Chain-in-Tree: Back to Sequential Reasoning in LLM Tree Search

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Abstract

Test-time scaling improves large language models (LLMs) on long-horizon reasoning tasks by allocating more compute at inference. Tree-Search (LITS) methods achieve strong performance but are highly inefficient, often running an order of magnitude slower than iterative approaches. We propose **Chain-in-Tree (CiT)**, a plug-in framework that decides *when* to branch during search rather than expanding at every step. CiT introduces lightweight **Branching Necessity (BN)** evaluations: **BN-DP** (Direct Prompting), where an auxiliary LLM judges branching needs, and **BN-SC** (Self-Consistency), which clusters candidate actions to assess agreement. Integrated into Tree of Thoughts, ReST-MCTS, and RAP, BN-DP achieves **75–85%** reductions in token generation, model calls, and runtime on GSM8K and Math500, with often negligible or no accuracy loss. BN-SC typically yields substantial savings (up to 80%) generally but shows instability in 1–4 out of 14 settings, caused by a small subset of examples that produce extremely long reasoning steps. We theoretically prove that BN-DP never increases policy invocations and release both modular LITS implementations and a lightweight CiT function applicable across all LITS variants. The full codebase is publicly available at https://github.com/xinzhel/chain_in_tree.

1 Introduction

Large language models (LLMs) excel at tasks such as mathematical and commonsense reasoning, but their performance often improves further when additional test-time compute is allocated. Recent work has shown that *test-time scaling* enables LLMs to explore multiple reasoning paths, thereby making better use of knowledge they already possess (Sprague et al., 2025). Among test-time scaling methods, tree-search–based approaches have achieved state-of-the-art results on benchmarks like GSM8K and Math500, by treating reasoning as sequential decision-making and exploring multiple candidate trajectories (Zhang et al., 2024a; Yao et al., 2023a). Such approaches naturally align with planning-style problems (Valmeekam et al., 2023).

However, tree-search–based frameworks are highly inefficient: compared to simpler iterative prompting methods, they are often 10–20 times slower (Chen et al., 2024). A central limitation is that they operate at a fixed granularity of reasoning steps. In some cases, this granularity is enforced explicitly, for example by treating each subquestion–answer pair as a node (Hao et al., 2023). Other approaches, such as MCTS with free-form thoughts (Zhang et al., 2024a; Yao et al., 2023a), allow more flexibility but still assume that every generated thought must branch independently. In practice, however, a reasoning step in mathematics may correspond to a single operation or a tightly coupled set of operations, while in domains with deterministic action spaces (e.g., board games) the step granularity is even more strictly defined. This rigidity forces branching even on trivial steps, resulting in excessive LLM calls during both expansion and simulation.

We address this limitation by proposing **Chain-in-Tree (CiT)**, a plug-in for LLM-in-the-loop tree search that adaptively decides *when* branching is necessary. The key idea is to introduce continuous nodes chained together: steps deemed confident or routine by the model are chained sequentially, while branching is reserved only for uncertain points where exploration is valuable. This reduces unnecessary expansion, lowers inference costs, and preserves the search capacity of existing frameworks.

Contributions. Our contributions are as follows:

- We formulate the decision of when to branch as a new component in tree search and propose two lightweight **Branching Necessity (BN) evaluation methods**: Direct Prompting (BN-DP) and Self-Consistency (BN-SC). These methods allow LLMs to autonomously determine whether branching is needed at each step.

- We provide a **theoretical guarantee** that BN-DP never increases runtime relative to the baseline, thereby ensuring efficiency by design.

- We conduct a comprehensive empirical study across 14 settings: two mathematical reasoning benchmarks (GSM8K, Math500), two base LLMs (Qwen3-32B, LLaMA3-8B) serving either as search policies or BN evaluators, and three representative LITS frameworks (ToT-BS, ReST-MCTS, RAP).

- Our experiments show that **BN-DP consistently reduces runtime by 75–85% across all settings with negligible accuracy loss and in some cases improved accuracy**, confirming its reliability. In contrast, **BN-SC achieves substantial savings in most settings but exhibits instability in a few cases**. Finally, we demonstrate that the overall effectiveness of CiT strongly depends on the accuracy of BN evaluation.

- We release a **unified implementation** of ToT-BS, RAP, and ReST-MCTS with modular LLM-profiled roles, enabling consistent comparison across frameworks and simplifying extension of CiT to future LITS variants.

2 Related Work

We situate our method within a unified view of LLM inference via tree search (LITS), showing how our plug-and-play module can be applied across different frameworks. In addition, we discuss two related lines of work that share a similar high-level motivation—reducing unnecessary branching—but operate in different settings and with distinct mechanisms.

LLM Inference via Tree Search (LITS). A growing line of work has explored performing LLM inference through tree-search (LITS) (Hao et al., 2023; Yao et al., 2023a). Following the unified view of Li (2025), these frameworks can be cast into a Markov Decision Process (MDP), where backbone LLMs are profiled into three main roles: (1) **Policy**: generative LLMs produce candidate actions a_t (e.g., reasoning steps) given a state s_t (e.g., the task with prior steps). This usage traces back to the ReAct paradigm (Yao et al., 2023b); (2) **Reward model**: either using generative LLMs to score candidate steps (Yao et al., 2023a; Hao et al., 2023) or employing dedicated non-generative/fine-tuned models (Dai et al., 2025; Luo et al., 2025); (3) **Transition model**: explicitly predicting the next state s_{t+1} and its confidence r_{conf} when a_t is executed (e.g., RAP (Hao et al., 2023)), or more commonly, updating the state by concatenating new thoughts (e.g., ToT (Yao et al., 2023a), ReST-MCTS (Zhang et al., 2024a)), in which case $r_{\text{conf}} = 1$. Our experiments span both types of reward models and both explicit and concatenation-based transition models, demonstrating that CiT is broadly compatible across frameworks.

Reducing Redundant Branching or Reasoning Steps. Our chaining mechanism is conceptually related to prior ideas that aim to reduce search complexity by avoiding unnecessary branching. Our chaining mechanism is conceptually related to *macro-operators* in automated planning, which collapse sequences of primitive operators into a single higher-level action (Chrpa and Vallati, 2022).

One concurrent work is Li et al. (2025), who proposed branching-on-demand in beam search decoding based on entropy over token-level probability distributions. While the high-level motivation is similar—branching only when necessary—the setting is fundamentally different. Their method operates at the token level in traditional sequence generation tasks such as machine translation and speech recognition (Sutskever et al., 2014), where beam search has long been standard. In contrast, our work addresses LLM reasoning and planning in LITS frameworks under a general MDP formulation, where states and actions correspond to semantically meaningful reasoning steps. Branching necessity in CiT is evaluated by clustering candidate actions into equivalence classes and measuring consistency, making it directly applicable to reasoning and planning tasks rather than token-level decoding.

In the context of sequential reasoning (not tree search), Sabbata et al. (2024) “train LLMs to selectively use intermediate reasoning steps only when necessary”.

Algorithm 1 Chain-in-Tree (CiT) with Branching Necessity Evaluation

Input: Depth limit L, BN budget k_{bn}, thresholds $R_{\text{bn}}, R_{\text{conf}}$,
LLM roles: Policy $\text{LLM}_{\text{policy}}$, Transition $\text{LLM}_{\text{trans}}$, Aggregator LLM_{agg}, Equivalence LLM_{eq}, BN evaluator LLM_{bn}
Output: Continued trajectory ending at a node that either triggers branching or is terminal

procedure BN-DP-EVAL(s_t, a_t)
  $r_{\text{bn}} \leftarrow \text{LLM}_{\text{bn}}(s_t, a_t)$
  return r_{bn}
end procedure

procedure BN-SC¹-EVAL($s_t, \mathcal{A}_t$)
  $\mathcal{C} \leftarrow \text{LLM}_{\text{agg}}(\mathcal{A}_t)$ ▷ Cluster candidates
  $r_{\text{bn}} \leftarrow \max_{C \in \mathcal{C}} \frac{|C|}{|\mathcal{A}_t|}$
  return r_{bn}
end procedure

procedure BN-SC²-EVAL($s_t, \mathcal{A}_t$)
  $\mathcal{P} \leftarrow$ pairs from $\mathcal{A}_t$
  $\mathcal{C} \leftarrow \{\text{LLM}_{\text{eq}}(a_i, a_j) : (a_i, a_j) \in \mathcal{P}\}$ ▷ Equivalence checks
  $r_{\text{bn}} \leftarrow \max_{C \in \mathcal{C}} \frac{|C|}{|\mathcal{A}_t|}$
  return r_{bn}
end procedure

procedure CIT-CHAIN($nd, R_{\text{bn}}, R_{\text{conf}}$)
  initialize path $\leftarrow [\,]$
  while nd is not terminal and $nd.depth \leq L$ **do**
    $\mathcal{A}_t \sim \text{LLM}_{\text{policy}}(nd.state, n = k_{\text{bn}})$
    $r_{\text{bn}} \leftarrow \text{BN-Eval}(nd.state, \mathcal{A}_t)$
    append nd to path
    if $r_{\text{bn}} < R_{\text{bn}}$ **then**
      return path ▷ branching required
    end if
    $(s', r_{\text{conf}}) \sim \text{LLM}_{\text{trans}}(nd.state, a)$
    if $r_{\text{conf}} < R_{\text{conf}}$ **then**
      return path ▷ low transition confidence
    end if
    $nd \leftarrow \langle s', a \rangle$
  end while
  append nd to path
  return path
end procedure

3 Chain-in-Tree

We introduce *Chain-in-Tree (CiT)*, a plug-and-play chaining phase inserted before tree expansion, i.e., before actually growing the search tree by attaching k new children at the next depth. [1] CiT adaptively decides whether to grow the tree structure versus to continue in-chain, thereby reducing unnecessary expansions.

We finally analyze the efficiency of *Chain-in-Tree* (CiT) under both Tree-of-Thoughts Beam Search (ToT-BS) and MCTS variants.

3.1 Chaining Phase

As shown in Algorithm 1, during the chaining phase, multiple nodes (actions and their resulting states) are generated and concatenated into a linear chain rather than expanded into branches. This occurs when the BN score r_{bn} exceeds a threshold R_{bn} and the confidence score r_{conf} is below a threshold R_{conf}.

Reusing Children. In standard LLM-in-the-loop tree-search (LITS) frameworks, the expansion phase always invokes the policy to generate a full set of k_{expand} children, regardless of whether a node already has children. CiT modifies this behavior: children generated during chaining are reused at expansion time, truncated to at most k_{expand}, and supplemented with new actions from the policy only if fewer than k_{expand} are available. This design is important to guarantee the efficiency of CiT methods, as specified in Section 3.3and 3.4. Besides, all children—whether reused or newly generated—are consistently assigned rewards, which are not always required during chaining.

Concretely: 1) If $r_{\text{bn}} < R_{\text{bn}}$, the tree is expanded by committing new nodes that contain only the actions produced during chaining; 2) If $r_{\text{bn}} \geq R_{\text{bn}}$ and $r_{\text{conf}} < R_{\text{conf}}$, both actions and their resulting states are retained for expansion.

3.2 Branching Necessity (BN) Evaluation

We now describe how BN scores r_{bn} are computed. We propose two methods: **Direct Prompting (DP)** and **Self-Consistency (SC)**. In both cases, the evaluation operates over k_{bn} candidate actions sampled from the policy model $\text{LLM}_{\text{policy}}$. By default, $k_{\text{bn}} = 1$ for BN-DP and k_{expand} for BN-SC.

Direct Prompting (DP). An auxiliary evaluator model LLM_{bn} is prompted to directly judge whether an action a_t should trigger branching given the current state s_t.

Self-Consistency (SC). A self-consistency strategy (Wang et al., 2023) is adopted by leveraging the diversity of multiple policy samples. From a state s_t, the policy generates a set of k_{bn} candidate actions $\mathcal{A}_t = \{a_1, \ldots, a_{k_{\text{bn}}}\}$. Candidates are clustered into equivalence classes. The BN score r_{bn} is then defined as the fraction of actions belonging to the largest cluster.

[1]While some search procedures (e.g., MCTS rollouts) may involve branching in the sense of simulating multiple continuations, these branches are not materialized in the tree.

$$r_{\mathrm{bn}} = \frac{\max_{C \in \mathcal{C}} |C|}{k_{\mathrm{bn}}}, \quad (1)$$

where $\mathcal{C}$ = Equivalence classes of $\mathcal{A}_t$.

Intuitively, if most candidates agree on the next step, the model is confident and chaining is applied. If candidates diverge, branching is triggered. By default, chaining occurs when $r_{\mathrm{bn}} \geq 0.5$ (i.e., more than half of the actions are consistent).

Two Implementations of BN-SC We explore two clustering implementations: 1) **BN-SC**[1] **(Aggregator-based).** An auxiliary model $\mathrm{LLM}_{\mathrm{agg}}$ clusters candidate actions into dictionaries of the form {canonical action, count}. 2) **BN-SC**[2] **(Pairwise-Equivalence).** A model $\mathrm{LLM}_{\mathrm{eq}}$ is queried as a binary oracle to decide whether two candidate actions are semantically equivalent. The union–find–style merging is the applied: each action maintains a representative index, and pairwise equivalences trigger unions. After processing, clusters are defined by representatives and counts are aggregated. In our case, the "representative index" is simply the first surviving index arbitrarily assigned during merging.[2]

In deterministic domains (e.g., board games with fixed move sets), $\mathrm{LLM}_{\mathrm{eq}}$ can be replaced by simple programmatic rules. Prompts for $\mathrm{LLM}_{\mathrm{bn}}$, $\mathrm{LLM}_{\mathrm{agg}}$, and $\mathrm{LLM}_{\mathrm{eq}}$ are detailed in Appendix A.

3.3 Efficiency Guarantee of Beam Search

While LITS frameworks involve multiple LLM roles—policy, reward, and transition models—the cost of policy invocations dominates overall inference and provides the most consistent analytical basis across frameworks. Supporting details are provided in Appendix B.1, with empirical validation in Section 5.

Assumption (Notation and Setup for ToT-BS (also applies to MCTS))**.** *Let the branching factor be $k_{\mathrm{expand}} \in \mathbb{N}_{>0}$, and let the depth limit be $D \in \mathbb{N}$.*

When a node v is first visited, its BN score *determines whether v is classified as* easy. *If v is easy, the chaining phase is applied: exactly one child is expanded. This consumes k_{bn} policy calls (with $k_{\mathrm{bn}} \leq k_{\mathrm{expand}}$), but only a single child is preserved. Chaining then continues forward until a node fails the BN threshold. At the stopping node (non-easy), a standard full expansion of k_{expand} children is performed, requiring k_{expand} policy calls.*

Expansion cost of ToT-BS. Figure 1 compares the number of policy invocations of Original ToT-BS vs ToT-BS with chaining. Let's assume a homogeneous layer, where every expanded node yields exactlyk_{expand} children (or at least k_{expand} exist) at every depth. At depth t, the frontier size satisfies $\min(B,\, k^t_{\mathrm{expand}}))$ for all $t \geq 0$. Define the per-depth cost as the number of LLM invocations for action generation, the total expansion cost up to depth D is

$$C_{\mathrm{bs}}(D) \;=\; \sum_{t=0}^{D-1} k_{\mathrm{expand}} \min(B, k^t_{\mathrm{expand}}). \quad (2)$$

Guarantee. Assume that D_{C1} is the first depth that normal beam expansion resumes. For all $t < D_{C1}$ we have $k_{\mathrm{bn}} \leq k_{\mathrm{expand}} \leq k_{\mathrm{expand}} \min(B, k^t_{\mathrm{expand}}) = C_t$, and for all $t \geq D_{C1}$,

$$\min(B,\, k^{t-D_{C1}}_{\mathrm{expand}}) \;\leq\; \min(B,\, k^t_{\mathrm{expand}}), \quad (3)$$

hence $C^{\mathrm{cont}}_t \leq C_t$. Summing over all depths shows

$$C_{\mathrm{bs+chain}}(D) \;\leq\; C_{\mathrm{bs}}(D). \quad (4)$$

Therefore, chaining never increases the number of policy invocations, and yields a strict reduction whenever some $k_{\mathrm{bn}} < k_{\mathrm{expand}}$. The detailed proof is demonstrated in Appendix B.

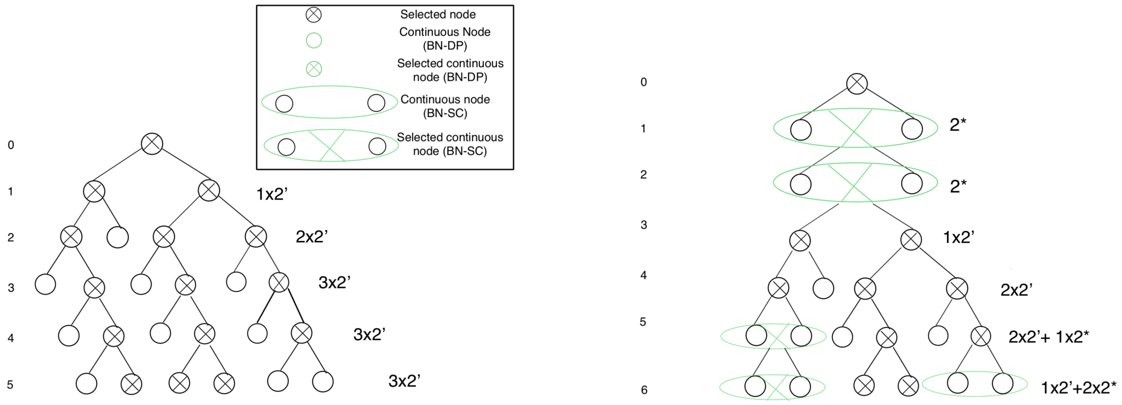
3.4 Efficiency Guarantee of MCTS

We only consider policy invocation under epxansion. Although there exist policy calls during the simulation phase, chaining shortens the remaining distance to a terminal node before rollout begins, so the simulation phase makes fewer policy calls on average.

Assumption (Notation and Setup for MCTS)**.** *In addition to the notation above, let $N \in \mathbb{N}$ denote the number of MCTS iterations (not fixed). Following prior work (Zhang et al., 2024a; Hao et al., 2023), we adopt the* full expansion on first visit *rule: an unexpanded node generates all k_{expand} actions at once when first expanded.*

Define $E(N)$ as the set of distinct nodes first-visited (i.e., expanded) within N MCTS iterations, and let $E^c(N) \subseteq E(N)$ be the subset of those nodes classified as easy under BN evaluation.

[2]In classical union–find, the root is the unique representative in a hierarchy, while no hierarchy is maintained in our case.



(a) ToT-Beam Search.

(b) ToT-Beam Search + Chaining (BN-SC).

Figure 1: Policy invocations in Original ToT-BS vs. ToT-BS + Chaining (BN-SC). Numbers with $\prime$ indicate beam search sampling size; those with $*$ indicate BN judge sampling size. The BN-DP variant is shown in Appendix B.

Expansion cost. Under the baseline rule, each new node incurs cost k_{expand}, hence

$$C_{\text{mcts}}(N) \;=\; k_{\text{expand}}\,|E(N)|. \tag{5}$$

With chaining, easy nodes expand with at most k_{bn} calls, while hard nodes expand with k_{expand}, so

$$C_{\text{mcts+chain}}(N) = k_{\text{expand}} \cdot \big(|E(N)| - |E^c(N)|\big) + k_{\text{bn}} \cdot |E^c(N)|. \tag{6}$$

Guarantee. Since $k_{\text{bn}} \leq k_{\text{expand}}$, it follows immediately that

$$C_{\text{mcts+chain}}(N) \;\leq\; C_{\text{mcts}}(N), \tag{7}$$

with strict inequality whenever at least one easy node is encountered. Thus adding chaining never increases the number of policy invocations and strictly decreases it in the presence of easy nodes.

4 Experimental Setup

Datasets. Prior work shows that test-time scaling is most effective when models already possess the required background knowledge (Snell et al., 2025). Accordingly, we evaluate on mathematical reasoning, a domain where Chain-of-Thought (CoT) prompting provides substantial improvements (Sprague et al., 2025). We select two standard benchmarks: **GSM8K** and **Math500** (Zhang et al., 2024b; Hendrycks et al., 2021). For strict evaluation, we retain only problems whose final answers are single numbers, yielding 316 usable examples out of the original 500. From both benchmarks, we use the first 100 test instances for evaluation.

Baselines. We compare CiT against three representative LLM-in-the-loop tree-search (LITS) frameworks. Each serves as the corresponding upper bound of computational cost for its CiT-augmented variant (details in Appendix C): **(1) ToT-BS** (Yao et al., 2023a): Beam search where $\text{LLM}_{\text{policy}}$ generates candidate thoughts (actions) and LLM_{rm} evaluates candidates. Transitions are realized by concatenation of actions. **(2) RAP** (Hao et al., 2023): MCTS with dynamic transitions and reward models. Each node is defined by a sub-question (action) and its predicted answer (for formulating the next state). We follow the original settings: policy with 4-shot prompting, temperature 0.8 (annealed to 0 at depth limit), generating three candidate branches at each expansion, and 10 MCTS iterations. Rewards are obtained by profiling LLMs for *usefulness*, augmented with an additional correctness check (Appendix D), which we also apply to ToT-BS. $\text{LLM}_{\text{trans}}$ is profiled to answer each sub-question. **(3) ReST-MCTS* (abbreviated as ReST)**: This method is an MCTS variant where each node corresponds to a free-form reasoning step ("thought"). For the *policy*, we use a modified prompt (Appendix A) with temperature 0.7. Other MCTS settings are the same as RAP. For the *transition model*, we follow the same concatenation-based approach as in ToT-BS. For the *evaluator*, we require a Process Reward Model (PRM). The original work introduces a PRM but does not release its trained model. Therefore, we adopt the publicly available PRM from Xiong et al. (2024), which is finetuned on GSM8K and Math500 training sets, making it a suitable substitute for evaluation in our experiments. **(4) CoT** serves as a lower bound for both efficiency and accuracy.

Base LLMs. Our main experiments use **Qwen3-32B-AWQ**, the strongest open-source model that fits on a single 40GB GPU at the time of writing. We also evaluate with **LLaMA3-8B-Instruct** as a small language model (SLM), consistent with prior findings that SLMs more clearly reveal the benefits of inference-time search (Qi et al., 2025; Zhang et al., 2024a). However, RAP requires a completion-style interface, while chat-formatted models (Qwen3-32B-AWQ, LLaMA3-8B-Instruct) enforce a `(role, content)` structure incompatible with RAP's design. Therefore, we use the completion model **LLaMA3-8B** for RAP. See Appendix E for details. The parameters for LLM inference, including GPU specifications, decoding temperatures, and maximum output token limits, are detailed in Appendix F.

Evaluation Settings. In total, we consider 14 configurations:

- 3 base-LLM settings (Qwen3-32B for all roles; LLaMA3-8B for all roles; LLaMA3-8B for LITS roles with Qwen3-32B for BN roles) $\times$ 2 frameworks (ReST-MCTS, ToT-BS) $\times$ 2 datasets (GSM8K, Math500) = 12 settings.
- Plus RAP with LLaMA3-8B (all roles) on both datasets = 2 additional settings.

The mixed setting (Qwen3-32B for BN roles only) is included to evaluate the impact of BN evaluator quality.

Metrics. Efficiency is measured by: 1) number of output tokens, 2) number of invocations, 3) wall-clock runtime of $\text{LLM}_{\text{policy}}$, and 4) total runtime. Accuracy is measured using a lightweight number-only evaluator adapted from RAP (Hao et al., 2023), extended with string-to-number normalization and a fallback verification step (via Qwen3-32B) to ensure robustness in parsing numeric answers embedded in text.

5 Analysis

We report percentage cost savings in Table 1, Table 2 (for ToT-BS and ReST), and Table 3 (for RAP). The complete set of raw measurements underlying these relative improvements are provided in Appendix G.

Overall Efficiency and Stability of BN Methods. Across all settings, **BN-DP** consistently achieves the efficiency guarantee predicted by our theoretical analysis. In particular, BN-DP reduces total runtime by 75–85% relative to the baselines, while maintaining accuracy comparable to the underlying LITS framework. This makes BN-DP the most reliable and stable choice among our BN evaluation methods.

By contrast, **BN-SC^1** performs well in most configurations but fails in 4 out of 14 settings. All failures occur within the ToT-BS framework: GSM8K and Math500 with both policy and BN roles handled by LLaMA (LLaMA+LLaMA), and GSM8K and Math500 with LLaMA as policy and Qwen as the BN evaluator (LLaMA+Qwen).

BN-SC^2 is more stable, failing in only 1 out of 14 settings, occurring in the ToT-BS framework on Math500 once with LLaMA+Qwen (**BN-SC^2+** in Table 2).

Analysis of Failure Settings. To better understand the observed failures, we conducted instance-level analyses for all four failure cases of **BN-SC^1** and the failure case of **BN-SC^2**. Two consistent patterns emerge: 1) BN methods remain more efficient than the baseline on most instances—for example, on 73% and 83% of Math500 cases with LLaMA+QWen under BN-SC^1 and BN-SC^2, respectively; 2) aggregate inefficiency is driven by the remaining small subset of instances, where BN methods incur more calls than the baseline. This pattern is consistent across all failure settings, as illustrated in the figures in Appendix H.

Impact of BN Evaluator Quality on Accuracy. Figure 2 illustrates that the quality of BN evaluation plays a critical role in the effectiveness of our CiT plug-in. When smaller LLMs (e.g., LLaMA-3-8B) are used as BN evaluators (*Poor BN*), the accuracy often drops below that of the baseline LITS methods and in some cases approaches the weaker CoT baseline. This suggests that underpowered BN evaluators may systematically overestimate node scores, leading to premature chaining and insufficient exploration, which propagates errors downstream.

In contrast, when stronger LLMs (e.g., Qwen-3-32B) are used as BN evaluators (*Accurate BN*), the performance recovers and in most cases approaches that of the baseline LITS methods. While in some settings with BN-SC^1 performance can even appear higher than baseline LITS, we caution against

Method	GSM8K Out	Inv	Time	Total	Acc	Math500 Out	Inv	Time	Total	Acc
Relative to ToT-BS	(baseline Acc: **0.98**; CoT: 0.96)					(baseline Acc: **0.87**; CoT: 0.79)				
+BN-SC^1	13.1%↓	11.8%↓	14.7%↓	16.0%↓	0.96	28.8%↓	2.8%↓	36.7%↓	32.5%↓	0.89
+BN-SC^2	35.2%↓	37.0%↓	38.0%↓	44.4%↓	0.96	62.8%↓	40.3%↓	72.8%↓	71.2%↓	0.84
+BN-DP	78.3%↓	78.3%↓	78.5%↓	77.3%↓	0.97	78.9%↓	80.0%↓	78.1%↓	78.2%↓	0.86
Relative to ReST	(baseline Acc: **0.97**; CoT: 0.96)					(baseline Acc: **0.87**; CoT: 0.79)				
+BN-SC^1	26.7%↓	27.6%↓	34.3%↓	12.1%↑	0.97	41.4%↓	43.7%↓	37.0%↓	25.2%↓	0.84
+BN-SC^2	41.7%↓	44.0%↓	49.0%↓	16.2%↓	0.97	60.7%↓	58.0%↓	58.8%↓	48.7%↓	0.85
+BN-DP	79.6%↓	80.1%↓	81.8%↓	80.3%↓	0.97	82.4%↓	84.9%↓	82.8%↓	82.4%↓	0.88

Table 1: Percentage cost savings relative to ToT-BS and ReST (Qwen3-32B). **In** = input tokens (policy), **Out** = output tokens (policy), **Inv** = number of model invocations (policy), **Time** = wall-clock running time in hours (policy), **Time (Total)** = overall LLM running time in hours (LLMs as policy, reward models, transition models and BN evaluators), **Acc** = accuracy. ↓indicates reductions; ↑indicates overhead.

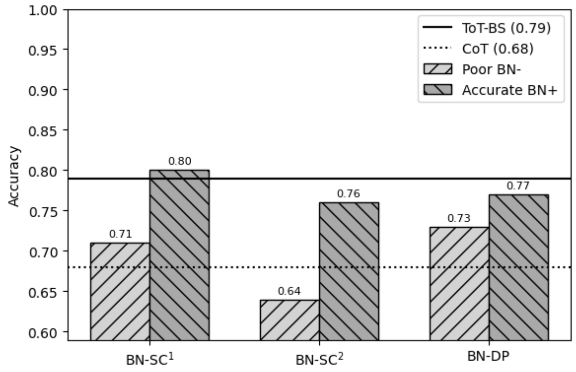
Method	GSM8K Out	Inv	Time	Total	Acc	Math500 Out	Inv	Time	Total	Acc
Relative to ToT-BS	(baseline Acc: **0.79**; CoT: 0.68)					(baseline Acc: **0.39**; CoT: 0.34)				
BN-SC^1-	14.9%↑	17.4%↑	13.5%↑	21.6%↓	0.71	34.7%↑	37.7%↑	36.7%↑	25.5%↑	0.35
BN-SC^2-	22.4%↓	22.4%↓	20.2%↓	80.9%↓	0.64	38.6%↓	24.8%↓	38.6%↓	76.6%↓	0.30
BN-DP-	68.8%↓	71.0%↓	68.5%↓	73.4%↓	0.73	69.9%↓	63.4%↓	69.7%↓	68.8%↓	0.27
BN-SC^1+	2.9%↓	1.6%↑	1.1%↓	2.3%↑	0.80	36.9%↑	25.5%↑	40.4%↑	62.9%↑	0.38
BN-SC^2+	29.2%↓	29.9%↓	28.1%↓	72.8%↓	0.76	81.2%↑	25.1%↑	87.5%↑	4.9%↓	0.39
BN-DP+	64.0%↓	69.5%↓	62.9%↓	70.9%↓	0.77	37.8%↓	37.8%↓	37.0%↓	39.9%↓	0.36
Relative to ReST	(baseline Acc: **0.80**; CoT: 0.68)					(baseline Acc: **0.39**; CoT: 0.34)				
+BN-SC^1-	22.8%↓	26.0%↓	21.7%↓	35.4%↓	0.70	23.3%↓	17.5%↓	22.4%↓	19.6%↓	0.33
+BN-SC^2-	47.9%↓	47.5%↓	47.2%↓	69.3%↓	0.73	62.8%↓	51.1%↓	63.4%↓	71.0%↓	0.29
+BN-DP-	77.5%↓	77.8%↓	76.4%↓	74.8%↓	0.68	82.4%↓	81.6%↓	82.4%↓	80.6%↓	0.36
+BN-SC^1+	41.0%↓	40.8%↓	40.6%↓	36.1%↓	0.84	65.5%↓	56.7%↓	66.5%↓	50.5%↓	0.43
+BN-SC^2+	50.2%↓	52.1%↓	49.1%↓	67.6%↓	0.80	39.8%↓	48.4%↓	40.9%↓	53.8%↓	0.34
+BN-DP+	78.8%↓	80.6%↓	78.3%↓	76.3%↓	0.76	66.7%↓	67.7%↓	67.1%↓	65.0%↓	0.37

Table 2: Percentage cost savings relative to ToT-BS and ReST (LLaMA3-8B Instruct), under both *Poor BN* evaluation (–, using LLaMA-3-8B Instruct) and *Accurate BN* evaluation (+, using Qwen-3-32B).

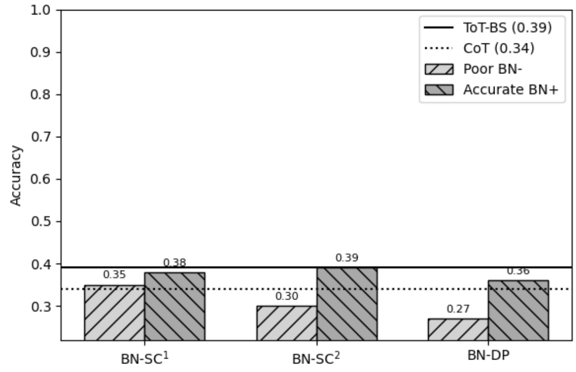
Method	GSM8K Out	Inv	Time	Total	Acc	Math500 Out	Inv	Time	Total	Acc
Relative to RAP	(baseline Acc: **0.61**; CoT: 0.32)					(baseline Acc: **0.18**; CoT: 0.17)				
BN-SC^1+	65.3%↓	69.9%↓	65.2%↓	47.9%↓	0.48	19.5%↓	34.5%↓	9.0%↓	2.4%↓	0.27
BN-SC^2+	78.0%↓	75.5%↓	78.3%↓	80.8%↓	0.46	63.4%↓	59.6%↓	61.2%↓	60.4%↓	0.21
BN-DP+	88.6%↓	86.4%↓	88.4%↓	77.4%↓	0.57	79.1%↓	80.5%↓	79.1%↓	60.8%↓	0.26

Table 3: Percentage cost savings relative to RAP (LLaMA3-8B), where *Accurate BN* evaluation (+) is performed by using Qwen-3-32B for BN roles.

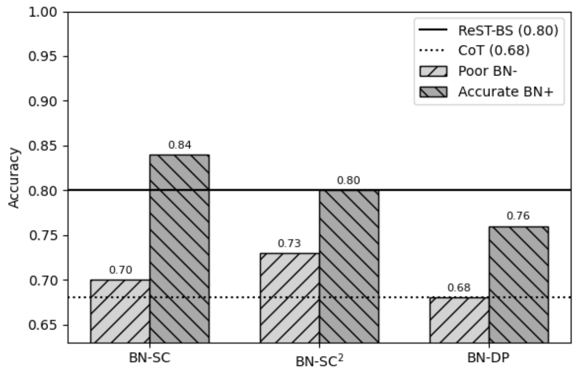
overinterpreting this result: it may partly reflect the ability of the BN aggregator to reformulate or improve upon actions generated by the policy rather than simply. Thus, we do not claim that BN-SC



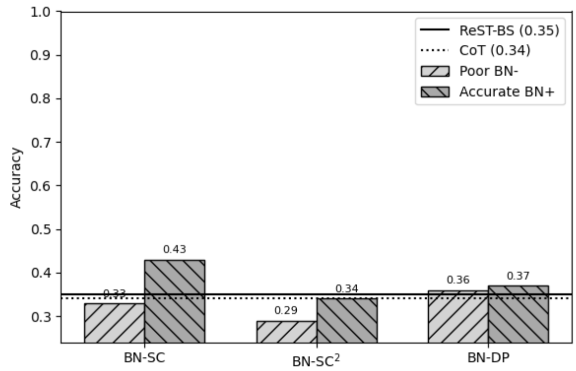
(a) ToT-BS + CiT on GSM8K



(b) ToT-BS + CiT on Math500



(c) ReST-MCTS* + CiT on GSM8K



(d) ReST-MCTS* + CiT on Math500

Figure 2: Accuracy comparison under CiT plug-in across two search frameworks (ReST-MCTS* and ToT-BS) and two datasets (GSM8K, Math500). Bars show BN evaluator quality (**Poor BN**: LLaMA-3-8B vs **Accurate BN**: Qwen-3-32B). Horizontal lines denote baselines (CoT, ReST, ToT-BS).

can outperform baseline LITS.

The consistent finding across both frameworks (ReST-MCTS* and ToT-BS) is that chaining can be effective when BN evaluation is sufficiently accurate, while poor BN evaluation can negate the benefits of chaining or even harm performance. A reasonable implication is that, for tasks with deterministic action spaces, reliable BN evaluation could in principle be implemented with rule-based or hard-coded checks, thereby eliminating the risks associated with poor BN evaluators.

6 Conclusion

We proposed **Chain-in-Tree (CiT)**, a plug-and-play framework that inserts a chaining phase into LLM tree search to avoid unnecessary branching. CiT theoretically guarantees non-increasing policy cost and achieves up to 85% runtime reduction across ToT-BS, ReST-MCTS, and RAP without accuracy loss. Overall, CiT emphasizes the importance of accurate BN evaluation for scaling LLM-based search.

6.1 Reproducibility

To support reproducibility, we release an open-source Python package that modularizes LLM-profiled roles across various search frameworks, along with scripts for running all experiments and evaluations. The chaining phase in CiT is implemented as a single Python function that is universally applicable across all three frameworks used in our experiments. Details are provided in Appendix J.

For transparency, we additionally provide evaluation datasets, detailed logs of LLM generations for each role and instance, JSON files for reconstructing search trees, and per-instance inference cost reports covering all search phases. [3]

Limitations

Coverage of LITS Frameworks. Our study considers beam search (ToT-BS) and two variants

[3]The complete package—including code, scripts, datasets, and example outputs from a representative run—is included in the supplementary material.

of MCTS (ReST-MCTS and RAP). Other search paradigms such as A* or heuristic-guided search are not evaluated. Nevertheless, our use of unified tasks and LLM-profiled roles (Li, 2025), together with modularized implementations, makes it straightforward to extend CiT to additional LITS frameworks in future work.

Scope of Empirical Evaluation. Following prior work (Snell et al., 2025; Zhang et al., 2024a), our experiments focus on mathematical reasoning, where LLMs already possess the necessary knowledge but still benefit from test-time scaling. We have not evaluated domains with deterministic action spaces (e.g., board games, navigation), where BN-SC's use of LLMs for clustering semantically equivalent actions may be unnecessary. Extending CiT to such domains is left for future work.

Accuracy Gains from CiT. Although CiT is designed for efficiency, we observe that it can also improve accuracy in several settings. Understanding why chaining sometimes enhances reasoning quality requires deeper analysis, which we leave for future investigation.

References

Ziru Chen, Michael White, Ray Mooney, Ali Payani, Yu Su, and Huan Sun. 2024. When is tree search useful for LLM planning? it depends on the discriminator. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 13659–13678, Bangkok, Thailand. Association for Computational Linguistics.

Lukas Chrpa and Mauro Vallati. 2022. Planning with critical section macros: theory and practice. *Journal of Artificial Intelligence Research*, 74:691–732.

Ning Dai, Zheng Wu, Renjie Zheng, Ziyun Wei, Wenlei Shi, Xing Jin, Guanlin Liu, Chen Dun, Liang Huang, and Lin Yan. 2025. Process supervision-guided policy optimization for code generation.

Arthur Guez, David Silver, and Peter Dayan. 2012. Efficient bayes-adaptive reinforcement learning using sample-based search. In *Proceedings of the 26th International Conference on Neural Information Processing Systems - Volume 1*, NIPS'12, page 1025–1033, Red Hook, NY, USA. Curran Associates Inc.

Shibo Hao, Yi Gu, Haodi Ma, Joshua Hong, Zhen Wang, Daisy Wang, and Zhiting Hu. 2023. Reasoning with language model is planning with world model. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 8154–8173, Singapore. Association for Computational Linguistics.

Dan Hendrycks, Collin Burns, Saurav Kadavath, Akul Arora, Steven Basart, Eric Tang, Dawn Song, and Jacob Steinhardt. 2021. Measuring mathematical problem solving with the MATH dataset. In *Thirty-fifth Conference on Neural Information Processing Systems Datasets and Benchmarks Track (Round 2)*.

Xianzhi Li, Ethan Callanan, Xiaodan Zhu, Mathieu Sibue, Antony Papadimitriou, Mahmoud Mahfouz, Zhiqiang Ma, and Xiaomo Liu. 2025. Entropy-aware branching for improved mathematical reasoning. *arXiv preprint arXiv:2503.21961*.

Xinzhe Li. 2025. A survey on LLM test-time compute via search: Tasks, LLM profiling, search algorithms, and relevant frameworks. *Transactions on Machine Learning Research*.

Liangchen Luo, Yinxiao Liu, Rosanne Liu, Samrat Phatale, Meiqi Guo, Harsh Lara, Yunxuan Li, Lei Shu, Lei Meng, Jiao Sun, and Abhinav Rastogi. 2025. Improve mathematical reasoning in language models with automated process supervision.

Zhenting Qi, Mingyuan Ma, Jiahang Xu, Li Lyna Zhang, Fan Yang, and Mao Yang. 2025. Mutual reasoning makes smaller LLMs stronger problem-solver. In *The Thirteenth International Conference on Learning Representations*.

C. Nicolò De Sabbata, Theodore Sumers, and Thomas L. Griffiths. 2024. Rational metareasoning for large language models. In *NeurIPS 2024 Workshop on Behavioral Machine Learning*.

Charlie Victor Snell, Jaehoon Lee, Kelvin Xu, and Aviral Kumar. 2025. Scaling test-time compute optimally can be more effective than scaling LLM parameters. In *The Thirteenth International Conference on Learning Representations*.

Zayne Rea Sprague, Fangcong Yin, Juan Diego Rodriguez, Dongwei Jiang, Manya Wadhwa, Prasann Singhal, Xinyu Zhao, Xi Ye, Kyle Mahowald, and Greg Durrett. 2025. To cot or not to cot? chain-of-thought helps mainly on math and symbolic reasoning. In *The Thirteenth International Conference on Learning Representations*.

Ilya Sutskever, Oriol Vinyals, and Quoc V Le. 2014. Sequence to sequence learning with neural networks. *Advances in neural information processing systems*, 27.

Karthik Valmeekam, Matthew Marquez, Alberto Olmo, Sarath Sreedharan, and Subbarao Kambhampati. 2023. Planbench: An extensible benchmark for evaluating large language models on planning and reasoning about change. In *Thirty-seventh Conference on Neural Information Processing Systems Datasets and Benchmarks Track*.

Xuezhi Wang, Jason Wei, Dale Schuurmans, Quoc V Le, Ed H. Chi, Sharan Narang, Aakanksha Chowdhery, and Denny Zhou. 2023. Self-consistency improves chain of thought reasoning in language models. In

The Eleventh International Conference on Learning Representations.

Wei Xiong, Hanning Zhang, Nan Jiang, and Tong Zhang. 2024. An implementation of generative prm. https://github.com/RLHFlow/RLHF-Reward-Modeling.

Shunyu Yao, Dian Yu, Jeffrey Zhao, Izhak Shafran, Thomas L. Griffiths, Yuan Cao, and Karthik Narasimhan. 2023a. Tree of thoughts: Deliberate problem solving with large language models. *Preprint*, arXiv:2305.10601.

Shunyu Yao, Jeffrey Zhao, Dian Yu, Nan Du, Izhak Shafran, Karthik R Narasimhan, and Yuan Cao. 2023b. React: Synergizing reasoning and acting in language models. In *The Eleventh International Conference on Learning Representations*.

Dan Zhang, Sining Zhoubian, Ziniu Hu, Yisong Yue, Yuxiao Dong, and Jie Tang. 2024a. ReST-MCTS*: LLM self-training via process reward guided tree search. In *The Thirty-eighth Annual Conference on Neural Information Processing Systems*.

Di Zhang, Xiaoshui Huang, Dongzhan Zhou, Yuqiang Li, and Wanli Ouyang. 2024b. Accessing gpt-4 level mathematical olympiad solutions via monte carlo tree self-refine with llama-3 8b. *arXiv preprint arXiv:2406.07394*.

A Prompts

The prompt use as policy, reward model and world model is summarized in Table 4.

Methods	Policy	Reward Model	Dynamic Model
RAP	QA-based policy (Table 5)	Usefulness logit-based evaluator (Table 7)	QA-based transition model (Table 5)
ReST-MCTS*	Thought generator (Table 6)	Fine-tuned reward models	NA
ToT-BF	Thought generator (Table 6)	Usefulness evaluator(Table 9) + Correctness evaluator (Table 8)	NA

Table 4: Prompt Summary for Different Frameworks.

Given a question, please decompose it into sub-questions. For each sub-question, please answer it in a complete sentence, ending with "The answer is". When the original question is answerable, please start the subquestion with "Now we can answer the question:"
(few-shot demonstrations are ignored)
Question 1: James writes a 3-page letter to 2 different friends twice a week. How many pages does he write a year?
Question 1.1: How many pages does he write every week?
Answer 1.1: James writes a 3-page letter to 2 different friends twice a week, so he writes 3 * 2 * 2 = 12 pages every week. The answer is 12.
Question 1.2: How many weeks are there in a year?
Answer 1.2: There are 52 weeks in a year. The answer is 52.
Question 1.3: Now we can answer the question: How many pages does he write a year?
Answer 1.3: James writes 12 pages every week, so he writes 12 * 52 = 624 pages a year. The answer is 624.
...

Question 5: Janet's ducks lay 16 eggs per day. She eats three for breakfast every morning and bakes muffins for her friends every day with four. She sells the remainder at the farmers' market daily for $2 per fresh duck egg. How much in dollars does she make every day at the farmers' market?
Question 5.1:

(Generation as a policy)
How many eggs does Janet have left after eating three for breakfast and baking muffins with four?

Answer 5.1:

(Generation as a transition model)
Janet starts with 16 eggs per day, consumes 3 for breakfast and 4 for baking, so she has 16 - 3 - 4 = 9 eggs left for the farmers' market. The answer is 9.

Table 5: A policy/transition model for RAP. Sourced from Hao et al. (2023).

System message:
Your task is to give the correct next step, given a science problem and an existing partial solution (not a complete answer). Assuming the input is n-steps, then the format of the input is: "Problem: ... Existing Steps: Step 1: ... Step 2: ... ... Step n: ..." where ... denotes omitted input information. Please follow the restricted output format: * If no existing steps are given, generate Step 1. * Otherwise, following the given step(s), output ONLY ONE step within 1000 tokens. SHOULD NOT output multiple steps. * DO NOT repeat Problem or any Existing Steps. * Your output should be a complete reasoning step that includes calculations, reasoning, choosing answers, etc. * When the final answer is/has been reached, begin the step with EXACTLY the phrase:"Now we can answer the question: The answer is ", followed by EXACTLY one number. Do not include any other words, punctuation, or explanation after the number.
User message:
Problem: How many positive whole-number divisors does 196 have? Existing Steps: None Step 1:

Table 6: A policy used for ReST and BFS. Sourced from Zhang et al. (2024a).

Given a question and some sub-questions, determine whether the last sub-question is useful to answer the question. Output 'Yes' or 'No', and a reason. **Question 1:** Four years ago, Kody was only half as old as Mohamed. If Mohamed is currently twice as 30 years old, how old is Kody? **Question 1.1:** How old is Mohamed? **Question 1.2:** How old was Mohamed four years ago? **New question 1.3:** How old was Kody four years ago? *Is the new question useful? Yes. We need the answer to calculate how old is Kody now.* *(Few-shot demonstrations are ignored.)* **Question 5:** Janet's ducks lay 16 eggs per day. She eats three for breakfast every morning and bakes muffins for her friends every day with four. She sells the remainder at the farmers' market daily for $2 per fresh duck egg. How much in dollars does she make every day at the farmers' market? **New question 5.1:** Now we can answer the question: How much in dollars does she make every day at the farmers' market? *Is the new question useful?*

Table 7: An LLM evaluator. Source from Hao et al. (2023)

System message:

Given a question and a chain of thoughts, determine whether the last thought is **correct**, where **correct** means factually accurate and mathematically accurate (all calculations and formulas are correct), and logically consistent with the question.
Instructions:
Output only a score:
- 0 if any correctness criterion is unmet.
- 1 if all correctness criteria are fully met.
The score must be parsable by Python's `float()` function, with no punctuation or additional text.

User message:

Problem: How many positive whole-number divisors does 196 have?
Existing Steps:
Step 1: Find the prime factorization of 196 as $2^2 \times 7^2$
Step 2: Apply the divisor formula $(a+1)(b+1)$ to the prime factorization $2^2 \times 7^2$ and calculate $3 \times 3 = 9$
New Step to be evaluated: Now we can answer the question: The answer is 9.

Table 8: A correctness evaluator used for BFS.

System message:

Given a question and a chain of thoughts, determine how **useful** the last thought is for answering the question, regardless of correctness.
Instructions:
Output only a score between 0 and 1:
- 0 if the step is entirely irrelevant or unhelpful.
- 1 if the step is essential and maximally useful.
- A value strictly between 0 and 1 if the step is partially useful. Larger values indicate more usefulness.
The score must be parsable by Python's `float()` function, with no punctuation or additional text.

User message:

Problem: How many positive whole-number divisors does 196 have?
Existing Steps:
Step 1: Find the prime factorization of 196 as $2^2 \times 7^2$
Step 2: Apply the divisor formula $(a+1)(b+1)$ to the prime factorization $2^2 \times 7^2$ and calculate $3 \times 3 = 9$
New Step to be evaluated: Now we can answer the question: The answer is 9.

Table 9: A usefulness evaluator used for BFS.

System message:
You are an expert at deciding whether a single reasoning step is *logically compulsory* given the task and the partial solution path. Input fields (A) Task description - one paragraph. (B) Partial reasoning path so far. (C) Candidate next step. ONLY output a single number from 1 to 4. Scale 4 - **Unavoidable next step**: given the current path, this step must come next to proceed logically. 3 - Strongly expected: skipping it now would be very unusual, though not impossible. 2 - Potentially useful but avoidable: alternative coherent next steps exist. 1 - **Optional**: the step is not logically required at this point. Think silently, then output the single line - nothing else.
User message:
(A) *(task)* (B) *(partial path)* (C) *(candidate step)*

Table 10: BN Evaluator.

System message for RAP:

You are given a QUESTION and its partial solution (Subquestions which have been answered).
Your task is to group the provided list of candidate next subquestions (After "List of Candidates for the following step") into clusters.

- Steps that are semantically equivalent must be grouped together.
- Paraphrase or stylistic differences are irrelevant
- Existing Steps are given only as context and MUST NOT appear in the clusters.

OUTPUT FORMAT (Python literal list only; must be parsable by ast.literal_eval):
OUTPUT FORMAT:

```
[
 { "canonical_action": "<a CONCRETE subquestion>", "count": <the number of the candidates grouped in that cluster> },
  ...
]
```

Rules:
- Each array element represents one cluster.
- No text outside the list.
- The total number of generated words should be NO more than 450 words.

System message for ReST-MCTS* and ToT-BS:

You are given a QUESTION and its partial solution (Existing Steps).
Your task is to group the provided list of candidate next steps (After "List of Candidates for the following step") into clusters.

- Steps that are semantically equivalent must be grouped together.
- Paraphrase or stylistic differences are irrelevant.
- Existing Steps are given only as context and MUST NOT appear in the clusters.

OUTPUT FORMAT:

```
[
 { "canonical_action": "<CONCRETE calculation(s) and outcome(s) after the Existing Steps>", "count": <the number of the candidates grouped in that cluster> },
  ...
]
```

Rules: Each array element represents one cluster. No text outside the list. The total number of generated words should be no more than 450 words.

Table 11: BN Aggregator .

System message for RAP: You are a strict semantic comparator. Given two sub-questions, decide if they are semantically overlapping given the context.
System message for ReST-MCTS* and ToT-BS: You are a strict semantic comparator. Given two action descriptions, decide if they are semantically overlapping given the context. Definition: - "Overlapping" means the two descriptions express the same underlying operation or one is a specific case/subsumption of the other or have the same effect on the context. - "Not overlapping" means the operations are mutually exclusive in meaning. Answer format: return only 'YES' or 'NO' with no punctuation, no explanation.
User message: Context: ======== {*context*} ======== New Step A: {*canonical_action*} New Step B: {*canonical_action*} Do these steps express the same underlying operation given the context?

Table 12: BN equivalence checker

B Theoretical Costs

B.1 Scope of Theoretical Analysis

This section clarifies why our theoretical efficiency analysis of *Chain-in-Tree* (CiT) focuses exclusively on policy invocations.

Justification for Focusing on Policy Invocations. 1) Cost of reward and transition models never increase: While LLMs may serve as *policy*, *reward*, and *transition* models, we only count invocations of $\text{LLM}_{\text{policy}}$. The reason is structural: every node generated by $\text{LLM}_{\text{policy}}$ necessarily triggers the use of LLM_{rm} and/or $\text{LLM}_{\text{trans}}$ if it exists. For example, in ToT-BS, every child node requires reward evaluation; in RAP, at least one transition evaluation is needed per depth to maintain expansion. By contrast, during the chaining phase, CiT invokes $\text{LLM}_{\text{trans}}$ exactly once per chaining node (i.e., per depth), which is no worse than the per-depth transition usage in the original frameworks; moreover, reward evaluation via LLM_{rm} can be deferred until branching. Thus, CiT consistently reduces reward/-transition overhead under the same policy budget.

(2) Additional BN evaluation roles are lightweight. Although CiT introduces additional roles—LLM_{bn}, LLM_{agg}, and LLM_{eq}—for Branching Necessity (BN) evaluation, their overhead is significantly smaller than that of $\text{LLM}_{\text{policy}}$ or $\text{LLM}_{\text{trans}}$ (when present). We confirm this empirically in Section 5.

Uniform Token Length Assumption. We assume the number of input and output tokens per $\text{LLM}_{\text{policy}}$ invocation is approximately uniform across steps and examples.

B.2 ToT-BS

Proposition 1. (Beam-search frontier size.) At depth t, the frontier size under beam search satisfies

$$|N_t| = \min(B, k^t_{\text{expand}}), \tag{8}$$

assuming each node generates at most k_{expand} children, pruning retains the top B nodes at each layer, and no terminals are reached.

Proof. The recurrence relation for the frontier is

$$|N_{t+1}| = \min\bigl(B,\ k_{\text{expand}}\,|N_t|\bigr). \tag{9}$$

For the base case, $|N_0| = 1 = \min(B, k^0_{\text{expand}})$ (assuming $B \geq 1$). For the inductive step, assume $|N_t| = \min(B, k^t_{\text{expand}})$. Then

$$\begin{aligned} |N_{t+1}| &= \min\bigl(B,\ k_{\text{expand}} \min(B, k^t_{\text{expand}})\bigr) \\ &= \min\bigl(B,\ \min(k_{\text{expand}}B,\ k^{t+1}_{\text{expand}})\bigr). \end{aligned} \tag{10}$$

Because $k_{\text{expand}}B \geq B$ for all integers $k_{\text{expand}} \geq 1$, the inner minimum simplifies to k^{t+1}_{expand} whenever $k^{t+1}_{\text{expand}} < B$, and otherwise the outer minimum enforces B. Thus

$$|N_{t+1}| = \min(B, k^{t+1}_{\text{expand}}).$$

□

Hence the frontier grows geometrically as k^t_{expand} until saturating at beam width B. An edge case is $k_{\text{expand}} = 1$, which yields a single chain $|N_t| = 1$ (if $B \geq 1$).

In the presence of terminals or variable branching, the relation holds as an upper bound rather than an equality, i.e., $|N_t| \leq \min(B, k^t_{\text{expand}})$.

Proposition 2. (Beam-search cumulative expansion cost.) Assume each node generates at most k_{expand} children, pruning retains the top B nodes after each layer, and no terminal states are encountered. Let $D \in \mathbb{N}$ be the maximum depth (number of layers). Define the per-depth expansion cost as the number of child-generation operations,

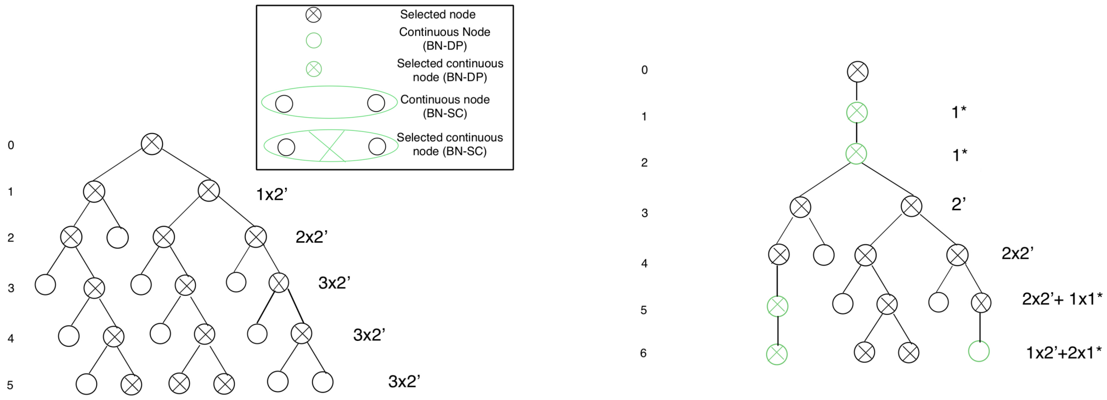
$$\begin{aligned} C_{\text{bs}}(t) &:= k_{\text{expand}}\,|N_t| \\ &= k_{\text{expand}}\ \min(B,\ k^t_{\text{expand}}), \\ &\quad t = 0, 1, \ldots, D-1. \end{aligned} \tag{11}$$

Then the total expansion cost up to depth D is

$$\begin{aligned} C_{\text{bs}}(D) &= \sum_{t=0}^{D-1} C_t \\ &= \sum_{t=0}^{D-1} k_{\text{expand}}\ \min(B,\ k^t_{\text{expand}}). \end{aligned} \tag{12}$$

Proposition 3. (Beam-search with chaining: cumulative expansion cost.) Suppose chaining is enabled for the first D_{C1} "easy" depths, where each expansion produces at most $k_{\text{bn}} \leq k_{\text{expand}}$ children ($k_{\text{bn}} = 1$ for direct prompting, $k^t_{\text{bn}} = k_{\text{expand}}$ for the self-consistency approach). After depth D_{C1}, standard beam search resumes with branching factor k_{expand} and beam size B. Then the per-depth expansion cost is

Hence the total expansion cost up to depth D is



(a) ToT-Beam Search.

(b) ToT-Beam Search + Chaining (BN-DP).

Figure 3: The number of policy invocations of Original ToT-BS vs ToT-BS + Chaining. The numbers suffixed by "'" indicate sampling size for beam search expansion, while The numbers suffixed by "*" indicate sampling size for BN judge.

$$
\begin{aligned}
&C_{\text{bs+chain}}(D) \\
&= \sum_{t=0}^{D_{C1}-1} k_{\text{bn}} \\
&\quad + \sum_{t=D_{C1}}^{D-1} k_{\text{expand}} \cdot \min\Big(B,\, k_{\text{expand}}^{t-D_{C1}}\Big).
\end{aligned} \tag{13}
$$

□

C Details of RAP and REST-MCTS

C.1 Task Formulation: RAP vs ReST-MCTS

Table 13 shows the distinction between task formulation.

C.2 Four Phases

As standard MCTS, four phases are included for RAP and REST-MCTS.

- Selection: Walk down the tree until a leaf or an unexpanded node is reached. UCT values will be used for selection when all the child nodes have been visited (i.e., node.state is not empty). Otherwise , the reward is estimated to select from unvisited nodes.
- Expansion: If the leaf is not terminal and not depth-limited, the selected node will be expaned by calling the policy. All its k children will be expanded at once.
  - Lazy Sampling: Following RAP implementation (Hao et al., 2023), lazy sampling (Guez et al., 2012) is used. After the policy generates multiple actions, RAP may leave action nodes unvisited for efficiency and only use the transition model to infer the next state if it is selected for expansion. Therefore, the sampled candidate nodes only maintain actions.
  - Non-empty state may reflect the existence of value: Once the state of a node is not empty, the node must have gone through backpropagation and thus contain rewards for selection. But this does not be the case for continuous nodes due to the requirement of inferring the state during continuation.
- Simulation (rollout): At each step, k actions are sampled from policy, and then most reward models are used to select the most valuable one.
  - In RAP, the sampling process will proceed iteratively until a terminal step is reached or a global depth limit is reached.
  - In ReST-MCTS, a fixed depth limit 2 is set specifically for roll-out.
- MCTS Backpropagation - Value Update: After each simulation returns a reward r, update the Q value as:

$$
Q_{\text{new}} = \frac{r + Q_{\text{old}} \cdot \text{Count}_{\text{new}}}{\text{Count}_{\text{new}}}, \tag{14}
$$

Reasoning via Concatenation from Rest-MCTS	Reasoning via QA from RAP
First, calculate the total number of eggs used by Janet each day for breakfast and baking.(Homogeneous Thought 1) Janet uses 3 eggs for breakfast and 4 eggs for baking, so the total number of eggs used each day is $3 + 4 = 7$. (Homogeneous Thought 2)	What is the total number of eggs used by Janet each day for breakfast and baking? (Question as action) Janet uses 3 eggs for breakfast and 4 eggs for baking, so the total number of eggs used each day is $3 + 4 = 7$. (Answer to form the next state)

Table 13: Formatting Difference Between Reasoning via Concatenation and QA under the same meaning.

r, depending on the task, can be a reward at the terminal state. In some cases,it can be an aggregated one, if each simulation step yields a reward. Specifically, if rewards r_t are discounted by γ, then the final sample reward r for backpropagation is:

$$r = G = \sum_{t=0}^{T-1} \gamma^t r_t. \tag{15}$$

These rewards from simulated nodes are then employed to update the Q values for non-simulated nodes, including the leaf nodes and those above. Q_{old} are the previous Q-value, and $\text{Count}_{\text{new}}$ is the total visit count after the current update.

During our implementation, each reward $r \in R_{\text{cum}}$ propagating from the terminal node is stored in a list R_{cum} , and average them when used. The procedure of value estimate, provides the initialized values for new actions or resulting states.

For RAP, the confidence of transition models is also included along with the usefulness score to be processed for backpropagation

$$r^w \cdot r_{\text{conf}}^{(1-w)}, \tag{16}$$

where w is the weight between 0 and 1.

- MCTS Backpropagation - Visit Update: Except for the estimated value $Q(s, a)$, the backpropagation also updates the visit count for every state on the path from the root to the leaf and each edge (s, a) along that path, denoted as Count (s_t) and Count (s_t, a_{t+1}), respectively.

D Reward Models

We profile LLMs as reward models, as RAP does. However, the original profiling only consider the contribution of solution steps to the input task. As suggested by Zhang et al. (2024a), we further improve the prompt to reflect the probability of correctness. Three constraints are enforced: bounded range, contribution-awareness, and correctness-awareness in the original paper.

E Incompatibility of Chat-Formatted LLMs with RAP

Firstly, the policy and transition model in RAP requires a raw completion interface: the LLM is repeatedly invoked with concatenated sub-questions and answers, such as "`Subquestion 1: ... Answer 1: ... Subquestion 2: ...`". This mismatch often leads to unstable generations (e.g., empty outputs, spurious punctuation, or off-task continuations), since the evolving transcript no longer resembles the conversational templates seen in training. Furthermore, the reward model requires the next token logically requiring "`yes`" or "no" for judgments (e.g., "`Is the new question useful?`"), however, the next token in the chat models tends to be a template one, which disrupts the intended binary evaluation.

F Parameters for LLM Inference

GPU Specification All experiments with LLaMA3 were conducted on NVIDIA A100-SXM4 40GB GPUs, while Qwen3 experiments were run on NVIDIA L40S 48GB GPUs.

Maximum Length. The maximum context length is set to 32,768 tokens (the upper limit of Qwen3) for all LITS roles and for CoT. In practice, 2,048 tokens are sufficient for all GSM8K instances, whereas Math500 often requires longer inputs and extended reasoning chains. For the policy models in ReST and ToT-BS, we instruct the model to keep each reasoning step within 1,000 tokens.

For BN evaluation, we enforce a maximum of 1,000 output tokens for the aggregator model used in BN-SC^1. For LLM_{eq} (BN-SC^2) and LLM_{bn} (BN-DP), the same limit is applied, but only single-word outputs are accepted: "yes/no" for LLM_{eq}, or a number between 1–4 for LLM_{bn}. Special tokens are ignored in this check.

Temperature. We follow the settings from prior work: RAP uses temperature 0.8 for LITS roles, ReST uses 0.7, and ToT-BS reuses the ReST policy with temperature 0.7.

G Raw Efficiency and Effectiveness Results

For completeness and reproducibility, we report the raw numbers underlying the relative efficiency tables in the main paper. These include input tokens, output tokens, number of invocations, policy runtime, total runtime, and accuracy.

H Additional Failure Analyses

In this section we provide the full set of instance-level visualizations for all failure cases of BN methods. Each figure reports the difference in the number of invocations between BN methods and the baseline across 100 instances, with filled markers indicating correct predictions and hollow markers incorrect ones.

I LLM Usage

Large Language Models (LLMs) were used in this work as **writing assistants** to support clarity and style. Their role was confined to the revision stage of the manuscript and did not extend to research ideation, algorithm design, proofs, experiments, or interpretation of results.

The revision process followed a structured, iterative workflow:

1. **Abstract revision:**
   - The LLM was asked to revise the abstract.
   - The authors manually revised the generated text, compared it against the original version, and selectively incorporated improvements.
   - For specific sentences, the LLM was prompted in-quote to suggest localized adjustments (e.g., rephrasing for clarity or conciseness).
   - The finalized abstract was authored by the authors after reviewing and merging both versions.

2. **Section-by-section revision:**
   - With the finalized abstract fixed, the same process was repeated sequentially for each section: Section 1, Section 2, Section 3, Section 4, Section 5, Section 6, and the Appendix.
   - At each stage: (i) the LLM was asked to revise the draft section, (ii) the authors manually revised and compared the LLM output with the original draft, and (iii) the LLM was used for fine-grained, sentence-level in-quote adjustments where needed.
   - The revised section was only finalized after careful author editing and approval.

3. **Formatting assistance:**
   - The LLM was occasionally used to generate LaTeX table skeletons, figure captions, and consistent notation formatting. All outputs were verified and edited by the authors.

This procedure ensured that the LLM functioned only as a **linguistic and formatting assistant**. All scientific content—including the conception of the *Chain-in-Tree* framework, technical derivations, algorithmic innovations, and empirical analysis—originated entirely from the authors.

The authors take **full responsibility** for the correctness, originality, and integrity of all content.

J Package Design

The LangAgent Python package modularizes LLM-profiled roles across various search frameworks.

Role Modularity. Specifically, LangAgent organizes all LLM-mediated reasoning roles behind stable interfaces so that different search frameworks can reuse the same components without behavioral drift. Core contracts for the *world model*, *policy*, and *reward/evaluator* roles are declared once in `langagent/reasoner_base.py`, together with the shared `BaseSearchConfig` structure that wires

Method	GSM8K Out	Inv	Time	Total	Acc	Math500 Out	Inv	Time	Total	Acc
ToT-BS	75.6k	738	1.63H	2.25H	0.98	594.5k	1266	19.6H	20.96H	0.87
+BN-SC^1	65.7k↓	651↓	1.39H↓	1.89H↓	0.96↓	423.3k↓	1230↓	12.40H↓	14.14H↓	0.89↑
+BN-SC^2	49.0k↓	465↓	1.01H↓	1.25H↓	0.96↓	221.3k↓	756↓	5.34H↓	6.03H↓	0.84↓
+BN-DP	16.4k↓	160↓	0.35H↓	0.51H↓	0.97↓	125.5k↓	253↓	4.29H↓	4.57H↓	0.86↓
ReST	83.5k	836	1.98H	1.98H	0.97↓	491.0k	1574	11.98H	11.99H	0.87=
+BN-SC^1	61.2k↓	605↓	1.30H↓	2.22H↑	0.97↓	287.9k↓	886↓	7.55H↓	8.97H↓	0.84↓
+BN-SC^2	48.7k↓	468↓	1.01H↓	1.66H↓	0.97↓	192.9k↓	661↓	4.93H↓	6.15H↓	0.85↓
+BN-DP	17.0k↓	166↓	0.36H↓	0.39H↓	0.97↓	86.4k↓	238↓	2.06H↓	2.11H↓	0.88↑
CoT	46.2k	100	0.96H	0.96H	0.96	78.1k	100	1.61H	1.61H	0.79

(a) Qwen3 32B.

Method	GSM8K Out	Inv	Time	Total	Acc	Math500 Out	Inv	Time	Total	Acc
ToT-BS	108.6k	1509	0.89H	6.91H	0.79	458.1k	2816	3.76H	14.68H	0.39
+BN-SC^1	124.8k↑	1771↑	1.01H↑	5.42H↓	0.71↓	617.0k↑	3877↑	5.14H↑	18.42H↑	0.35↓
+BN-SC^2	84.3k↓	1171↓	0.71H↑	1.32H↓	0.64↓	281.2k↓	2119↓	2.31H↓	3.44H↓	0.30↓
+BN-DP	33.9k↓	438↓	0.28H↓	1.84H↓	0.73↓	137.8k↓	1032↓	1.14H↓	4.58H↓	0.27↓
+BN-SC^1+	105.4k↓	1533↑	0.88H↓	7.07H↑	0.80↑	627.1k↑	3534↑	5.28H↑	23.92H↑	0.38↓
+BN-SC^2+	76.9k↓	1058↓	0.64H↓	1.88H↓	0.76↓	830.0k↑	3523↑	7.05H↑	13.96H↓	0.39(=)
+BN-DP+	39.1k↓	460↓	0.33H↓	2.01H↓	0.77↓	284.9k↓	1751↓	2.37H↓	8.83H↓	0.36↓
ReST	130.4k	1828	1.06H	10.44H	0.80	640.8k	3976	5.41H	25.98H	0.37
+BN-SC^1-	100.7k↓	1352↓	0.83H↓	6.74H↓	0.70↓	491.4k↓	3281↓	4.20H↓	20.89H↓	0.33↓
+BN-SC^2-	68.0k↓	960↓	0.56H↓	3.21H↓	0.73↓	238.5k↓	1944↓	1.98H↓	7.53H↓	0.29↓
+BN-DP-	29.4k↓	406↓	0.25H↓	2.63H↓	0.68↓	112.8k↓	731↓	0.95H↓	5.04H↓	0.36↓
+BN-SC^1+	76.9k↓	1082↓	0.63H↓	6.67H↓	0.84↑	221.1k↓	1722↓	1.81H↓	12.87H↓	0.43↑
+BN-SC^2+	65.0k↓	875↓	0.54H↓	3.38H↓	0.80=	386.0k↓	2053↓	3.20H↓	12.01H↓	0.34↓
+BN-DP+	27.6k↓	354↓	0.23H↓	2.47H↓	0.76↓	213.4k↓	1285↓	1.78H↓	9.10H↓	0.37=
CoT	20.0k	100	0.16H	–	0.68	121.5k	316	1.01H	–	0.34

(b) LlaMa3 8B Instruction. **BN-SC-**, **BN-DP-** uses the incompetent small LLaMA3-8B for the action aggregator or BN judge, respectively, whereas **BN-SC+** and **BN-DP+** employ the stronger Qwen3-32B for these roles.

Table 14: Efficiency and effectiveness of of ToT-BS (or ReST-MCTS*) +CiT on GSM8K and Math500. **Out** = output tokens (policy), **Inv** = number of model invocations (policy), **Time** = wall-clock running time in hours (policy), **Time (Total)** = overall LLM running time in hours (LLMs as policy, reward models, transition models and BN evaluators), **Acc** = accuracy.

termination and continuation settings across algorithms.

Concretely, `WorldModel` methods are defined for initialization, state transitions, and terminal checks. The policies inherit from the common `QAPolicy` skeleton, while evaluator variants specialize `QAEvaluator.fast_reward` to add correctness or usefulness signals.

Functional Search Pipelines. Search algorithms in `langagent/search` follow a functional design that keeps each phase explicit and composable. Breadth-first search exposes pure helpers for expansion, continuation-aware expansion and terminal checks that the top-level `bfs_topk` function orches-

Method	GSM8K					Math500				
	Out	Inv	Time	Total	Acc	Out	Inv	Time	Total	Acc
RAP	67.8k	4606	0.69H	5.53H	0.61	70.4k	3583	0.67H	8.03H	0.18
+BN-SC+	23.5k↓	1388↓	0.24H↓	2.88H↓	0.48↓	56.7k↓	2347↓	0.61H↓	7.84H↓	0.27↑
+BN-SC^2+	14.9k↓	1128↓	0.15H↓	1.06H↓	0.46↓	25.8k↓	1449↓	0.26H↓	3.18H↓	0.21↑
+BN-DP+	7.7k↓	625↓	0.08H↓	1.25H↓	0.57↓	14.7k↓	697↓	0.14H↓	3.15H↓	0.26↑
CoT	69.4k	100	0.57H	–	0.32	71.2k	100	0.57H	–	0.17

Table 15: Efficiency and effectiveness of RAP+CiT on GSM8K and Math500.

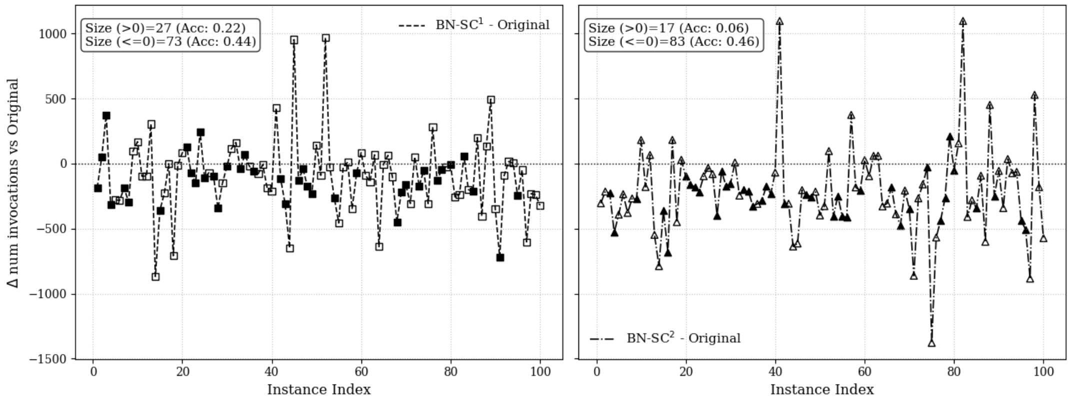


Figure 4: Instance-level analysis of a failure case on Math500 with LLaMA+Qwen (policy = LLaMA, BN = Qwen). Each point shows the relative change in the number of invocations compared to the baseline; negative values indicate higher efficiency (fewer output tokens required). Filled markers correspond to correct predictions, while hollow markers correspond to incorrect ones.

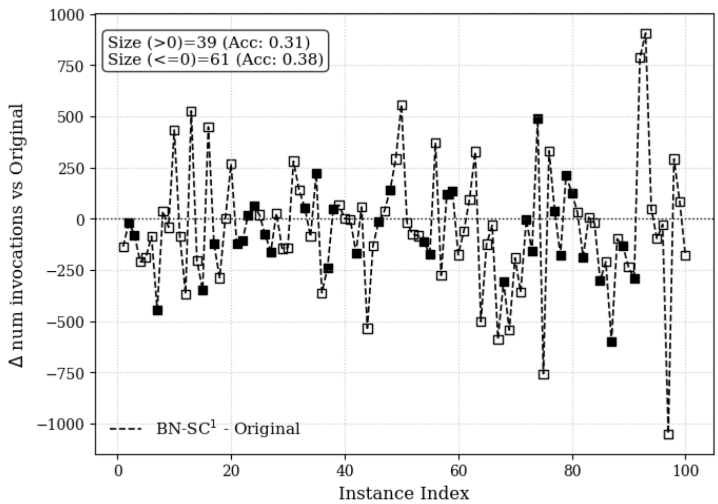


Figure 5: Instance-level analysis of failure for Math500 with LLaMA+LLaMA (BN-SC^1).

trates. Likewise, the Monte Carlo tree search implementation separates selection, expansion, simulation, and backpropagation.

Identical role objects can drive either algorithm, and new planners can reassemble the same primitives to instrument alternative search behaviors without duplicating logic.

Utilities. Auxiliary utilities—answer extraction, dataset loading, and evaluation—live in `langagent/langreason/common.py`, ensuring that any new framework automatically gains the same output handling.

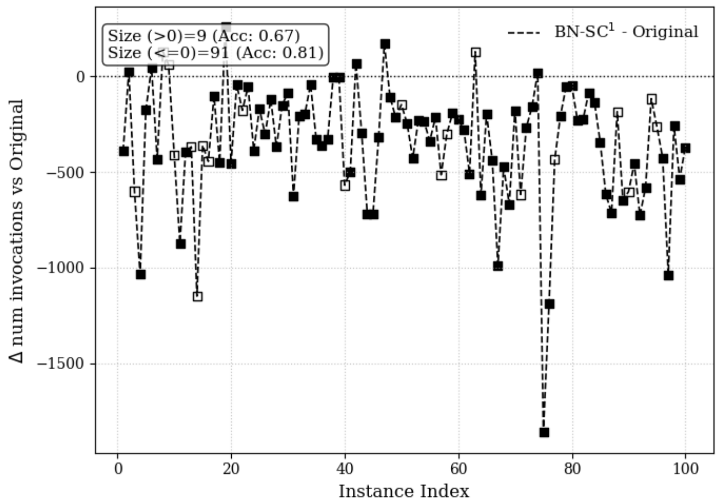


Figure 6: Instance-level analysis of failure for GSM8K with LLaMA+Qwen (BN-SC^1).

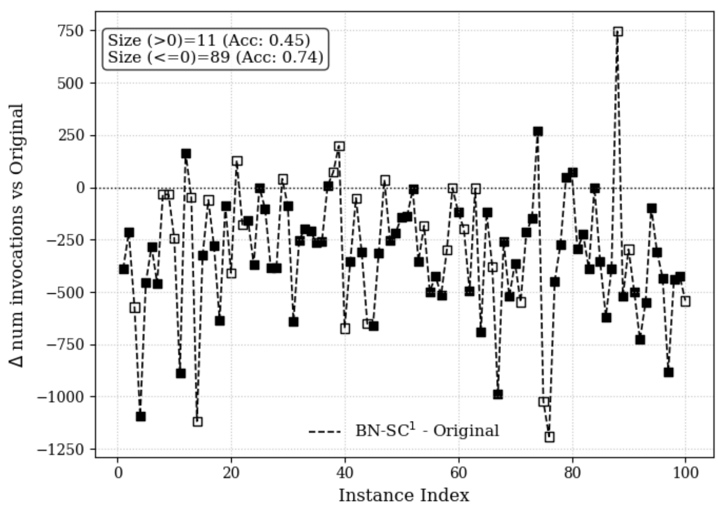


Figure 7: Instance-level analysis of failure for GSM8K with LLaMA+LLaMA (BN-SC^1).