Cognitive Loop of Thought: Reversible Hierarchical Markov Chain for Efficient Mathematical Reasoning

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Abstract

Multi-step Chain-of-Thought (CoT) has significantly advanced the mathematical reasoning capabilities of LLMs by leveraging explicit reasoning steps. However, the widespread adoption of Long CoT often results in sequence lengths that exceed manageable computational limits. While existing approaches attempt to alleviate this by reducing KV Cache redundancy via Markov chain-like structures, they introduce two critical limitations: inherent memorylessness (loss of context) and limited backward reasoning capability. To address these limitations, we propose a novel Chain-of-Thought framework based on Reversible Hierarchical Markov Chain, termed Cognitive Loop of Thought (CLoT), and a backward reasoning dataset CLoT-Instruct. In CLoT, problems are decomposed into sub-problems with hierarchical dependencies. Inspired by human cognitive processes—where reasoning is revisited to verify conclusions—we introduce a backward verification mechanism at each hierarchical layer. Furthermore, we implement a pruning strategy: once higher-level sub-problems are verified, redundant lower-level sub-problems are pruned to maximize efficiency. This approach effectively mitigates error propagation and enhances reasoning robustness. Experiments on four mathematical benchmarks demonstrate the effectiveness of our method. Notably, on the AddSub dataset using GPT-4o-mini, CLoT achieves 99.0% accuracy, outperforming traditional CoT and CoT-SC by 4.1% and 2.9%, respectively. Our code is publicly available at: https://anonymous.4open.science/r/CLoT-7EBD.

1 Introduction

Large Language Models (LLMs) have achieved remarkable breakthroughs across a broad spectrum of Natural Language Processing (NLP) tasks, such as question answering, automatic summarization, and machine translation (Achiam et al., 2023; Chowdhery et al., 2023; Touvron et al., 2023; Huang et al., 2023; Zhao et al., 2023). Despite these achievements, LLMs continue to exhibit notable limitations in reasoning performance when compared to human cognitive capabilities. Empirical evidence suggests that merely increasing model scale through parameter expansion is insufficient to bridge the gap in complex reasoning abilities between current LLMs and human-level intelligence. (Zhou et al., 2024).

To enhance the model's reasoning capabilities, researchers have explored various strategies to enhance the logical coherence and step-by-step inference processes of LLMs. One of the most influential approaches is Chain-of-Thought (CoT) reasoning (Kojima et al., 2022), which enables models to generate intermediate reasoning steps before arriving at a final answer. By mimicking human-like problem-solving patterns, CoT not only improves model performance on complex reasoning tasks, but also enhances the interpretability of model decisions. The transparency afforded by explicit reasoning traces allows users to inspect, validate, and potentially correct the model's logic, thereby fostering trust and facilitating debugging.

However, when facing real-world application scenarios, CoT still encounters the challenge that intermediate reasoning steps may contain errors. To address this challenge, one approach to improve performance is intrinsic self-correction (Kamoi et al., 2024; Pan et al., 2024), which allows the model to check and revise its own generated answers without external feedback—a process highly analogous to human thinking. Nevertheless, negative views on self-correction also exist. (Stechly et al., 2023; Tyen et al., 2024; Jiang et al., 2024) finds that large language models are even unable to determine the correctness of answers, often changing correct answers into incorrect ones or failing to correct originally erroneous responses. The debates in prior research indicate that the self-correction mechanisms of large models still lack in-depth ex-

ploration.

To address these limitations and obviate the need for extensive training on verification tasks, we propose a novel reverse self-verification method named CLoT (Cognitive Loop of Thought). Humans often employ "reverse engineering" or self-validation to confirm inferred conclusions. Drawing inspiration from this cognitive process and reversible Markov chains, we treat the forward refinement and backward verification steps as a single closed loop, iteratively executing this process to ensure the validity of intermediate reasoning. Specifically, in the forward refinement phase, the LLM progressively generates sub-questions and answers via CoT. Subsequently, each sub-question undergoes backward verification: the original conditions are treated as unknown variables, while the generated answer serves as a known condition to deduce the original premises. Consistency between the backward inference and the original condition validates the step; discrepancies trigger a root-cause analysis. This bidirectional verification minimizes error propagation in the reasoning chain. We evaluate our method using gpt-4o-mini and gpt-4-1106-preview across multiple mathematical, commonsense, and logical reasoning datasets. Our contributions are summarized as follows:

- We propose a novel self-reflective verification method for reasoning chains, named CLoT (Cognitive Loop of Thought). CLoT is capable of verifying both intermediate steps and the final answer, as well as analyzing the causes of errors.

- We introduce a hierarchical pruning strategy that removes redundant verification steps at lower layers, reducing CLoT's resource consumption by 41.8% without compromising performance.

- We construct CLoT-Instruct, an instruction-tuning dataset designed to facilitate the learning of "Backward Verification" capabilities in LLMs.

- Extensive experiments across six diverse tasks demonstrate that CLoT effectively identifies and corrects reasoning errors, consistently outperforming baseline methods.

2 Related Work

Since training LLMs requires enormous resources, effectively improving model performance without retraining has become a key research focus. (Wei et al., 2022) introduced the concept of CoT reasoning, emphasizing the importance of deriving conclusive answers through multi-step logical pathways. (Kojima et al., 2022) found that simply adding the phrase "let's think step by step" to prompts enables LLMs to perform zero-shot logical reasoning without any additional human-designed prompts. Subsequently, (Wang et al., 2023b) proposed Self-Consistency (SC) to replace the greedy decoding strategy. (Zhang et al., 2023) developed an automatic CoT framework based on the input problem, eliminating the instability caused by manual prompting. (Fu et al., 2023) employed complexity-based multi-step reasoning estimation to execute CoT. (Zhu et al., 2025) further enhanced performance by applying pre-prompting in the form of a plugin. However, standard chain-like reasoning still struggles with highly complex logical problems. Variants such as Tree-of-Thoughts (Yao et al., 2023), Graph-of-Thoughts (Besta et al., 2024), and Markov-chain-inspired reasoning frameworks have effectively enhanced the model's reasoning capabilities (Teng et al., 2025). Nevertheless, in practical applications, large models often fail to recognize their own errors and tend to repeat mistakes, limiting their applicability in real-world scenarios.

To expand the application scenarios of LLMs by enhancing their ability to identify and correct errors, researchers have developed various methods to improve their self-correction capabilities. (Wang et al., 2023a) verifies answers by integrating inputs from both humans and other models. (Weng et al.) employs backward verification to evaluate and score multiple candidate answers generated during a tree-of-thought reasoning process. (Li et al., 2024) enables models to effectively distinguish between confident and uncertain responses using a simple "Self-Verifying" prompt (e.g., "If you are very confident about your answer, maintain your answer. Otherwise, update your answer"). (Zheng et al., 2024) relies on ground truth to determine if a question needs to be answered again. (Chen and Li, 2024) identifies and corrects errors by having the LLMs analyze the intermediate steps of a CoT for mistakes and pinpoint the source of the error. While these methods have improved

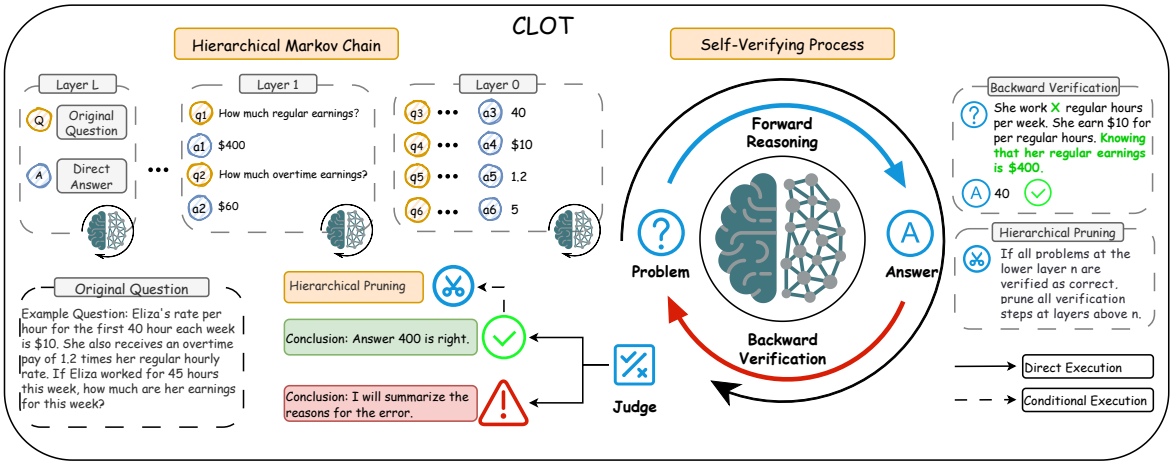


Figure 1: Overview of the CLoT Framework.

self-correction to varying degrees, they often face the challenges summarized by (Yang et al., 2024): (1) reliance on high-quality external feedback, (2) lack of comparison with baselines that consume the same number of tokens, and (3) prompts that are strictly designed and potentially complex.

To address these challenges, we propose the CLoT. Our approach achieves self-correction without requiring any external high-quality feedback. It demonstrates a significant performance improvement compared to a baseline with equivalent token consumption and operates in a zero-shot manner, eliminating the need for designing complex prompt examples.

3 Method

In this section, we provide a detailed description of the design of the CLoT method. CLoT guides the model to perform backward verification, identifies potential failures in backward verification, and ultimately summarizes the causes of errors and corrects them. Additionally, we construct a CLoT-Instruct Dataset based on the CLoT approach to help train models to learn "Backward Verification" approach.

3.1 Reversible Hierarchical Markov Chain

The architecture of CLoT is illustrated in Figure 1. The left panel delineates the Hierarchical Markov Process, where the top tier comprises the initial problem and its corresponding answer generated via direct CoT reasoning; subsequent layers execute iterative, step-by-step verification. The right panel details the backward verification mechanism: the model-generated answer is reformulated as a premise, while a specific condition from the original problem is selected by the LLMs to serve as a target variable for backward inference. For non-numerical tasks, the model identifies and validates key semantic entities. By reasoning through this reconfigured problem, CLoT determines whether the reconstructed condition aligns with the original input. This dual-loop design empowers CLoT to not only detect erroneous outputs but also to locate and rectify reasoning flaws, thereby substantially bolstering the model's interpretability, safety, and reliability.

For a mathematical problem q, we observe that successful reasoning involves not only a sequential simplification of the problem through derivation steps but also an implicit hierarchical organization of cognitive processes—such as conceptual abstraction, subproblem decomposition, and strategic planning. To capture this structure, we propose a Hierarchical Markov Chain framework, which models reasoning as a multi-level stochastic process where each level corresponds to a distinct granularity of problem understanding or solution strategy. Let the original problem be denoted by $q_1^{(L)}$ at the max layer $l = L$. At each lower layer $l < L$ (down to $l = 1$), the problem is refined into increasingly concrete and actionable representation $q_t^{(l)}$, forming a hierarchical structure that transitions from abstract strategies to specific derivations. State transitions within each layer satisfy the Markov property, while cross-layer transitions are jointly governed by top-down refinement and bottom-up generalization mechanisms. Specifically, given a state $q_{t-1}^{(l)}$ and a derivation step $s_{t-1}^{(l)}$ at layer l , the

next state is generated via:

$$p(q_t^{(l)} \mid q_{t-1}^{(l)}, s_{t-1}^{(l)}), \tag{1}$$

and inter-layer propagation is modeled as:

$$p(q_t^{(l+1)} \mid q_t^{(l)}) \quad \text{(abstraction)}, \tag{2}$$

$$p(q_t^{(l)} \mid q_t^{(l+1)}) \quad \text{(refinement)}, \tag{3}$$

this hierarchical structure allows the model to maintain long-range dependencies across reasoning steps through high-level semantic anchors, while still enabling local decision-making at fine-grained levels. Crucially, unlike standard Markov chains, we introduce reversibility in the reasoning trajectory by incorporating a backward verification process, ensuring logical consistency and reducing error accumulation.To quantitatively assess the reliability of a generated reasoning path $\tilde{q}_1 \to \cdots \to \tilde{q}_T \to a$, we propose a bi-directional coherence score rather than a standard training objective. Specifically, we evaluate the joint likelihood of the derivation steps s_t and states $\tilde{q}_t$ through the following scoring metric:

$$\begin{aligned} \mathcal{S}_{\text{RHMC}} = &\sum_{t=1}^{T} \log p(s_t, \tilde{q}_{t+1} \mid \tilde{q}_t) \\ &+ \sum_{t=1}^{T} \log p^{\leftarrow}(s_t, \tilde{q}_t \mid \tilde{q}_{t+1}). \end{aligned} \tag{4}$$

This metric aggregates two complementary perspectives:

- **Forward Consistency** $\log p(s_t, \tilde{q}_{t+1} \mid \tilde{q}_t)$: Measures the deductive validity of deriving the next state $\tilde{q}t + 1$ from the current state $\tilde{q}_t$, reflecting the model's confidence in its local decision-making.
- **Backward Justification** $\log p^{\leftarrow}(s_t, \tilde{q}_t \mid \tilde{q}_{t+1})$: Evaluates whether the preceding state $\tilde{q}_t$ can be logically reconstructed given the result $\tilde{q}_{t+1}$. This acts as a semantic check: "Is the premise necessary and justifiable given the conclusion?"

Ideally, a valid reasoning step should exhibit high probability in both directions. The backward term is not merely an inverse operation but a semantic-level backtracking mechanism that assesses whether the predecessor state $\tilde{q}_t$ remains consistent if the consequent $\tilde{q}_{t+1}$ holds true. By integrating these directional checks, CLoT provides a fine-grained diagnostic signal to identify invalid assumptions or non sequiturs without requiring external supervision or parameter updates.

3.2 Hierarchical Pruning

Building upon the RHMC framework, we introduce a Consistency-Aware Hierarchical Pruning strategy. This method exploits the dependency structure of hierarchical reasoning to minimize computational redundancy while maintaining rigorous verification standards.

The fundamental assumption is that global semantic consistency at the highest abstraction level serves as a high-fidelity proxy for the validity of the underlying granular steps. Unlike traditional forward-only models where a correct plan might mask local arithmetic errors, CLoT utilizes a backward reconstruction mechanism ($p^{\leftarrow}$). Since the top-most layer represents the most complete task representation (mapping the final conclusion back to the initial query), a high consistency score $\mathcal{V}^{(L)}$ implies that the entire reasoning trajectory has formed a closed logical loop. In this context, if the "global loop" is verified, the probability of a "locally-broken but globally-consistent" error—such as a lucky guess or a self-canceling calculation error—is statistically minimized.

Formally, consider a reasoning hierarchy with L layers. We define the backward consistency metric $\mathcal{V}^{(l)}$ for layer l as the aggregate reconstruction likelihood:

$$\mathcal{V}^{(l)} = \sum_{t=1}^{T_l} \log p^{\leftarrow}(s_t^{(l)}, \tilde{q}_t^{(l)} \mid \tilde{q}_{t+1}^{(l)}) \tag{5}$$

where T_l is the number of steps in layer l. This metric acts as a rigorous gatekeeper rather than a soft heuristic. We implement a dynamic protocol that prioritizes "Global Confirmation" before "Local Scrutiny":

Macro-Verification (Top Layer L): The system first computes $\mathcal{V}^{(L)}$. Because Layer L encapsulates the comprehensive logic of the problem, a successful verification here indicates that the final output is logically anchored to the input. If $\mathcal{V}^{(L)} > \tau$ (where τ is a strict confidence threshold), the system considers the reasoning chain robust and prunes all lower-layer verification ($l < L$). This reflects the insight that if the "big picture" is mathematically and logically reconstructible, the fine-grained derivations are implicitly validated.

Recursive Refinement: If $\mathcal{V}^{(L)}$ fails verification, it signals a potential "hallucination" or a "logical

gap" that the abstract layer cannot resolve. The system then descends to Layer $L-1$ to perform a granular, step-by-step validation. This process repeats until consistency is either confirmed at a more detailed level or the system identifies a specific step-wise failure in the finest-grained layer.

To address concerns regarding subtle low-level errors (e.g., arithmetic slips in a correct plan), CLoT's pruning is not purely plan-based but outcome-dependent. If a low-level arithmetic error leads to an incorrect final answer, the backward reconstruction at the top layer will inevitably fail ($p^{\leftarrow} \approx 0$), thus triggering a mandatory descent into fine-grained verification. This hierarchical gatekeeping ensures that pruning only occurs when the reasoning is "correct for the right reasons" across the entire semantic scope.

3.3 CLoT-Instruct Dataset

3.3.1 Dataset Construction

Building upon the theoretical framework of the RHMC, we introduce CLoT-Instruct, a specialized instruction-tuning dataset designed to train language models with bidirectional reasoning and self-verification capabilities. Unlike conventional cot datasets that focus solely on forward reasoning, CLoT-Instruct explicitly encodes the backward verification mechanism central to our CLoT framework, enabling models to develop intrinsic self-consistency checking abilities.

Theoretically, our construction methodology is applicable to any mathematical reasoning dataset, as it does not rely on any specific problem type but instead builds upon a general hierarchical reasoning structure and bidirectional verification logic. Currently, we have implemented and released three high-quality subsets based on this approach, using GSM8K, SVAMP, and AddSub as the foundational datasets. The construction of CLoT-Instruct follows a two-stage pipeline designed to jointly ensure the quality of forward reasoning and the integrity of backward verification:

- Forward Reasoning: Creation of hierarchical problem-solving trajectories
- Backward Verification: Generation of logically inverted validation questions

3.3.2 Dataset Structure

Formally, let $\mathcal{D}_{\text{origin}}$ denote the original mathematical reasoning dataset, where each instance follows the format $\tau_1 = (q_1, s_{1:T}, a)$. Here, q_1 represents the initial problem, $s_{1:T}$ denotes a sequence of T reasoning steps ($T \geq 1$), and a is the final answer.

In contrast to conventional approaches that treat the entire reasoning chain as a monolithic unit, our CLoT framework explicitly decomposes reasoning into hierarchical components, each augmented with bidirectional verification signals. To support this, we construct the CLoT-Instruct dataset, in which every sample is uniformly structured as:

$$\mathcal{X} = \Big(q_{\text{origin}},\ a_{\text{gt}},\ \{\tau^{(l)}\}_{l=0}^{L},\ max\_layer\Big), \quad (6)$$

where q_{origin} is the original problem, and a_{gt} is its ground-truth answer. max_layer denotes the maximum reasoning depth required. For each layer $l \in \{0, 1, \ldots, L\}$, $\tau^{(l)}$ represents the reasoning trajectory at that layer, defined as

$$\tau^{(l)} = \Big(q^{(l)},\ s^{(l)}_{1:T_l},\ \big\{(q^{(l)}_{\text{verify},t},\ a^{(l)}_{\text{verify},t})\big\}_{t=1}^{T_l}\Big), \quad (7)$$

where $q^{(l)}$ is the problem at layer l (either the original question or a sub-question), $s^{(l)}_{1:T_l}$ is its sequence of reasoning steps, and each pair $(q^{(l)}_{\text{verify},t}, a^{(l)}_{\text{verify},t})$ constitutes a bidirectional verification instance: $q^{(l)}_{\text{verify},t}$ is a logically inverted question derived from the forward step, and $a^{(l)}_{\text{verify},t}$ is its expected answer. This unified representation enables hierarchical dependency tracking, dynamic verification, and scalable supervision across reasoning depths—while maintaining a consistent and extensible data schema.

In this section, we conduct comprehensive experiments to thoroughly investigate CLoT through extensive benchmark evaluations on six standard datasets, efficiency analysis, data result analysis, and ablation studies.

4 Experiment

4.1 Experimental Settings

4.1.1 Datasets

We evaluate CLoT using gpt-4o-mini, gpt-4-1106-preview and deepseek-v3 as backbone models. Our evaluation covers three types of reasoning tasks: mathematical QA reasoning (MATH_{900}, (Hendrycks et al., 2021), GSM8K_{1319}, (Cobbe et al., 2021), Addsub_{395}, (Hosseini et al., 2014), and SVAMP_{1000}, (Patel et al., 2021)), mathematical multiple-choice (AQUA_{254}, (Ling et al., 2017)), and commonsense reasoning ($\text{CommonsenseQA}_{1220}$, (Talmor et al., 2019)). For

Models	AddSub	GSM8K	SVAMP	MATH	AQuA	CSQA	Avg.
gpt-4o-mini							
CoT	94.9	90.9	93.4	78.3	81.4	81.5	86.7
CoT-SC(n=5)	96.1	92.0	93.5	81.0	83.1	83.4	88.3
AR	82.3	91.7	92.4	73.1	77.5	78.7	81.0
C-CoT	97.2	92.4	93.4	76.9	83.3	81.0	87.4
ISP-CoT	96.1	92.4	93.9	77.9	83.7	81.9	87.7
CLoT(ours)	99.0	94.6	94.9	80.7	85.8	82.3	89.6
gpt-4							
CoT	98.0	93.1	93.4	73.0	82.7	84.9	87.5
CoT-SC(n=5)	98.4	94.2	93.5	81.6	83.1	85.6	89.4
AR	87.1	93.4	92.7	73.1	79.5	79.1	84.2
C-CoT	98.4	94.2	93.6	80.6	82.7	83.9	88.9
ISP-CoT	97.7	93.3	93.5	77.7	84.2	83.4	88.3
Tr	97.5	94.2	91.3	71.9	79.9	79.4	85.7
CLoT(ours)	99.0	95.4	95.0	81.6	86.9	84.9	90.5
deepseek-v3							
CoT	97.7	94.1	93.9	90.2	84.2	81.1	90.2
CoT-SC(n=5)	98.5	94.5	94.3	91.3	87.4	82.2	91.4
AR	93.9	93.3	93.1	89.7	86.6	81.0	89.6
C-CoT	97.9	94.2	93.8	89.7	88.1	81.2	90.5
CLoT(ours)	99.0	95.5	95.6	91.7	91.8	82.6	92.7

Table 1: Accuracy of CLoT and baselines on six mainstream datasets. Higher is better for all metrics. The best score, and second best score are red, and orange, respectively.

the large datasets Math and SVAMP, we adopt the same data processing procedure as in Study (Chen and Li, 2024), evaluating the first 900 and 1,000 questions from their respective test sets. On mathematical datasets, CLoT employs exact numeric matching—i.e., an answer is considered correct only if it exactly matches the numeric value in the original question. On commonsense datasets, it uses synonym-based judgment—i.e., an answer is deemed correct if it is a synonym or near-synonym of the answer in the original question.

4.1.2 Baseline

Our baselines include classical prompting methods (CoT, (Kojima et al., 2022)), CoT with Self-Consistency (CoT-SC, n = 5, (Wang et al., 2023b)), CoT with Iterative Summarization Pre-Prompting (ISP-CoT, (Zhu et al., 2025)), Analogical Reasoning (AR, (Yasunaga et al., 2024)), Complex-CoT (C-CoT, (Fu et al., 2023)) and Thought Rollback (Tr, (Chen and Li, 2024)).

4.2 Main Results

Table 1 summarizes the performance of CLoT and various baselines across six benchmarks using three different model backbones: GPT-4o-mini, GPT-4, and DeepSeek-V3. Overall, CLoT consistently demonstrates competitive performance, outperforming all competitive baselines in terms of average accuracy.

Under the GPT-4o-mini setting, CLoT achieves an average accuracy of 89.6%, surpassing the most competitive baseline, CoT-SC (n=5), by a margin of 1.3%. Notably, CLoT establishes new performance ceilings on AddSub (99.0%), GSM8K (94.6%), SVAMP (94.9%), and AQuA (85.8%), demonstrating its robust reasoning capabilities across both straightforward arithmetic and complex multi-step reasoning tasks.

When evaluated on the more powerful GPT-4 backbone, CLoT further extends its lead, attaining the highest average accuracy of 90.5%. Compared to the best-performing baseline, it delivers substantial gains on GSM8K (+1.2%), SVAMP (+1.5%), and AQuA (+3.8%). These results underscore CLoT's ability to effectively leverage its iterative generate-and-verify mechanism to rectify subtle errors in the reasoning chain, particularly in challenging datasets like AQuA.

Furthermore, CLoT demonstrates superior scalability and generalization on DeepSeek-V3, achieving a peak average accuracy of 92.7%. The consistent improvements across diverse tasks—ranging from symbolic arithmetic (AddSub) to complex

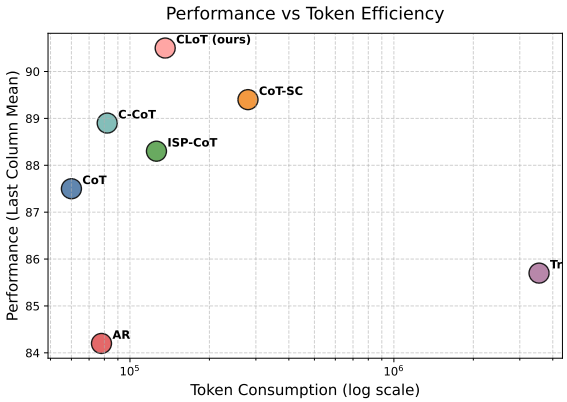


Figure 2: The results of CLoT efficiency. The token consumption corresponds to the total number of tokens used to solve the same 100 gsm8k problems (idx0 – idx99).

mathematical reasoning (MATH) and commonsense QA (CSQA)—validate the effectiveness and versatility of our proposed verification-driven framework.verification-driven framework.

4.3 Efficiency Analysis

We further evaluate the efficiency of different methods in terms of token consumption. The results are shown in Figure 2 and were obtained using the gpt-4o-mini API. Traditional methods such as CCoT and CoT-SC consume approximately 280k tokens. In contrast, Tr uses chain-of-thought for self-verification and requires as many as 3.3M tokens, resulting in very high computational costs. AR is more token-efficient, using only 78k tokens. However, its overall performance still lags behind other approaches. Notably, CLoT achieves performance on par with or even better than existing methods while consuming just 136k tokens. This highlights its strong reasoning efficiency under low token overhead. This efficiency stems from its hierarchical pruning strategy, which selectively removes redundant verification steps at lower reasoning layers. This design enables high reasoning efficacy with minimal token overhead, making CLoT particularly suitable for large-scale and resource-constrained applications.

4.4 Datasets Analysis

To systematically evaluate our model's verification capability on mathematical reasoning, we built verification datasets from four standard math QA benchmarks: AddSub, SVAMP, GSM8K, and AQuA (see Figure 3). We analyze four key metrics:

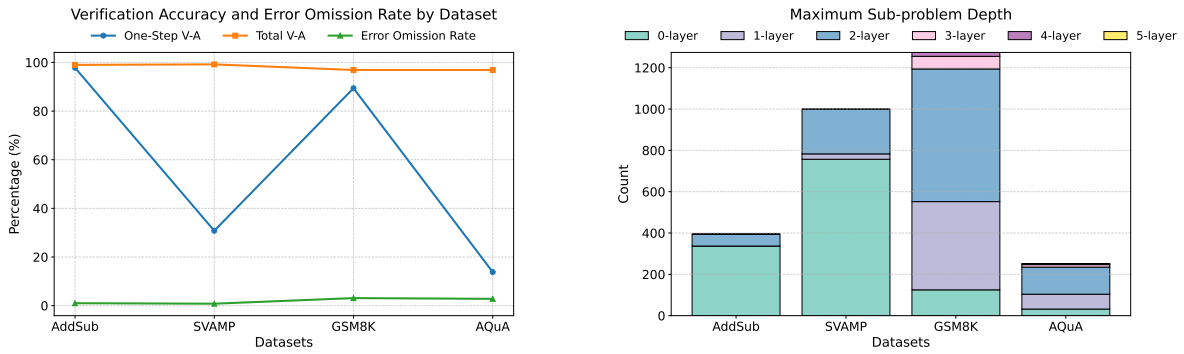
- One-Step Verification Accuracy: the fraction of problems whose initial solution is both correct and verified on the first attempt.
- Total Verification Accuracy: the proportion of problems that are either correctly solved or whose errors are successfully detected.
- Error Omission Rate: the fraction of incorrect solutions missed by the verifier.

One-Step Verification Accuracy is high on AddSub (97.8%) and GSM8K (89.4%), indicating strong self-verification on problems with simple or clear reasoning paths. It drops sharply on SVAMP (30.8%) and AQuA (13.8%), reflecting the difficulty of generating verifiable solutions in a single pass for semantically complex or multi-step problems—often requiring iterative refinement.

In contrast, Total Verification Accuracy remains consistently high across all datasets, demonstrating that CLoT reliably ensures output correctness by either producing correct answers or flagging errors. Correspondingly, the Error Omission Rate is low, confirming the verifier's high recall. Notably, AQuA achieves an omission rate of only 2.8%, comparable to GSM8K, despite its low one-step accuracy. This highlights the effectiveness of multi-round verification in catching errors even from poor initial solutions. Finally, the maximum layer counts are shown in Figure 3b. The results indicate that AddSub and SVAMP have at most two layers of subproblems, whereas GSM8K and AQuA exhibit three or more layers, demonstrating that more challenging tasks require multiple rounds of the "generate-and-verify" cycle.

4.5 Ablation analysis

To systematically evaluate the effectiveness of each component in our proposed method, we conduct a series of ablation studies using the gpt-4o-mini model. As shown in Table 2, we incrementally introduce four key designs: (1) standard Chain-of-Thought (CoT) with a single direct answer verification (CoT + Self-Verifying, or CoT + SV), serving as the baseline; (2) CoT enhanced with Hierarchical Markov Chain decomposition (CoT + HMC) without any verification, to assess the benefit of structured reasoning alone; (3) CoT with Reversible Hierarchical Markov Chain (CoT + RHMC), which adds step-by-step verification at each reasoning level to improve overall reliability; and (4) CoT + RHMC further augmented with



(a) (b)

Figure 3: We present a visualization of the dataset analysis. Figure (a) shows the various accuracy metrics on the dataset, where V-A denotes Verification Accuracy. Figure (b) shows the maximum number of layers in the multi-layer Markov chains used in the dataset.

Models	Token	AddSub	GSM8K	SVAMP	AQuA	Avg.
CoT (baseline)	60k	94.9	90.9	93.4	81.4	90.2
CoT + SV	98k	92.0	93.5	87.3	81.4	88.6
CoT + HMC	112k	94.9	90.9	93.4	81.0	90.1
CoT + RHMC	325k	94.4	93.5	93.9	84.6	91.6
CoT + RHMC + HP	136k	99.0	94.6	94.9	85.8	93.6

Table 2: Ablation study results of CLoT based on gpt-4o-mini. The experiment used four datasets and token consumption to evaluate the contributions of three components. The token consumption corresponds to the total number of tokens used to solve the same 100 GSM8K problems (idx0 – idx99).

Hierarchical Pruning (HP), where lower-level verification steps are skipped once all subproblems at a higher level are confirmed correct.

The results show that CoT + SV achieves limited performance across datasets, with an average accuracy of 88.6%. Adding the HMC structure yields slightly unstable results but produces more organized reasoning paths. With RHMC, the model shows clear improvements on AddSub, GSM8K, and SVAMP, reaching an average accuracy of 91.6%. Finally, our full method (CoT + RHMC + HP) further boosts average accuracy to 93.6% while reducing total token consumption from 325k to 136k (41.8%). This demonstrates that hierarchical pruning effectively balances efficiency and performance. Overall, the results confirm the importance of layered verification and dynamic pruning in complex reasoning tasks.

5 Conclusion

In this paper, we introduced Cognitive Loop of Thought (CLoT), a novel reasoning framework that addresses the inherent "memorylessness" and error propagation issues in traditional Chain-of-Thought (CoT) prompting. By modeling the reasoning process as a Reversible Hierarchical Markov Chain (RHMC), we bridge the gap between sequential token generation and human-like cognitive verification. Our core contribution, the backward verification mechanism, enables LLMs to treat reasoning as a closed loop, where conclusions are validated by reconstructing original premises. To ensure this process remains computationally viable, we implemented a hierarchical pruning strategy that leverages the dependency structure of subproblems to bypass redundant checks. Our experiments across six benchmarks demonstrate that CLoT consistently achieves state-of-the-art performance, notably reaching 99.0% accuracy on the AddSub dataset. Furthermore, our ablation studies confirm that the synergy between reversible logic and hierarchical pruning allows for a 41.8% reduction in token overhead without sacrificing reasoning integrity. The release of CLoT-Instruct provides a foundational resource for the community to further explore bidirectional instruction tuning. We believe that shifting from purely forward-moving chains to cognitive loops is a critical step toward developing more reliable, self-correcting, and autonomous reasoning agents.

Limitations

This study has two main limitations. First, CLoT relies on the model's intrinsic ability to perform backward reasoning. Our experiments show that while large-scale models like GPT-4o excel at this, smaller or less capable models may struggle with the logical inversion required for effective self-verification, potentially leading to false negatives during the pruning process. second, our current evaluation focuses primarily on mathematical, logical, and commonsense reasoning tasks where conclusions are relatively deterministic. In more subjective or open-ended tasks, such as creative writing or legal argumentation, defining a clear backward verification logic is more challenging, as there may not be a unique set of premises that lead to a specific conclusion.

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A datasets

A.1 Mathematical Reasoning Datasets

We evaluate CLoT on four mathematical QA datasets and one multiple-choice dataset:

1) MATH & SVAMP: Given the extensive size of these benchmarks, we follow the established data processing procedure from prior research (Chen and Li, 2024), specifically evaluating the first 900 samples of MATH and the first 1,000 samples of SVAMP to ensure consistent comparison.

2) GSM8K & AddSub: We utilize the full test sets (1,319 and 395 samples, respectively) to assess the model's ability to handle grade-school level multi-step arithmetic word problems.

3) AQuA: A mathematical multiple-choice dataset requiring algebraic reasoning. This helps evaluate CLoT's performance when the solution space is constrained by predefined options.

A.2 Commonsense Reasoning Dataset

CommonsenseQA (CSQA): We use 1,220 samples from CSQA to test the framework's ability to leverage world knowledge and semantic relationships.

B Answer Formation

The following section illustrates the multi-stage reasoning process of CLoT, where discrete steps are facilitated through Chain-of-Thought (CoT) prompting. Specifically, Tables 5 and 6 exemplify the detailed reasoning trajectories for mathematical problems. To ensure consistency and facilitate evaluation, the final output generation phase adheres to the standardized formats presented in Table 4.

C Algorithm

This section delineates the procedural execution of the **Cognitive Loop of Thought** (CLoT) framework, as formalized in Algorithm 1. The efficacy of CLoT stems from its structured hierarchical state transitions and a specialized reversibility-based scoring mechanism, which is theoretically grounded in Reversible Hierarchical Markov Chains (RHMC).

Dataset	Reasoning Task	Answer Type	Example	Number
MATH (Hendrycks et al., 2021)	Mathematical QA	Number	4	900
GSM8K (Cobbe et al., 2021)	Mathematical QA	Number	4	1,319
AddSub (Hosseini et al., 2014)	Mathematical QA	Number	4	395
SVAMP (Patel et al., 2021)	Mathematical QA	Number	4	1,000
AQuA (Ling et al., 2017)	Mathematical MC	Multi-choice	4	254
CommonsenseQA (Talmor et al., 2019)	Commonsense	Multi-choice	4	1,220

Table 3: Overview of datasets utilized in CLoT experiments.

Task	Answer-format Instructions
GSM8K, SVAMP, AddSub, math	You can freely reason in your response, but please enclose the final answer within <answer></answer>tags(pure number without units and explanations)
AQuA, CommonsenseQA	You can freely reason in your response, but please enclose the final option within <answer></answer>tags(pure uppercase option without explanations)

Table 4: Answer-format instructions for different tasks.

SVAMP Problem
Q: Kylar went to the store to buy glasses for his new apartment. One glass costs $5, but every second glass costs only 60% of the price. Kylar wants to buy 16 glasses. How much does he need to pay?
Step 1, First CoT
Q: Lets think step by step. ***Thought*** <answer> 64 </answer>
Step 2, Backward Verification
Q: Please replace one numerical value in the original problem with X and incorporate the answer as a known condition. Kylar went to the store to buy glasses for his new apartment. One glass costs X, but every second glass costs only 60% of the price. Kylar wants to buy 16 glasses. Knowing that he need to pay $64 for them. What's the X?
Step 3, Solve the new problem
Q: Lets think step by step. ***Thought*** <answer> 5 </answer>
Step 4, Judge
$5 = 5$
Answer: 64

Table 5: Examples of Successful Verification by CLoT on Mathematical Problem Datasets.

SVAMP Problem
Q: Kylar went to the store to buy glasses for his new apartment. One glass costs $5, but every second glass costs only 60% of the price. Kylar wants to buy 16 glasses. How much does he need to pay?
Step 1, First CoT
Q: Lets think step by step. ***Thought*** <answer> 96 </answer>
Step 2, Backward Verification
Q: Please replace one numerical value in the original problem with X and incorporate the answer as a known condition. Kylar went to the store to buy glasses for his new apartment. One glass costs X, but every second glass costs only 60% of the price. Kylar wants to buy 16 glasses. Knowing that he need to pay $64 for them. What's the X?
Step 3, Solve the new problem
Q: Lets think step by step. ***Thought*** <answer> 10 </answer>
Step 4, Judge
$4 \neq 5$
Step 5, Decompose sub-problems
Q: You are teasked with breaking down a math problem reasoning process into sub-problems. q1, q2, q3,...
Step 6, For each subproblem, iteratively execute Steps 1–4.
If all subproblems at the same level pass verification, exit the loop.
Step 7, Second CoT
Q: Lets think step by step. Please refer tp the following sub-problems and sub-answers. ***Thought*** <answer> 64 </answer>
Answer: 64

Table 6: Examples of CLoT's verification failures on mathematical problem datasets.

Algorithm 1: CLoT Reasoning

Input: Original problem $q_1^{(L)}$ at top layer L
Output: Reasoning trajectory $\{\tilde{q}_1, \ldots, \tilde{q}_{T+1}\}$ and score $\mathcal{L}_{\text{RHMC}}$

Initialization: Set $t \leftarrow 1$, current layer $l \leftarrow L$, and initial state $q_1^{(L)}$;
while $t \leq T$ **do**
    `// Intra-layer transition`
    Sample next state $q_t^{(l)} \sim p(q_t^{(l)} \mid q_{t-1}^{(l)}, s_{t-1}^{(l)})$;
    `// Cross-layer propagation`
    for $l = L$ **to** 1 **do**
        Refine: $q_t^{(l)} \sim p(q_t^{(l)} \mid q_t^{(l+1)})$;
        Abstract: $q_t^{(l+1)} \sim p(q_t^{(l+1)} \mid q_t^{(l)})$;
    end
    `// Record trajectory`
    Set $\tilde{q}_t \leftarrow q_t^{(l)}$ with derivation step s_t;
    $t \leftarrow t + 1$;
end
Forward path: $\tilde{q}_1 \rightarrow \cdots \rightarrow \tilde{q}_T \rightarrow a = \tilde{q}_{T+1}$;
Scoring with Reversibility:;
$\mathcal{L}_{\text{RHMC}} \leftarrow 0$;
for $t = 1$ **to** T **do**
    $\mathcal{L}_{\text{RHMC}} \leftarrow \mathcal{L}_{\text{RHMC}} + \log p(s_t, \tilde{q}_{t+1} \mid \tilde{q}_t)$;
    $\mathcal{L}_{\text{RHMC}} \leftarrow \mathcal{L}_{\text{RHMC}} + \log p^{\leftarrow}(s_t, \tilde{q}_t \mid \tilde{q}_{t+1})$;
end
return $\{\tilde{q}_1, \ldots, \tilde{q}_{T+1}\}, \mathcal{L}_{RHMC}$