construct a trajectory-specific DAG:

$$\mathcal{G}_{\text{gen}}^{(i)}(\boldsymbol{x}_{\texttt{in}}) = \big(\mathcal{V}_{\text{gen}}^{(i)}(\boldsymbol{x}_{\texttt{in}}), \mathcal{E}_{\text{gen}}^{(i)}(\boldsymbol{x}_{\texttt{in}})\big), \quad 1 \le i \le N,$$

where the the object (DAG, node, or edge) with subscript $\texttt{gen}$ indicates it is extracted from the generated CoT trajectory. Each trajectory-specific DAG is a sub-DAG of $\mathcal{G}(\boldsymbol{x}_{\texttt{in}})$, and the reasoning ability of each trajectory can be evaluated using a new metric, termed **logical closeness**, and the concept of *perfect reasoning*, introduced in our framework.

**Definition 1** (Logical closeness and perfect reasoning)**.** *Under Assumption 1, consider an input prompt $\boldsymbol{x}_{\texttt{in}}$ and the DAG $\mathcal{G}_{gen}(\boldsymbol{x}_{\texttt{in}})$. For each node $v \in \mathcal{G}_{gen}(\boldsymbol{x}_{\texttt{in}})$, define its out-degree as*

$$\texttt{deg}\big(v \mid \mathcal{G}_{gen}(\boldsymbol{x}_{\texttt{in}})\big) := \Big|\big\{u \in \mathcal{G}_{gen}(\boldsymbol{x}_{\texttt{in}}) \mid (v \to u) \in \mathcal{E}_{gen}(\boldsymbol{x}_{\texttt{in}})\big\}\Big|.$$

*We say that $\mathcal{G}_{gen}(\boldsymbol{x}_{\texttt{in}})$ is **logically closed** if*

$$\texttt{deg}\big(v \mid \mathcal{G}_{gen}(\boldsymbol{x}_{\texttt{in}})\big) \ge 1, \quad \forall\, v \in \mathcal{V}_{gen}(\boldsymbol{x}_{\texttt{in}}),$$

*i.e., only the final nodes have no outgoing edges. Furthermore, if the sink node corresponds to the correct answer, we call the associated CoT trajectory a case of **perfect reasoning**.*

Now we can formally define the mathematical reasoning ability of LLMs as follows.

**Definition 2** (Mathematical reasoning ability)**.** *Under Assumption 1, let an LLM be given a prompt $\boldsymbol{X}_{\texttt{in}} \in \mathcal{P}$, sampled from an underlying distribution $\mathcal{D}$ over mathematical problem prompts. We define two indicator functions for a trajectory-specific DAG $\mathcal{G}_{gen}(\boldsymbol{X}_{\texttt{in}})$:*

$$\delta_{\texttt{close}}\big(\mathcal{G}_{gen}(\boldsymbol{X}_{\texttt{in}})\big) := \begin{cases} 1, & \text{if } \mathcal{G}_{gen}(\boldsymbol{X}_{\texttt{in}}) \text{ is logically closed}, \\ 0, & \text{otherwise}, \end{cases}$$

$$\delta_{\texttt{final}}\big(\mathcal{G}_{gen}(\boldsymbol{X}_{\texttt{in}})\big) := \begin{cases} 1, & \text{if the sink node of } \mathcal{G}_{gen}(\boldsymbol{X}_{\texttt{in}}) \text{ is correct}, \\ 0, & \text{otherwise}. \end{cases}$$

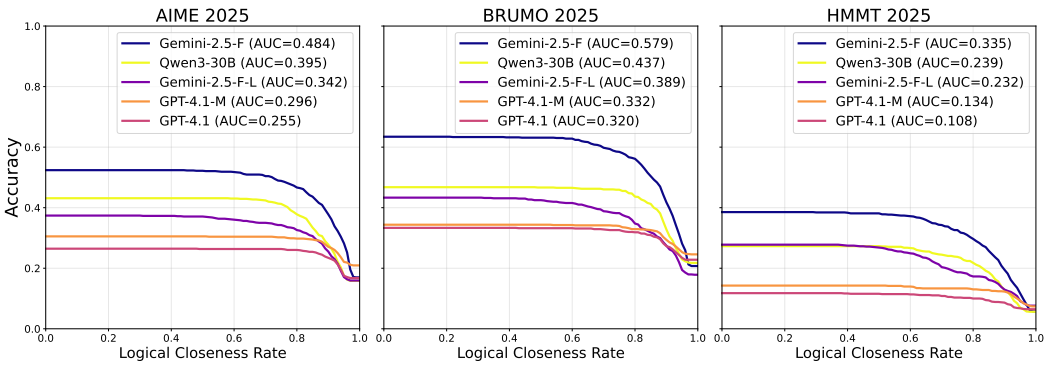


Figure 1: The AUC curves of averaged accuracy under the logical closeness rate over three datasets for five selected LLMs.

*Then, the **Perfect Reasoning Rate (PRR)** of an LLM w.r.t. a given prompt $\boldsymbol{X}_{\texttt{in}}$ is defined as*

$$\mathrm{PRR}(\boldsymbol{X}_{\texttt{in}}) := \mathbb{E}_{\mathbb{P}}\Big[\delta_{\texttt{close}}\big(\mathcal{G}_{gen}(\boldsymbol{X}_{\texttt{in}})\big) \times \delta_{\texttt{final}}\big(\mathcal{G}_{gen}(\boldsymbol{X}_{\texttt{in}})\big)\Big].$$

*The overall **mathematical reasoning ability** of an LLM over the distribution $\mathcal{D}$ is then measured as*

$$\mathcal{R} := \mathbb{E}_{\boldsymbol{X}_{\texttt{in}}\sim\mathcal{D}}\big[\,\mathrm{PRR}(\boldsymbol{X}_{\texttt{in}})\big] = \mathbb{E}_{\mathbb{P},\,\boldsymbol{X}_{\texttt{in}}\sim\mathcal{D}}\Big[\delta_{\texttt{close}}\big(\mathcal{G}_{gen}(\boldsymbol{X}_{\texttt{in}})\big) \times \delta_{\texttt{final}}\big(\mathcal{G}_{gen}(\boldsymbol{X}_{\texttt{in}})\big)\Big].$$

In practice, given a dataset with $M$ problems and $N$ independent CoT trajectories per problem, one can approximate $\mathrm{PRR}\,(\boldsymbol{x}_{\texttt{in}})$ and $\mathcal{R}$ by

$$\widehat{\mathrm{PRR}}\,(\boldsymbol{x}_{\texttt{in}}) := \frac{1}{N}\sum_{i=1}^{N} \delta^{(i)}_{\texttt{close}}\,(\boldsymbol{x}_{\texttt{in}}) \times \delta^{(i)}_{\texttt{final}}\,(\boldsymbol{x}_{\texttt{in}})\,, \quad \widehat{\mathcal{R}} := \frac{1}{M}\sum_{j=1}^{M} \widehat{\mathrm{PRR}}\left(\boldsymbol{x}^{(j)}_{\texttt{in}}\right).$$

**AUC socres:** By relaxing $\delta_{\texttt{close}}$ to permit a certain proportion of nodes that do not satisfy logical closeness, we obtain the corresponding AUC scores (with proportion of logic closeness from 0% to 100%), which serves as a comprehensive measure of mathematical reasoning performance.

Furthermore, Section B presents an example from AIME 2025 (Art of Problem Solving, 2025a,b) where the final answer is correct, but logic-closeness fails due to mixing two solution paths.

## 4 Evaluation of Mathematical Reasoning Ability

To make the DAG structure of standard CoT trajectories explicit, we introduce a structured CoT format via prompting called the *DAG-MATH* format. For illustration, below is one step in the DAG-MATH format (more example steps are presented in Section C).

> **Step 4** **`Edge`**: Since the left-hand side of the equation in Step 1 contains $\log(x-1)$, the domain restriction for a logarithm requires $x-1>0$, i.e., $x>1$.
> **`Parents`**: Step 1. **`Node`**: $\log(x-1)$ requires $x>1$.

For evaluation, we first construct a benchmark which contains 2,894 gold-standard formatted CoTs (see Section D), then we employ few-shot prompting (see Section E for details) to guide LLMs in generating formatted CoTs/DAGs for test problems.

**Models and datasets:** We evaluate five LLMs: `Gemini-2.5-Flash` (Gemini-2.5-F), `Gemini-2.5-Flash-Lite` (Gemini-2.5-F-L), `GPT-4.1`, `GPT-4.1-mini` (GPT-4.1-M), and `Qwen3-30B-A3B-Instruct-2507` (Qwen3-30B). These models demonstrate strong mathematical performance even without long thinking (White et al., 2025), also are more efficient and economical than other thinking-focused models due to lower token usage. We evaluate these models on three recently adopted datasets for high-difficulty, answer-based problems: AIME 2025 (Art of Problem Solving, 2025a,b), BRUMO 2025 (BRUMO, 2025), and HMMT 2025 (HMMT, 2025).

Table 1: Averaged graph-level statistics of sampled DAGs across selected LLMs on AIME 2025.

| Model | Class | #nodes | #edges | density | $\mathrm{d}_{\mathtt{in}}^{\max}$ | $\mathrm{d}_{\mathtt{out}}^{\max}$ |
|---|---|---|---|---|---|---|
| Gemini-2.5-F | All | 32.8 | 48.9 | 11.2% | 4.3 | 7.0 |
| | Incorrect | 35.6 | 53.3 | 10.6% | 4.6 | 8.6 |
| | Correct | 30.2 | 45.1 | 11.6% | 4.1 | 5.5 |
| | Perfect | 23.3 | 30.8 | 13.0% | 3.3 | 3.6 |
| Gemini-2.5-F-L | All | 33.0 | 54.0 | 13.4% | 3.6 | 9.7 |
| | Incorrect | 40.5 | 68.6 | 11.9% | 3.9 | 12.8 |
| | Correct | 21.5 | 31.6 | 15.7% | 3.2 | 4.8 |
| | Perfect | 16.1 | 21.4 | 18.4% | 3.0 | 3.2 |
| GPT-4.1 | All | 17.8 | 21.4 | 16.2% | 2.6 | 3.0 |
| | Incorrect | 18.4 | 22.2 | 15.6% | 2.6 | 3.1 |
| | Correct | 15.9 | 19.3 | 17.5% | 2.7 | 2.9 |
| | Perfect | 14.1 | 16.8 | 19.0% | 2.5 | 2.4 |
| GPT-4.1-M | All | 22.8 | 31.3 | 14.2% | 3.2 | 4.0 |
| | Incorrect | 25.0 | 34.7 | 13.3% | 3.3 | 4.3 |
| | Correct | 17.9 | 23.6 | 16.6% | 3.0 | 3.4 |
| | Perfect | 16.5 | 21.5 | 17.4% | 3.0 | 3.1 |
| Qwen3-30B | All | 21.4 | 31.1 | 16.0% | 3.3 | 4.9 |
| | Incorrect | 23.4 | 34.3 | 14.9% | 3.4 | 5.5 |
| | Correct | 18.9 | 27.2 | 17.2% | 3.1 | 4.1 |
| | Perfect | 14.7 | 19.6 | 20.2% | 2.9 | 3.0 |

We extract the generated DAGs and evaluate five graph-level statistics introduced in Section D, as well as model performance metrics (PASS@1 and $\widehat{\mathcal{R}}$). The sampled DAGs are then partitioned into four classes: **All** (no filtering), **Incorrect** (ending at an incorrect sink), **Correct** (ending at the correct sink), and **Perfect** (logically closed and ending at the correct sink).

Fig. 1 reports AUC scores across three datasets, with PASS@1 as the starting point and $\widehat{\mathcal{R}}$ as the end point (see more details in Table 2 in Section F), as the logic closeness rate increases. Besides, we also report averaged graph-level statistics for AIME 2025 in Table 1, with additional results for BRUMO 2025 and HMMT 2025 in Section F. We have the following observations:

- **Search improves raw accuracy while perfect reasoning ability remains similar.** Search can inflate raw accuracy, while the models' inherent perfect reasoning ability is broadly comparable. The AUC scores suggests that outputs, while correct, are superficially consistent at some point, which aligns with users' impressions when using these LLMs.
- **Graph structure reflects problem difficulty and reasoning quality.** Harder problems induce larger, sparser, and more branchy DAGs (see Section D). Gemini's **Correct** cohort exhibits larger but sparser graphs with slightly higher branching when compared to the GPT family, indicating that effective exploration and task planning can increase the likelihood of reaching correct answers without fully closed, deeper reasoning.
- **Identifying the "difficulty boundary".** Each model's effective difficulty ceiling corresponds to the regime where it can maintain compact, low-branching DAGs; beyond this point—when branching explodes and density drops-accuracy sharply declines.

## 5 Conclusion

This paper proposes a novel DAG-MATH framework for modeling and evaluating mathematical reasoning, introducing the concepts of logical closeness and perfect reasoning over DAGs. We demonstrate how DAG graph statistics vary with problem difficulty and how models' perfect-reasoning ability and AUC curve behaves across these tasks. The framework provides an accessible mathematical formalization of reasoning and memorization in LLMs, paving the way for future work on reasoning guarantees, analogous to generalization guarantees in supervised learning.

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# A Illustration and Definition of CoT Step

In this section, we first discuss execution correctness as a measure of LLM reasoning performance and emphasize that our framework addresses the key challenge of tracking logical dependencies. To facilitate understanding, we first provide an intuitive illustration of a CoT step using the logarithmic count problem, i.e.

**Logarithmic Count Problem (LCP)**

For how many integers $k \in [-300, 300]$ does the equation $2\log(x-1) = \log k$ have exactly one real solution $x$?

We illustrate a single step in the LCP below.

**One CoT Step in the Logarithmic Count Problem (LCP)**

If two logarithmic expressions are equal, then their arguments must also be equal.

Hence, from $2\log(x-1) = \log k$, we can conclude $(x-1)^2 = k$.

followed by a formal mathematical definition of a CoT step.

## A.1 Remark on Execution Correctness

We note that accurate calculation and symbolic execution remain essential for evaluating an LLM's mathematical reasoning. In practice, LLMs may make stepwise errors, such as computational slips or misreading problem statements. Our framework, however, assumes that each step is correct. This simplification is justified because step-level errors can be automatically detected using Process Reward Models (Lightman et al., 2023; Wang et al., 2024; Zhang et al., 2025) or SymPy validation.

Focusing on correct steps allows us to capture the trajectory of model capabilities: with recent advances (Kavukcuoglu, 2025; OpenAI, 2025; Yang et al., 2025; DeepSeek Team, 2025), the main bottleneck in complex mathematical reasoning lies less in local step fidelity and more in the higher-level logical structure. Our framework addresses this challenge by: (1) perceiving the full logical structure of a problem, and (2) navigating it to construct a coherent solution path. By abstracting away from local step errors, we can isolate and analyze the structural core of CoT reasoning.

## A.2 Intuitive Understanding of Steps in CoT

In this illustration, the blue part corresponds to the previous conclusion (parent node), the green part represents the new conclusion for the current node, and the orange part highlights the logical reasoning (Edge) that connects the parent to the current node. Note that the edge may be latent when the model only outputs the conclusion without explicitly stating the reasoning.

## A.3 Mathematical Definition of Steps in CoT

We now formalize the definition of a single CoT step. Let $\mathcal{V}$ denote the semantic domain of mathematical objects in *semantic normal form* (SNF). A raw CoT step is a sequence of tokens, i.e., a string $\boldsymbol{c} \in \mathcal{P}$. We introduce a *canonicalization map*

$$\kappa : \mathcal{P} \to \mathcal{V}$$

that maps any textual span to its SNF representation:

$$\boldsymbol{c} \xrightarrow{\kappa} \kappa(\boldsymbol{c}) \in \mathcal{V}\,.$$

The canonicalization map satisfies the following properties:

- **Idempotent:** $\kappa(\kappa(\boldsymbol{c})) = \kappa(\boldsymbol{c})$.

- **Presentation-invariant:** It does not perform substantive algebraic manipulations (e.g., expanding or factoring), which are treated as separate reasoning steps.

Canonicalization removes superficial variations such as synonyms, spacing differences, commutativity, and $\alpha$-equivalent variable names, ensuring semantic consistency.

Intuitively, a CoT step can be mapped to a normalized SymPy object that captures its underlying mathematical semantics. A concrete example of this canonicalization is provided below.

- *Input:* Raw CoT step as text tokens (e.g., "The value of our target is $x + y$." or "The target value is $(y + x)$.").
- *Canonicalization ($\kappa$):* Maps the input to a normalized form by removing superficial variations such as synonyms, spacing, commutativity, and $\alpha$-equivalent variable names.
- *Output:* A semantic object (e.g., SymPy object `Add(x,y)`) that consistently encodes the meaning.

Accordingly, let $\mathcal{F}$ denote a signature of *primitive inference rules/operations*. Each $f \in \mathcal{F}$ is associated with an arity $\mathrm{ar}(f) \in \mathbb{N}$ (i.e., the number of inputs the rule or operation takes) and a (partial) semantic operator $[\![f]\!] : \mathcal{V}^{\mathrm{ar}(f)} \rightharpoonup \mathcal{V}$. Intuitively, $\mathcal{F}$ represents the atomic reasoning steps allowed at the CoT level, such as a single algebraic operation, one application of a named lemma, or a single substitution. We now formally define a CoT step.

**Definition 3** (Atomic Step of CoT)**.** *Given an input prompt $\boldsymbol{x}_{\mathtt{in}} \in \mathcal{P}$, a CoT trajectory of length $\ell$ is a sequence of steps $\mathcal{C} = (\mathbf{c}_1, \ldots, \mathbf{c}_\ell)$. Suppose $\kappa : \mathcal{P} \to \mathcal{V}$ is a canonicalization map. Then, a* step *$\mathbf{c}_i$ can be formulated as a triple $(\Gamma_i, f_i, v_i)$ denoted by $\Gamma_i \xrightarrow{f_i} v_i$, where:*

1. ***Canonicalization:** Each string $\boldsymbol{c}_i \in \mathcal{P}$ produced in the CoT trajectory is mapped by $\kappa$ to the corresponding SNF object $v_i = \kappa(\boldsymbol{c}_i) \in \mathcal{V}$.*
2. ***Premises:** $\Gamma_i \subseteq \{v_1, v_2, \ldots, v_{i-1}\}$ is the finite set of previously established SNF objects (from the prompt or earlier steps) directly used to infer the current step.*
3. ***Primitive operation:** $f_i \in \mathcal{F}$ and $v_i = [\![f_i]\!](\Gamma_i)$, i.e., $v_i$ is obtained by exactly one application of a primitive operator to the premises.*

Accordingly, each step in a CoT can be viewed as the reasoning pattern:

$$\text{(Premises used)} + \text{(inference rule applied)} \longrightarrow \text{(new result)}.$$

Next, we provide a concrete algebra example on expanding $(x + y)^2$ for better intuition.

**Step $c_i$: Expand the square**

$$\Gamma_i = \{(x+y)^2\}, \quad f_i = \text{"expand square"}, \quad v_i = [\![f_i]\!](\Gamma_i) = (x+y)(x+y).$$

So we have:

$$\{(x+y)^2\} \xrightarrow{\text{expand square}} (x+y)(x+y).$$

**Step $c_{i+1}$: Distribute the product**

$$\Gamma_{i+1} = \{(x+y)(x+y)\}, \quad f_{i+1} = \text{"distributive law"}, \quad v_{i+1} = [\![f_{i+1}]\!](\Gamma_{i+1}) = x^2+xy+yx+y^2.$$

So we have:

$$\{(x+y)(x+y)\} \xrightarrow{\text{distribute}} x^2 + xy + yx + y^2.$$

**Step $c_{i+2}$: Simplify like terms**

$$\begin{aligned}
&\Gamma_{i+2} = \{x^2 + xy + yx + y^2\,, \\
&f_{i+2} = \text{"commutativity + combine like terms"}\,, \\
&v_{i+2} = [\![f_{i+2}]\!](\Gamma_{i+2}) = x^2 + 2xy + y^2\,.
\end{aligned}$$

So we have:

$$\{x^2 + xy + yx + y^2\} \xrightarrow{\text{simplify}} x^2 + 2xy + y^2.$$

Combining the above steps, the CoT trajectory is

$$(x+y)^2 \xrightarrow{\text{expand square}} (x+y)(x+y) \xrightarrow{\text{distribute}} x^2 + xy + yx + y^2 \xrightarrow{\text{simplify}} x^2 + 2xy + y^2.$$

This example follows Definition 3 and precisely characterizes a CoT trajectory at the step level. Note that this step-level formalization is not essential for understanding the main text, which primarily focuses on DAG-level reasoning rather than the specifics of individual nodes and edges. Nonetheless, for readers interested in how nodes and edges are defined or how they influence a CoT trajectory, this definition and the accompanying example provide a useful reference.

### A.4 Intuitive Example of Step-Level CoT under Framework in Section 2

**Phase 1:** Applied to our logarithmic count problem, we use `LLaMA-3.1-8B-Instruct` (Grattafiori et al., 2024) to generate four CoT trajectories, where each trajectory consists of its own steps leading to correct/incorrect answers. The task-specific DAG shown in Fig. 2 are performed by the authors, but can also be carried out by LLMs through appropriate prompting (see Section 4).

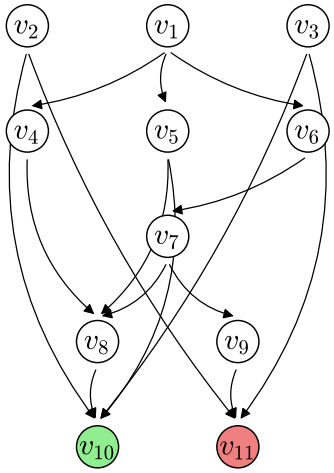


Figure 2: Task-specific DAG via `LLaMA-3.1-8B-Instruct`.

**Task – specific DAG for the logarithmic count problem**

- $v_1$ : "$2\log(x-1) = \log k$" (target equation);
- $v_2$ : "$k \in [-300\,, 300]$" (range constraint);
- $v_3$ : "exactly one solution" (task requirement);
- $v_4$ : "$\log(x-1)$ requires $x > 1$" (constraint inferred from the equation);
- $v_5$ : "$\log k$ requires $k > 0$" (constraint inferred from the equation);
- $v_6$ : "$2\log(x-1) = \log k \;\Rightarrow\; (x-1)^2 = k$" (re-arranged equation);
- $v_7$ : "$x = 1 \pm \sqrt{k}$" (solve the quadratic equation);
- $v_8$ : "$1 + \sqrt{k}$ is the only solution" (correct check);
- $v_9$ : "For any $k$, there are two solutions" (incorrect check);
- $v_{10}$ : "There are 300 valid values for $k$" (the correct answer);
- $v_{11}$ : "There are 0 valid value for $k$" (the incorrect answer).

**Phase 2:** The transition rule defined in Eq. (1) enforces valid transitions over the nodes. For instance, after collecting $\{v_1, v_2, v_3, v_4, v_5\}$, the next admissible node should be $v_6$; while nodes $v_7$ through $v_{11}$ remain inaccessible until $v_6$ has been visited. Accordingly, the LLM's final CoT output can be split into three classes (only representative examples are presented):

- **Perfect reasoning** $(v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8, v_{10})$: The trajectory only includes the correct sink node and its ancestors. We formally define this in the next section.
- **Imperfect reasoning**[7], e.g., $(v_1, v_2, v_3, v_4, v_5, v_6, v_7, \boxed{v_9}, v_8, v_{10})$: The trajectory still reaches the correct answer but also includes the irrelevant node $v_9$, which is not an ancestor of the correct node. Such case may occur when the LLM explores multiple directions and eventually arrives at the correct answer either by chance or through subsequent derivation. We give an example from AIME 2025 (Art of Problem Solving, 2025a,b) for this case in Section B where two solution paths are mixed.
- **Wrong reasoning**, e.g., $(v_1, v_2, v_3, v_6, v_7, v_9, v_{11})$: The final answer is incorrect.

[7]The LLM may reason imperfectly during its thinking process, e.g., dead-ends, self-correction, but is expected to output only the finalized, perfect, correct reasoning results to the user. The reasoning evaluation in this paper is based on the entire final output (while PASS@$k$ just considers the final answer).

## B Example of Logical Closeness

There are several reasons why LLMs may generate unclosed nodes even though the final answer is correct:

- Assertions stemming from an alternative strategy that is not the one leading to the final answer in the trajectory.
- Qualitative axioms that are implicitly used. When forming edges, the model tends to link parents that provide numerical values from earlier calculations, since quantitative conclusions are easier to cite than qualitative ones.
- Irrelevant information drawn from the problem statement.
- Additional commentary based on previous conclusions but not required for the solution.

We aim to analyze specific DAG-MATH formatted CoT trajectory which has the correct final answer but unclosed DAG. To justify the rationale, we take the following geometry problem from AIME 2025 I (Art of Problem Solving, 2025a) as an example.

**Area of Heptagon Problem**

On $\triangle ABC$, points $A, D, E$, and $B$ lie in that order on side $\overline{AB}$ with $AD = 4$, $DE = 16$, $EB = 8$. Points $A, F, G$ and $C$ lie in that order on side $\overline{AC}$ with $AF = 13$, $FG = 52$, and $GC = 26$. Let $M$ be the reflection of $D$ through $F$, and let $N$ be the reflection of $G$ through $E$. Quadrilateral $DEGF$ has area 288. Find the area of heptagon $AFNBCEM$.

We have 4 correct CoT trajectories over 32 total trajectories generated by `Gemini-2.5-Flash`. We provide a detailed analysis of one trajectory that contains multiple unclosed patterns and has a moderate graph size. There are two trajectories that exhibit similar characteristics, while the last trajectory consists of 121 nodes.

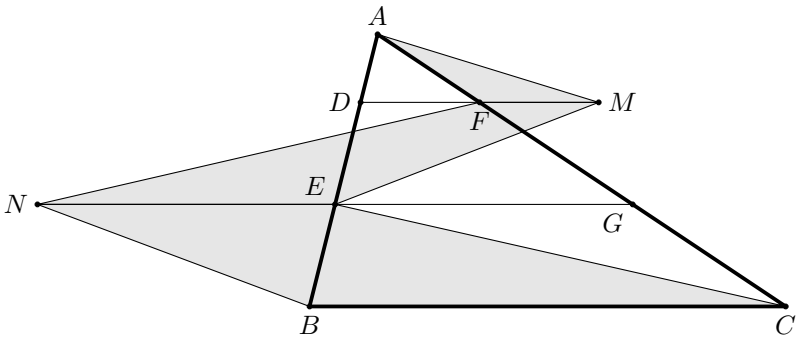


Figure 3: Visualization of the heptagon problem.

We plot Fig. 3 for better illustration and present the first trajectory-specific DAG shown in Fig. 4. We summarize each node's conclusion below.

1. States the ordering/collinearity $A$ , $D$ , $E$ , $B$ on $\overline{AB}$.
2. States $AD = 4$.
3. States $DE = 16$.
4. States $EB = 8$.
5. Computes $AE = AD + DE = 20$.
6. Computes $DB = DE + EB = 24$.
7. Computes $AB = AD + DE + EB = 28$.
8. States the ordering/collinearity $A - F - G - C$ on $\overline{AC}$ (global setup).
9. States $AF = 13$.

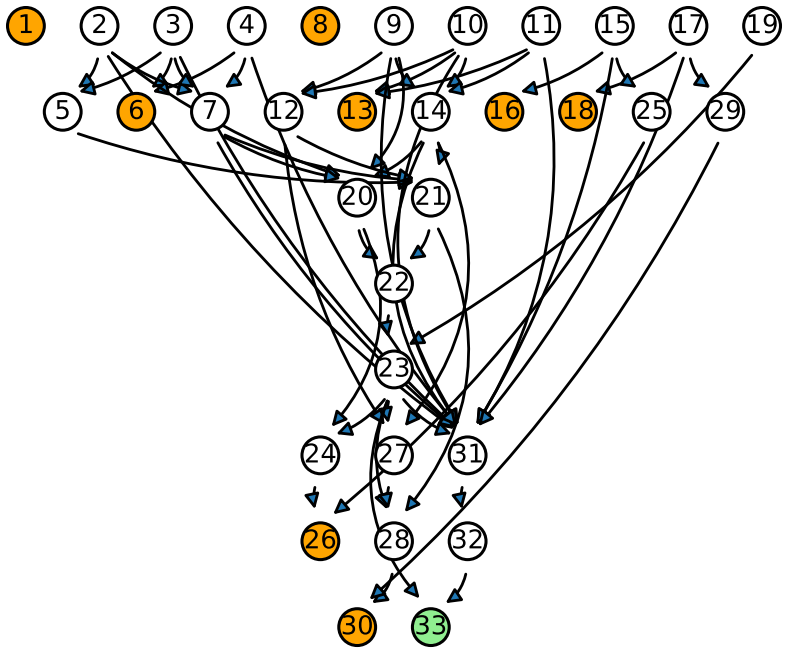


Figure 4: A trajectory-specific DAG for the Area of Heptagon problem, whose DAG-MATH–formatted CoT trajectory is generated by `Gemini-2.5-Flash` and has the correct final node. Nodes without any children are highlighted in orange.

10. States $FG = 52$.
11. States $GC = 26$.
12. Computes $AG = AF + FG = 65$.
13. Computes $FC = FG + GC = 78$.
14. Computes $AC = AF + FG + GC = 91$.
15. Defines $M$ as the reflection of $D$ across $F$ (so $F$ is midpoint of $DM$).
16. Elaborates reflection at $F$; observes $F$ midpoint of $DM \Rightarrow$ Area$(AFM) =$ Area$(ADF)$.
17. Defines $N$ as the reflection of $G$ across $E$ (so $E$ is midpoint of $GN$).
18. Notes explicitly that $E$ is the midpoint of $GN$.
19. States Area$(DEGF) = 288$.
20. Sets Area$(ADF) = \frac{AD}{AB} \cdot \frac{AF}{AC} \cdot$ Area$(ABC) = \frac{S}{49}$.
21. Sets Area$(AEG) = \frac{AE}{AB} \cdot \frac{AG}{AC} \cdot S = \frac{25S}{49}$.
22. Relates Area$(DEGF) =$ Area$(AEG) -$ Area$(ADF) = \frac{24S}{49}$.
23. Solves $\frac{24S}{49} = 288 \Rightarrow S =$ Area$(ABC) = 588$.
24. Computes Area$(ADF) = S/49 = 12$.
25. Uses reflection at $F \Rightarrow$ Area$(AFM) =$ Area$(ADF)$.
26. Concludes Area$(AFM) = 12$.
27. Computes Area$(ABG) = \frac{AG}{AC} \cdot S = 420$.
28. Computes Area$(BEG) =$ Area$(ABG) -$ Area$(AEG) = 420 - 300 = 120$.
29. Uses reflection at $E \Rightarrow$ Area$(BEN) =$ Area$(BEG)$.
30. Concludes Area$(BEN) = 120$.
31. Chooses coordinates $A = (0, 0), B = (28, 0), C = (0, 42)$; derives $D, E, F, G, M, N$ coordinates.

32. Applies the shoelace formula to the heptagon $AFNBCEM$ and gets area $588$.

33. States the final result: $\boxed{588}$.

We can observe that the DAG has 8 non-closed nodes. We diagnose the reasons of uncloseness for each node:

- **Nodes** $1$ **&** $8$: These two nodes state the global setup on collinearity/ordering, which are directly provided by the problem statement. The later steps implicitly use collinearity to add segment lengths on $\overline{AB}$ and $\overline{AC}$, but the LLM does not recognize that it has used these two nodes in its subsequent reasoning.

- **Nodes** $6$ **&** $13$ **&** $16$ **&** $18$: These nodes derive or state extra commentary of their previous step, which are not needed in the subsequent steps.

Then, the message conveyed by **Nodes** $26$ **&** $30$ is *crucial*. In this problem, the area of the heptagon $AFNBCEM$ can be computed via two distinct strategies:

- **Reflection-swap strategy**: The core idea is to replace two interior triangles ($\triangle ADF$, $\triangle BEG$) of $\triangle ABC$ with their exterior reflected counterparts ($\triangle AFM$, $\triangle BEN$), showing that the net area change is zero. Consequently, the heptagon's area is obtained by a straightforward "remove + add" bookkeeping.

- **Shoelace strategy**: This coordinate-based, algebraic method requires only listing the vertices $A, F, N, B, C, E, M$ in order and then applying the determinant sums to compute the area.

Nodes 20 through 30 derive the areas required for the final "remove + add" computation in the reflection-swap strategy, namely

$$\text{Area}(AFNBCEM) = \underbrace{\text{Area}(ABC)}_{\textbf{Node } 23} - \underbrace{\text{Area}(ADF)}_{\textbf{Node } 24} - \underbrace{\text{Area}(BEG)}_{\textbf{Node } 28} + \underbrace{\text{Area}(AFM)}_{\textbf{Node } 26} + \underbrace{\text{Area}(BEN)}_{\textbf{Node } 30}.$$

If the model had continued with this strategy, **Node 31** would correspond to the above equation, with **Nodes** $26$ **&** $30$ as its parents. However, the model instead switches to the shoelace strategy at **Node 31** and successfully obtains the correct answer, leaving **Nodes** $26$ **&** $30$ unclosed.

This provides evidence that the model generates elements of an alternative strategy that remain unused in the current trajectory and switches strategies during the generation process.

Next, the second and third trajectories exhibit node structures similar to the first. They also contain nodes such as **Nodes** $1$ **&** $8$ in the first trajectory, which are not recognized as being used. However, unlike the first trajectory, they rely solely on the reflection-swap strategy to obtain the final answer without switching strategy.

The final trajectory consists of 121 nodes in total. We provide a comprehensive review of its reasoning process: it begins by copying the givens, constructing segment sums, and recording the reflection, analogous to **Nodes** 1–19 in the first trajectory. It then attempts a parametric area strategy via trigonometric parametrization but halts after approximately 20 steps. Subsequently, it searches over many polygon decompositions of heptagon $AFNBCEM$, repeatedly proposing and discarding formulas—clear evidence of exploratory search—until it identifies the structural invariant $AD : DE : EB = AF : FG : GC = 1 : 4 : 2$, from which it correctly infers $DF \parallel EG \parallel BC$. At this stage, the strategy shifts to a similarity/area-ratio approach for triangles sharing angle $A$ and successfully derives the area of $\triangle ABC$. Finally, the strategy switches once more to the reflection-swap method, yielding the correct answer.

## C Example DAG-MATH Formatted CoT

**Example DAG-MATH Formatted CoT for the logarithmic count problem**

**Step 1**

**Edge**: Restate the target equation from the problem statement, $2\log(x-1) = \log k$, which is the central equation to solve for $x$ in terms of $k$.

**Parents**: Null

**Node**: $2\log(x-1) = \log k$.

⋮

**Step 4**

**Edge**: Since the left-hand side of the equation in Step 1 contains $\log(x-1)$, the domain restriction for a logarithm requires $x - 1 > 0$, i.e., $x > 1$.

**Parents**: Step 1

**Node**: $\log(x-1)$ requires $x > 1$.

⋮

**Step 8**

**Edge**: Using Step 7, the candidate solutions are $1 \pm \sqrt{k}$; Step 4 requires $x > 1$, and Step 5 ensures $k > 0$, so $\sqrt{k} > 0$, making $1 - \sqrt{k} < 1$ invalid. Therefore, $1 + \sqrt{k}$ is the only admissible solution.

**Parents**: Step 4,5,7

**Node**: $1 + \sqrt{k}$ is the only admissible solution.

**Step 9**

**Edge**: From Step 8, each positive integer $k$ yields exactly one solution $x = 1 + \sqrt{k}$. Step 5 requires $k > 0$, and Step 2 restricts $k$ to integers in $[1, 300]$. Therefore, there are 300 valid $k$ values, satisfying Step 3's requirement of exactly one solution.

**Parents**: Step 2,3,5,8

**Sink Node**: There are $\boxed{300}$ valid values for $k$.

## D Benchmark Construction

We prompt LLMs to generate CoT trajectories in the DAG-MATH format for existing mathematical datasets, such as Omni-MATH (Gao et al., 2024), and construct the corresponding DAGs. By verifying both logical closeness (Definition 1) and the correctness of the final answers, we compile a benchmark consisting of 2,894 gold-standard DAGs. The primary **purpose of this benchmark** is to characterize the statistical properties of these gold-standard DAGs across different problem difficulty levels, providing valuable insights for evaluating and enhancing LLM mathematical reasoning.

The benchmark comprises problems from Omni-MATH (Gao et al., 2024), which are categorized into difficulty levels ranging from 1 (easiest) to 10 (hardest). To ensure high solvability by LLMs, we only consider problems with difficulty levels below 6. For generating DAG-MATH formatted CoTs, we employ `GPT-o4-mini` and `Qwen3-235B-A22B-Thinking-2507`, both recognized as leading models in mathematical problem solving (LMArena, 2025). Gold-standard CoTs are constructed using a three-stage prompting strategy in **reverse order** (Node → Parents → Edge):

**Stage 1:** We prompt `GPT-o4-mini` to generate *only* the Node set, one step at a time, using the instructions in Section D.1. To enhance correctness, we adopt a supervised setup that provides both the problem and its correct solution. Because standard CoT can skip arithmetic or combine multiple results in a single step, we require that each Node consist of exactly one sentence containing a single mathematical or logical assertion (i.e., one primitive action per step) to normalize granularity. The

complete Node set is then validated using SymPy and LLM-as-Judge; if the final answer or any intermediate assertion is incorrect, the Nodes are resampled and re-validated.

**Stage 2:** Given the verified Node set from Stage 1, we prompt `GPT-o4-mini` (per Section D.2) to assign, for each Node, a minimal set of direct Parents sufficient to derive it via a primitive operation. We enforce acyclicity and well-typed arity constraints, then assemble the full DAG. The resulting DAG is checked for logical closeness relative to the sink node; if checks fail, dependencies are resampled. Simultaneously, irrelevant Nodes flagged in Stage 1 are pruned so that non-contributing leaves do not persist in the gold graph.

**Stage 3:** Conditioned on the generated [Parent(s), Node] pairs, we prompt `Qwen3-235B-A22B-Thinking-2507`[8] (per Section D.3) to generate the Edge content that justifies how each Node is inferred from its Parents. The justification must introduce no new facts beyond the problem statement and the cited Parents. After this step, the triplets are merged into a gold-standard DAG-MATH formatted CoT in forward order.

This approach fixes the node set first, making verification easier with SymPy or LLM-as-Judge and minimizing error propagation, thereby ensuring high-quality trajectories.

We consider five representative **graph-level statistics**: (1) the total number of nodes (#Nodes); (2) the total number of edges (#Edges); (3) graph density, defined as the ratio of #Edges to the maximum possible number of edges in an acyclic graph, i.e., $\frac{2\#\text{Edges}}{\#\text{Nodes}(\#\text{Nodes}-1)}$; (4) the maximum in-degree, denoted $\mathrm{d}_{\mathtt{in}}^{\max}$; and (5) the maximum out-degree, denoted $\mathrm{d}_{\mathtt{out}}^{\max}$. Fig. 5 shows the distributions of these five statistics across problem difficulty levels. Our key observations as **problem difficulty increases from 0 to 6** are as follows:

- **More nodes and edges with heavier tails:** The distributions of #Nodes and #Edges shift noticeably to the right and develop heavier tails, indicating that harder problems produce larger graphs, while simpler problems yield much smaller ones.
- **Sparser structure:** The graph becomes sparse when problem difficulty increases. Harder reasoning produces broader, less connected structures, reflecting modular sub-reasoning where semi-independent chains (e.g., sub-tasks or lemmas) are later combined.
- **Logic complexity reflected in maximum out-degree:** As difficulty increases, the distributions of maximum in-degree and out-degree shift rightward with heavier tails. Maximum in-degree grows slowly, suggesting most steps rely on few inputs, whereas maximum out-degree rises more sharply, indicating that certain key steps support multiple inferences. This implies that logical complexity scales primarily through branching rather than aggregation. The average in- and out-degree remains around 1.3 across difficulty levels, as most nodes have small degrees while a few pivotal steps exhibit large connectivity.

Accordingly, as problems become harder, their DAGs grow larger and sparser, with complexity arising primarily from branching into modular sub-reasoning chains. This underscores the importance of LLMs being able to decompose problems into sub-tasks, track longer dependencies, and recombine intermediate results to solve challenging problems effectively.

### D.1 Prompt for Stage 1

**Stage 1 - Instructions for Refined Step-by-Step Answer**

**Task:**

You are an expert in mathematical logic and reasoning. Your job is to take rough multi-step math solutions and rewrite them in a detailed, structured, and logical step-by-step format. Follow these guidelines:

- Each step must be exactly one sentence, and that sentence may contain only one mathematical or logical assertion.
- Do not combine multiple assertions in one step.

[8] We choose `Qwen3` as it provides a clearer description of the inference from Parents to Nodes than `GPT-o4`.

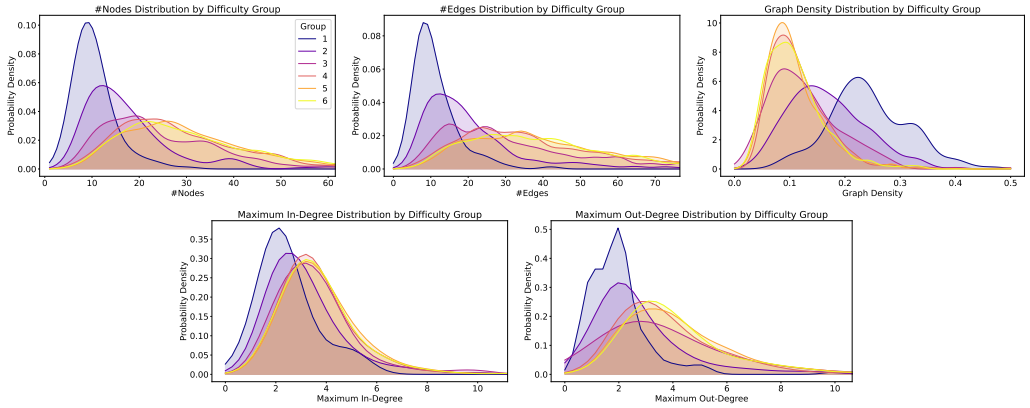


Figure 5: Empirical distributions of DAG statistics across problem difficulty groups, where group $k$ corresponds to problems with difficulty in $(k-1, k]$. Shown are the distributions of #Nodes, #Edges, graph density $\left(\text{i.e., } \frac{2\#\text{Edges}}{\#\text{Nodes}(\#\text{Nodes}-1)}\right)$, maximum in-degree, and maximum out-degree.

- Show every tiny inference—setting up equations, solving for variables, converting units, etc.—each in its own step.
- Any fact, formula, problem detail, or intermediate result must itself be stated in its own individual step.
- Avoid including irrelevant steps that do not contribute to the solution.
- The final step should be the answer statement in the form: `The final answer is \boxed{xxx}.`
- Use LaTeX format enclosed in dollar signs for all mathematical expressions.

**Problem:** `{problem statement}`
**Solution:** `{original step-by-step solution}`
**Refined Step-by-Step Answer:**

### D.2 Prompt for Stage 2

**Stage 2 - Instructions for Step Dependency Analysis**

**Role and Objective**
You are an expert in mathematical logic and stepwise reasoning. Your primary role is to analyze the detailed solution steps for a mathematical problem and annotate each step with its minimal set of direct dependencies.

**Instructions**

1. **Input Structure:**
   - Each problem appears as a JSON object with fields:
     `problem_text` (string): Problem description.
     `final_answer` (string): The solution.
     `steps` (array): Each is an object containing:
       `step_id` (integer): Unique step identifier.
       `text` (string): Reasoning or mathematical operation.
2. **Dependency Annotation:**
   - Add a `direct_dependent_steps` field for every step.
   - For each step:
     If stated directly from the problem statement, assign `null`.

Otherwise, list the minimal, directly required prior `step_id` values in *ascending order*, e.g., `[2, 3]`.

- **Dependency Rules:**

  1. Every dependency ID in `direct_dependent_steps` **MUST** exist in the original set of `step_id` values of the input.
  2. Every listed dependency must be a prior step—its `step_id` must be strictly less than the current step (i.e., no self- or future-dependency is allowed).

3. **Self-Validation for Step Closure:**
   - After assigning dependencies, check for unclosed intermediate steps:
     - An unclosed step is any non-final step not referenced in `direct_dependent_steps` by any subsequent step.
     - If any exist, refine dependencies until all intermediate steps are "closed" (each is used at least once by a later step).
4. **Post-action Validation:**
   - After annotating dependencies and closing all steps, validate that each intermediate step is referenced at least once by a subsequent step before finalizing the output. If any issues are found, self-correct and repeat the closure process.
5. **Structured Output and Consistency:**
   - The number of steps in the structured output **MUST** match exactly the number of steps in the original input.

**Application Process**

- When presented with a new problem in valid JSON:
  1. Iterate through steps in order of `step_id`.
  2. For each step, determine if it relies on previous steps or the problem statement and annotate `direct_dependent_steps` as specified.
  3. Validate dependencies (all dependency IDs exist; all point to a prior step).
  4. Check for unclosed steps and adjust as necessary.
  5. Validate closure and present the final modified problem.

**Error Handling**

- If the input is malformed (e.g., required fields missing, `step_id` missing, or `step_id` values not strictly ascending):
  - Return only a JSON object with an `error` field and a concise message. For example: `"error": "Input data malformed: missing step_id in step 3."`

**Output Format**

- Output the structured response with all steps mirroring the original order and count, each annotated with `direct_dependent_steps`. If there is an error, output only the error object as described.

```
{JSON text of refined step-by-step answer with problem
statement from Stage 1}
```

### D.3 Prompt for Stage 3

**Stage 3 - Instructions for Constructing Edge Inference**

**Role and Objective**

- You serve as a mathematics solution explainer. For each step in a solved mathematics problem (provided as structured JSON), generate a detailed and explanatory justification paragraph (`edge` string) clarifying the correctness and logical progression.

**Instructions**

- For each step in the provided `"steps"` array within the problem JSON, write a `edge` string that satisfies the rules below.
- If `direct_dependent_steps` is not `null`, explicitly justify how `direct_dependent_steps` support the current one, citing their IDs. If `null`, note that the step is given by the problem statement or background knowledge (definition, theorem, lemma, fact, or general knowledge not originally in the problem statement).
- Clearly explain the mathematical or logical principle, operation, or procedure used (e.g., counting rule, algebraic manipulation, definition, theorem, arithmetic operation) applied in the step.
- Strict Rule: Do not omit any referenced dependency, the `edge` **MUST** include every step in `direct_dependent_steps`.
- Clearly illustrate why we need to do this step and how we arrive at this step (acts like planning).
- For numeric calculations, perform the arithmetic clearly and include a brief sanity check as appropriate.
- Use neutral, present-tense, explanatory sentences with active voice.
- Ensure each justification is self-contained, needing only the current step and referenced prior steps to be understandable.

**Context**

- Input: JSON object representing a solved math problem with an array of steps, each with `step_id`, `text`, and `direct_dependent_steps`.
- Output: Return only the `edge` for each step, ordered to match the original steps array.
- Do **NOT** include internal model reasoning or any execution commentary in the output.

**Demonstration Example**

Here is a demonstration of the style and format of the edge field. You need to follow this style and format.

- "We plan to exclude numbers divisible by 2, 3, or 5. To do that systematically we first express the count of multiples of each relevant divisor in the domain. The number of multiples of $k$ up to $n$ is $\left\lfloor \frac{n}{k} \right\rfloor$. Applying that with $n = 999$ (from Step 1) and $k = 2$ gives $\lfloor 999/2 \rfloor$. Writing it as a floor expression is precise and handles the non-divisible endpoint gracefully."
- "Since numbers divisible by 2, 3, and 5 are overlapping, we need to subtract the count of numbers divisible by pairwise combinations of 2, 3, and 5 then add back the count of numbers divisible by all three, i.e., inclusion-exclusion. The least common multiple of 2 and 3 is 6, so count multiples of 6. Recall we have 999 integers in the domain from Step 1, count multiples of 6 up to 999 via $\lfloor 999/6 \rfloor$. This uses the same floor-division approach but applied to the least common multiple of the pair."
- "We convert the expression in Step 8 into a concrete number to use in later arithmetic. Compute $999/6 = 166.5$; taking the floor yields 166. Quick cross-check: $166 \times 6 = 996$, so the last multiple is exactly 996."
- "We now have all the building blocks: counts of singles, pairwise intersections, and the triple intersection. The immediate plan is to apply the inclusion-exclusion formula for three sets to compute the size of the union $A \cup B \cup C$ where $A =$ multiples of 2, $B =$ multiples of 3, $C =$ multiples of 5. Inclusion-exclusion avoids overcounting and is the rigorous combinatorial tool for unions of overlapping sets. The three-set inclusion-exclusion identity is $|A \cup B \cup C| = |A| + |B| + |C| - (|A \cap B| + |A \cap C| + |B \cap C|) + |A \cap B \cap C|$. Substitute the numerical values computed from Steps 3, 5, 7, 9, 11, 13, 15,: $499 + 333 + 199 - (166 + 99 + 66) + 33$. Writing it explicitly as $499 + 333 + 199 - 166 - 99 - 66 + 33$ lays out the arithmetic to be performed next."

- "Cite the standard definition: 1 has exactly one positive divisor (1 itself), so it is neither prime (requires two distinct divisors) nor composite (requires more than two). In partitioning the 266 numbers not divisible by 2,3,5 into primes and composites, we must also handle the special case 1, which is counted among the 266 but is neither prime nor composite; failing to account for 1 would misclassify one element."
- "We now simplify the complex expression from Step 12, which is $(48 \times 15) - (320 \div 8) + 27$. The order of operations dictates multiplication and division before addition or subtraction. First compute $48 \times 15 = 720$. Next compute $320 \div 8 = 40$. Substituting these back into the expression gives $720 - 40 + 27$. This reduction preserves equivalence while making the next step—performing the remaining subtraction and addition—more straightforward."

**Core Language Style Requirements**

- Match the tone, sentence flow, and level of detail in the demonstration examples provided below.
- Write in a way that reads naturally to a human reasoner, not like a formal audit log.

**Self-Validation**

- **IMPORTANT**: After each `edge` is generated, validate that whether it includes every step in `direct_dependent_steps`. If not, you need to re-generate the `edge` for the step. Notice that you need to check for all steps, not just a subset of steps.
- For each step, internally determine the applicable mathematical principle, identify dependencies, clarify evaluation or logic, and succinctly state both justification and role in the broader problem.
- Clearly state mathematical justifications, and follow the required language style. If a numeric evaluation is performed, confirm a brief sanity check is present.

**Verbosity**

- `edge` should be **detailed**, allowing for expansion if the step is complex or multi-part.

**Stop Conditions**

- Complete when every step has a well-justified `edge` field, following all style and content rules. Escalate for ambiguous or incomplete input only.

**Output Format**

- Return only a `edge` field for each step populated as described. Do not include extra fields, wrappers, or commentary.

EXAMPLE JSON OUTPUT:

```
{
    "edges": [
      {
        "step_id": 1,
        "edge": "We define ..."
      },
      {
        "step_id": 2,
        "edge": "Building on the definition of ..."
      },
      {
        "step_id": 3,
        "edge": "Using the expression for ..."
      }
}
```

`{JSON text of refined step-by-step answer with problem statement from Stage 1 and dependencies from Stage 2}`

## E Few-Shot Prompt for DAG-MATH Formatted CoT

**Instructions for DAG-MATH Formatted CoT Generation**

**Role and Objective**
You are an expert mathematical reasoner and logician. For the given problem, you must produce a single, valid JSON object containing a list of solution steps. Each step in the list must be an object with the following four fields: `step_id`, `edge`, `direct_dependent_steps`, and `node`.

**Requirements**
Each step has **exactly**:

- `step_id` (int; unique; strictly increasing)
- `edge` (sentences; describe *why/how* this step follows; reference prior steps with Step's `step_id` tags, e.g., `Step 1`, `Step 3`)
  - State the goal of the current step.
  - Cite the *minimal* **direct** dependent previous steps used, with *how* these steps are used for the current step. **IMPORTANT**: every direct dependent step *must* be cited in the form Step's `step_id`.
  - State clearly the mathematical principle being applied (e.g., inclusion–exclusion, algebraic manipulation, definition), which turns those inputs into the asserted output.
- `direct_dependent_steps` (array of ints **or** `null`)
  - This field must contain a list of `step_id`s representing the minimal set of prior steps directly used to derive the current step in `edge`.
  - The list must be in ascending order (e.g., `[2, 5]`).
  - If a step is a fact taken directly from the problem statement, this field should be `null`.
  - Topological order: every dependency ID $<$ current `step_id`.
  - Closure: every nonfinal step's `step_id` must appear in some later step's `direct_dependent_steps`.
- `node` (one execution sentence)
  - Each step's `node` field must contain a **single, atomic** sentence making exactly one logical assertion (e.g., stating an equation, defining a variable, presenting a calculation result) which acts as the results inferred from `edge`.
  - All information, including facts from the problem statement and intermediate results, must be broken down into these atomic steps.
  - Avoid including irrelevant steps that do not contribute to the solution.
  - The final step **must** be the answer statement in the form: "The final answer is $\boxed{\ldots}$".

**Global Constraints**

- Use LaTeX format enclosed in dollar signs for all mathematical expressions.
- Your entire output must be a single, valid JSON object. Do not include any text or commentary outside of the JSON structure. You will be provided with high-quality examples to demonstrate the required format and reasoning style.

**Demonstration Examples**
`{Gold-standard demonstration examples}`

**Bad Examples**

1. The example below is bad since Step's `step_id` are missing in `edge`.

```
{
  "steps": [
    ...
    {
```

```
      "step_id": 36,
      "edge": "Using the confirmed digit values--
        K=0, L=5, M=3, and N=9, the sum K + L + M + N
        is expressed as 0 + 5 + 3 + 9. This step
        prepares the expression for final evaluation.",
      "direct_dependent_steps": [
        8,
        15,
        26,
        32,
        35
      ],
      "node": "The sum of the digits $K + L + M + N$
        is $0 + 5 + 3 + 9$."
    },
    ...
  ]
}
```

2. The example below is bad since plural "Steps 8, 9, and 10" is used in `edge` instead of singular "Step 8, Step 9, and Step 10".

```
{
  "steps": [
    ...
    {
      "step_id": 11,
      "edge": "From Steps 8, 9, and 10, we have
        c(b - a) = 1 + 2k, b(c - a) = -3 + 6k,
        a(c - b) = -4 + 4k. To find relationships,
        assume a, b, c are such that differences are
        proportional. Let d = b - a, e = c - a,
        then c = a + e, b = a + d. Substitute into
        the equations.",
      "direct_dependent_steps": [
        8,
        9,
        10
      ],
      "node": "Define d = b - a and e = c - a. Then
      the equations become: (a + e) * d = 1 + 2k,
      (a + d) * e = -3 + 6k, a * (e - d) = -4 + 4k."
    },
    ...
  ]
}
```

**Problem:** `{Test problem statement}`
**Solution:**

## F Additional Details and Results for Evaluation

The results for final-answer accuracy (PASS@1) and empirical mathematical reasoning ability ($\widehat{\mathcal{R}}$) on three benchmarks across five LLMs are reported in Table 2. The averaged graph-level statistics for BRUMO 2025 and HMMT 2025 are reported in Tables 3 and 4, respectively. The overall trend is similar to the analysis in Section 4. Additionally, we can obtain the following findings:

- **The change in graph-level statistics is monotonic in $\Delta$.** The variations in the #nodes, #edges, density, and maximum out-degree from **Correct** to **Perfect** increase monotonically

Table 2: Final-answer accuracy (PASS@1) and empirical mathematical reasoning ability ($\widehat{\mathcal{R}}$) across three math benchmarks. Parentheses show the gap ($\Delta := \text{PASS@1} - \widehat{\mathcal{R}}$).

| **Model** | **AIME 2025** | | **BRUMO 2025** | | **HMMT 2025** | |
|---|---|---|---|---|---|---|
| | PASS@1 | $\widehat{\mathcal{R}}$ ($\Delta \downarrow$) | PASS@1 | $\widehat{\mathcal{R}}$ ($\Delta \downarrow$) | PASS@1 | $\widehat{\mathcal{R}}$ ($\Delta \downarrow$) |
| Gemini-2.5-F | 52.4 | 17.0 (35.4$\downarrow$) | 63.4 | 20.7 (42.7$\downarrow$) | 38.5 | 5.7 (32.8$\downarrow$) |
| Gemini-2.5-F-L | 37.4 | 15.9 (21.5$\downarrow$) | 43.2 | 17.8 (25.4$\downarrow$) | 28.8 | 7.5 (21.3$\downarrow$) |
| GPT-4.1 | 26.5 | 16.8 (9.7$\downarrow$) | 33.3 | 22.8 (10.5$\downarrow$) | 11.8 | 6.5 (5.3$\downarrow$) |
| GPT-4.1-M | 30.5 | 20.9 (9.6$\downarrow$) | 34.4 | 24.6 (9.8$\downarrow$) | 14.3 | 7.4 (6.9$\downarrow$) |
| Qwen3-30B | 43.1 | 15.8 (27.3$\downarrow$) | 46.8 | 21.8 (25.0$\downarrow$) | 27.3 | 5.6 (21.7$\downarrow$) |
| Std | 10.3 | 2.1 | 12.2 | 2.5 | 11.0 | 0.9 |

Table 3: Averaged graph-level statistics of sampled DAGs across selected LLMs on BRUMO 2025.

| Model | Class | #nodes | #edges | density | $\mathrm{d}_{\mathtt{in}}^{\max}$ | $\mathrm{d}_{\mathtt{out}}^{\max}$ |
|---|---|---|---|---|---|---|
| Gemini-2.5-F | All | 26.6 | 39.8 | 13.0% | 4.1 | 5.3 |
| | Incorrect | 29.2 | 47.4 | 13.0% | 4.8 | 6.2 |
| | Correct | 25.1 | 35.9 | 13.1% | 3.8 | 4.8 |
| | Perfect | 20.5 | 26.1 | 14.1% | 3.0 | 3.2 |
| Gemini-2.5-F-L | All | 27.9 | 47.7 | 15.5% | 3.8 | 8.3 |
| | Incorrect | 33.2 | 61.5 | 14.5% | 4.0 | 11.1 |
| | Correct | 21.2 | 30.4 | 16.7% | 3.4 | 4.8 |
| | Perfect | 14.1 | 17.4 | 20.1% | 2.6 | 2.9 |
| GPT-4.1 | All | 14.9 | 18.1 | 19.4% | 2.4 | 2.9 |
| | Incorrect | 15.9 | 19.6 | 18.4% | 2.5 | 3.0 |
| | Correct | 13.0 | 15.1 | 21.4% | 2.3 | 2.5 |
| | Perfect | 12.0 | 13.8 | 23.0% | 2.3 | 2.3 |
| GPT-4.1-M | All | 17.1 | 24.1 | 18.7% | 3.0 | 3.7 |
| | Incorrect | 18.6 | 27.2 | 17.7% | 3.1 | 4.1 |
| | Correct | 14.3 | 18.3 | 20.6& | 2.7 | 3.1 |
| | Perfect | 13.1 | 16.6 | 22.1% | 2.7 | 2.9 |
| Qwen3-30B | All | 18.4 | 27.7 | 19.8% | 3.4 | 4.7 |
| | Incorrect | 21.7 | 34.4 | 17.8% | 3.7 | 5.7 |
| | Correct | 14.7 | 20.1 | 22.1% | 3.1 | 3.6 |
| | Perfect | 12.1 | 15.4 | 25.3% | 2.8 | 3.0 |

with the gap $\Delta$ between PASS@1 and $\widehat{\mathcal{R}}$. When $\Delta$ is small, the statistics of these two classes are nearly identical.

- **Graph-level statistics remain similar across the four classes when raw accuracy is low.** In particular, when PASS@1 is low, their variations across classes are minimal.

Table 4: Averaged graph-level statistics of sampled DAGs across selected LLMs on HMMT 2025.

| Model | Class | #nodes | #edges | density | $\mathrm{d}_{\mathtt{in}}^{\max}$ | $\mathrm{d}_{\mathtt{out}}^{\max}$ |
|---|---|---|---|---|---|---|
| Gemini-2.5-F | All | 36.8 | 60.4 | 10.9% | 4.7 | 7.9 |
| | Incorrect | 36.6 | 61.4 | 11.4% | 4.7 | 8.4 |
| | Correct | 37.4 | 59.8 | 10.1% | 4.9 | 7.1 |
| | Perfect | 30.1 | 48.4 | 12.0% | 5.9 | 6.1 |
| Gemini-2.5-F-L | All | 35.8 | 63.0 | 14.0% | 4.1 | 11.2 |
| | Incorrect | 40.4 | 73.3 | 13.4% | 4.1 | 13.1 |
| | Correct | 26.5 | 42.7 | 15.2% | 4.0 | 7.1 |
| | Perfect | 16.8 | 25.9 | 20.6% | 3.9 | 4.2 |
| GPT-4.1 | All | 17.0 | 20.7 | 17.8% | 2.5 | 3.2 |
| | Incorrect | 16.9 | 20.8 | 17.8% | 2.5 | 3.1 |
| | Correct | 17.5 | 20.6 | 17.4% | 2.6 | 3.5 |
| | Perfect | 14.7 | 17.3 | 19.8% | 2.5 | 2.7 |
| GPT-4.1-M | All | 21.1 | 30.2 | 16.0% | 3.0 | 4.2 |
| | Incorrect | 21.1 | 30.2 | 15.9% | 3.0 | 4.1 |
| | Correct | 21.1 | 30.5 | 16.6% | 3.0 | 4.4 |
| | Perfect | 17.2 | 24.3 | 19.4% | 2.9 | 3.6 |
| Qwen3-30B | All | 22.8 | 34.6 | 16.1% | 3.6 | 5.6 |
| | Incorrect | 22.8 | 34.5 | 16.4% | 3.6 | 5.7 |
| | Correct | 22.8 | 35.0 | 15.2% | 3.7 | 5.5 |
| | Perfect | 18.7 | 28.5 | 18.8% | 4.6 | 5.0 |