# Markov Chain of Thought for Efficient Mathematical Reasoning

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# Abstract

Chain of Thought (CoT) of multi-step benefits from the logical structure of the reasoning steps and task-specific actions, significantly enhancing the mathematical reasoning capabilities of large language models. As the prevalence of long CoT, the number of reasoning steps exceeds manageable token limits and leads to higher computational demands. Inspired by the fundamental logic of human cognition, "derive, then reduce", we conceptualize the standard multi-step CoT as a novel Markov Chain of Thought (MCoT). In this study, we consider the mathematical reasoning task, defining each reasoning step as text accompanied by a Python code snippet. To facilitate a longer reasoning path, self-correction is enabled through interactions with the code interpreter. Our MCoT aims to compress previous reasoning steps into a simplified question, enabling efficient nextstep inference without relying on a lengthy KV cache. In our experiments, we curate the MCoTInstruct dataset, and the empirical results indicate that MCoT not only significantly enhances efficiency but also maintains comparable accuracy. While much remains to be explored, this work paves the way for exploring the long CoT reasoning abilities of LLMs.

# 1 Introduction

With the rapid advancement of large language models (LLMs), these models have demonstrated remarkable progress in a wide range of language tasks (Brown et al., 2020; Ouyang et al., 2022; Taori et al., 2023; Yang and Klein, 2021). However, they still face significant challenges when engaging in complex and symbolic reasoning tasks, particularly in mathematical reasoning (Cobbe et al., 2021; Hendrycks et al., 2021).

Most existing works have sought to enhance the mathematical reasoning capabilities of LLMs.

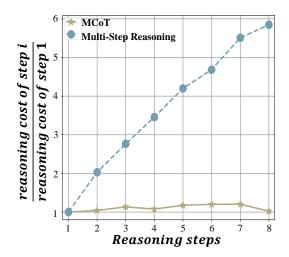


Figure 1: Comparison of reasoning efficiency between MCoT and Multi-Step Reasoning (MSR), showing the variation in reasoning time costs for both methods relative to *step 1* as the number of reasoning steps increases.

These efforts can be broadly categorized into two approaches: single-step reasoning (Yu et al., 2023; Yue et al., 2023) and multi-step reasoning (Gou et al., 2023; Wang et al., 2023a; Liao et al., 2024; Lu et al., 2024; Chen et al., 2024a,b). Single-step reasoning completes the reasoning task through one inferential step; Multi-step reasoning, which utilizes the reasoning traces (CoT) and task-specific actions (Code Interpreter), has been empirically demonstrated to boost the complex reasoning abilities of LLMs. Nevertheless, as the number of reasoning steps increases, Levy et al. (2024) finds that multi-step reasoning may become susceptible to accumulative errors or hallucinations. Furthermore, multi-step reasoning involving processing long CoT demands greater computational resources, which renders the inference process practically inefficient.

To address the inefficiency inherent in multi-step reasoning, our approach is deeply influenced by understanding how humans navigate complex reasoning tasks. Research on human cognition (Simon and Newell, 1971; Polya, 2004; Meadows, 2008)

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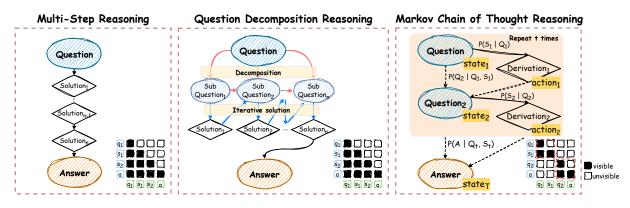


Figure 2: Schematic illustrating various approaches to mathematical reasoning with LLMs and their reasoning efficiency. The masked demonstrations across different approaches show that the efficiency of MCoT is similar to that of the blockwise masking approach, while the efficiency of MSR and question decomposition reasoning is more akin to that of the vanilla masking.

highlights two pivotal phases: derivation and re*duction*. When tackling a complex problem, the process often starts with deriving intermediate variables or partial solutions, rather than seeking an immediate full solution. These intermediate steps help clarify key aspects of the problem, which can then be simplified through reduction. The process of derivation and reduction is not linear but rather iterative. After each reduction, the newly simplified problem becomes an independent question, prompting further exploration for solutions. These new solutions could facilitate further reductions, gradually simplifying the problem and moving it toward the final answer. To formalize this reasoning process, we utilize the Markov chain to model the entire sequence of reasoning. This innovative approach is termed Markov Chain of Thought (MCoT).

The Markovian property has been explored in the mathematical proof of formal languages (FL), such as Lean (Moura and Ullrich, 2021). For example, executing a Lean tactic-equivalent to a reasoning step-transforms an original hypothesis (which may be none) into a new one while discarding the original. We aim to extend this idea to natural language (NL) for mathematical reasoning. Figure 2 illustrates the principle of MCoT approach. In MCoT, we initially frame the question as a particular state and consider the first derivation step as an associated action, then envision the complete solution as a sequential series of transitions between states. In contrast to question decomposition approaches (Zhou et al., 2022; Dua et al., 2022; Huang et al., 2023; Radhakrishnan et al., 2023), the Markov property inherent in MCoT framework guarantees that any state (question) can directly lead to the final answer. However, question decomposition breaks down a problem

into multiple sub-questions, each yielding only a partial answer. It is the cumulative aggregation of these partial answers that ultimately generates the final answer. Unlike multi-step reasoning, MCoT clears the KV cache of the context after simplifying questions, enabling it to support longer CoT. Therefore, MCoT offers the notable advantage that the reasoning's time or memory demands do not linearly or quadratically increase with the number of reasoning steps.

Empirically, we have developed a dataset specifically designed for MCoT reasoning, called MCoTInstruct. In order to maximize the utilization of existing data resources, we provide a reproducible pipeline starting from the multi-step reasoning datasets to construct the MCoT dataset. This dataset, originating from GSM8K (Cobbe et al., 2021) and MATH (Hendrycks et al., 2021), has been further refined through a combination of GPT-4 annotations and self-distillation processes.

In summary, Our contributions are as follows: **1.** We propose an innovative framework Markov Chains of Thought (MCoT), by exploiting the Markov property and envisioning the solution pro-

**2.** We constructed a MCoTInstruct dataset on mathematical reasoning task to facilitate research community.

cess as a series of transitions between states.

**3.** Extensive experiments demonstrate that, with a maximum number of eight steps, MCoT achieves an average reasoning efficiency that is  $1.90 \times$  faster than traditional multi-step reasoning and maintains superior to multi-step reasoning accuracy.

**4.** As MCoT provides a new pathway for exploring advanced reasoning abilities, we will release our dataset and code to facilitate further research and development within the community.

### Algorithm 1 Construction of the MCoT Seed Dataset

1:  $\mathcal{D}_{origin} \leftarrow Load$  initial GSM8K and MATH dataset

2: Define data format in  $\mathcal{D}_{\text{origin}}$ :  $\tau_1 = (\mathbf{q}_1, \mathbf{s}_{1:T}, \mathbf{a})$ , where T > 1.3: Train model  $M_{\text{verify}}$  using  $\mathcal{D}_{\text{origin}}$ 4:  $\mathcal{D}_{seed} = []$ 5:  $\mathcal{D}_{\text{origin}} = []$ 6: for each instance in  $\mathcal{D}_{origin}$  do 7: if T = 1 then 8: Add  $(\mathbf{q}_1, \mathbf{s}_1, \mathbf{a})$  to  $\mathcal{D}_{seed}$ Q٠ else 10: Use GPT-4 to generate reduced question  $q_2$  from  $(q_1, s_1)$ 11: Inference mode:  $M_{\text{verify}}(\mathbf{q}_2)$  to obtain  $(\mathbf{s}'_{1:T'}, \mathbf{a}')$ 12: if  $\mathbf{a}' = \mathbf{a}$  then ▷ Independence Test 13: Add  $(\mathbf{q}_1, \mathbf{s}_1, \mathbf{q}_2)$  to  $\mathcal{D}_{\text{seed}}$ Add new multi-step reasoning path  $\tau_2 =$ 14:  $(\mathbf{q}_2,\mathbf{s}'_{1:T'},\mathbf{a})$  to  $\mathcal{D}_{ ext{origin}}$ 15:  $\mathcal{D}_{\text{origin}} \leftarrow \tilde{\mathcal{D}}_{\text{origin}}$  then go to Line 5

# 2 Markov Chain of Thought Enable Mathematical Reasoning

#### 2.1 Markov Chain of Thought Reasoning

For mathematical problem  $\mathbf{q}$ , we assume that with each successful derivation step, the original problem can be incrementally simplified into a series of less complex problems, eventually leading to the final answer  $\mathbf{a}$ . Concretely, if we denote the original problem by  $\mathbf{q}_1$  and the first derivation step as  $\mathbf{s}_1$ , we can define the generation of new problems as  $p(\mathbf{q}_t | \mathbf{q}_{t-1}, \mathbf{s}_{t-1})$ . Consequently, the subsequent derivation step relies entirely on the newly formulated question. This indicates that the process adheres to the Markov property, which implies memorylessness (*i.e.*, the future state depends only on the current state and not on the sequence of events that preceded it).

$$p(\mathbf{s}_t | \mathbf{q}_{t' \le t}, \mathbf{s}_{t' < t}) = p(\mathbf{s}_t | \mathbf{q}_t)$$
(1)

For a question with T derivation steps, we are interested in maximizing the log-likelihood of the joint distribution of all steps. With the above assumption, we have the following objective.

$$\mathcal{L} = \log p(\mathbf{a}, \mathbf{s}_{1:T} | \mathbf{q}_1)$$
  
=  $\log \left( p(\mathbf{s}_1 | \mathbf{q}_1) \mathbb{E}_{\mathbf{q}_{2:T}} \left[ p(\mathbf{a} | \mathbf{q}_T, \mathbf{s}_T) \right] \right)$   
×  $\prod_{t=2}^T p(\mathbf{s}_t | \mathbf{q}_t) p(\mathbf{q}_t | \mathbf{q}_{t-1}, \mathbf{s}_{t-1}) \right]$  (2)

However, this objective is intractable due to the requirement of integrating latent variables  $q_{2:T}$ . As a surrogate, we turn to Monte Carlo integration, employing sampling techniques for feasibility. When we set the sampling size to 1, and if  $\tilde{\mathbf{q}}_{2:T}$  represents the sequence of sampled reduction questions of intermediate derivation steps, the objective  $\mathcal{L}$  can be approximated as follows.

$$\log \left( p(\mathbf{s}_{1} | \mathbf{q}_{1}) p(\mathbf{a} | \tilde{\mathbf{q}}_{T}, \mathbf{s}_{T}) \prod_{t=2}^{T} p(\mathbf{s}_{t} | \tilde{\mathbf{q}}_{t}) p(\tilde{\mathbf{q}}_{t} | \mathbf{q}_{t-1}, \mathbf{s}_{t-1}) \right)$$
Denote  $\mathbf{q}_{1} = \tilde{\mathbf{q}}_{1}$ ,  

$$= \log p(\mathbf{a} | \tilde{\mathbf{q}}_{T}, \mathbf{s}_{T}) + \sum_{t=1}^{T} \log p(\mathbf{s}_{t} | \tilde{\mathbf{q}}_{t})$$

$$+ \sum_{t=1}^{T-1} \log p(\tilde{\mathbf{q}}_{t+1} | \mathbf{q}_{t}, \mathbf{s}_{t})$$

$$= \log p(\mathbf{s}_{T}, \mathbf{a} | \tilde{\mathbf{q}}_{T}) + \sum_{t=1}^{T-1} \log p(\mathbf{s}_{t}, \tilde{\mathbf{q}}_{t+1} | \tilde{\mathbf{q}}_{t})$$
Denote  $\mathbf{a} = \tilde{\mathbf{q}}_{T+1}$ ,  

$$= \sum_{t=1}^{T} \log p(\mathbf{s}_{t}, \tilde{\mathbf{q}}_{t+1} | \tilde{\mathbf{q}}_{t})$$
(3)

In Eq. (3), the first equation unfolds the approximated loss into the summation of 2T independent log-likelihoods. The second equation applies expression re-organization with the rule of conditional probability  $p(\mathbf{s}_t | \mathbf{q}_t) p(\mathbf{q}_{t+1} | \mathbf{q}_t, \mathbf{s}_t) = p(\mathbf{s}_t, \mathbf{q}_{t+1} | \mathbf{q}_t)$ , resulted in *T* new independent log-likelihoods, signifying that these components can be optimized independently. The third equation is to rewrite the loss into a more concise representation. To sum up, if **multi-step reasoning** can be transformed into **multiple independent single-step reasoning**, the training and inference become very efficient. This is also the core intuition to build our dataset.

#### 2.2 MCoTInstruct Dataset

Our MCoTInstruct dataset is comprised of two components: the seed data, denoted as  $\mathcal{D}_{seed}$ , and the augmented self-distillation data, referred to as  $\mathcal{D}_{self}$ . To construct our dataset, we start from an available multi-step reasoning dataset, denoted as  $\mathcal{D}_{origin}$ , which includes the multi-step solutions from GSM8k and MATH datasets that have been further refined through GPT-4 annotations, e.g., MathCodeInstruct (Wang et al., 2023a). The data format of  $\mathcal{D}_{\text{origin}}$  is represented as  $\tau_1 =$  $(\mathbf{q}_1, \mathbf{s}_{1:T}, \mathbf{a})$ , where **a** stands for the final answer, and  $s_t$  signifies the intermediate derivation step at time t. Particularly, we assume that  $T \ge 1$ , implying the solution includes at least one derivation step. Furthermore, this derivation step adheres to the REACT (Yao et al., 2022) style, with customized <Text, Code, Observation> format that integrates text analysis with executable code blocks within the process of crafting a response, effectively enhancing the precision of reasoning.

**Seed data** To fully leverage available data resources, we have established a reproducible pipeline that iteratively extracts the required seed training instance and updates the multi-step reasoning dataset  $\mathcal{D}_{\text{origin}}$ . Algorithm 1 presents the overall pipeline designed to generate seed dataset.

First, we train a model based on DeepSeekMath 7B base model, denoted as  $M_{\text{verify}}$ , using the initially original dataset  $\mathcal{D}_{\text{origin}}$ . This model serves dual purposes: generation and verification. In the generation phase,  $M_{\text{verify}}$  produces multiple multistep solution samples for a given reduction question. During verification, if any final answer within these sampled solutions aligns with the answer to the original question, the corresponding reduction question is deemed acceptable.

Then, given an instance  $(\mathbf{q}_1, \mathbf{s}_{1:T}, \mathbf{a})$  in  $\mathcal{D}_{\text{origin}}$ , if T = 1, we directly incorporate this triplet  $(\mathbf{q}_1, \mathbf{s}_1, \mathbf{a})$  into our seed dataset. For other cases, we employ GPT-4-1106-preview (Achiam et al., 2023) to produce the reduction question  $q_2$  from  $(q_1, s_1)$ . The details of GPT-4 prompt can be found in Appendix I. We employ  $M_{\text{verify}}$  to assess whether  $q_2$  can yield the correct answer. If the outcome is accurate, it demonstrates that the reduction question is independent and does not rely on information from the previous questions and derivation steps, satisfying the required Markovian property. In this case, we include triplet  $(q_1, s_1, q_2)$  in the seed dataset, and a new multi-step reasoning pathway is generated as  $\tau_2 = (\mathbf{q}_2, \mathbf{s}'_{1:T'}, \mathbf{a})$ , which is then updated to the original dataset for the next round construction. This implies that we continuously iterate through the process to generate triplet data until we no longer obtain any multi-step reasoning solutions with a length exceeding two. Unlike previous works (Yue et al., 2023; Gou et al., 2023; Wang et al., 2023a; Liao et al., 2024), our approach relies solely on GPT-4 for generating a new question, typically a single sentence, instead of crafting a complete solution that includes text analysis and code snippets. Consequently, this method incurs significantly lower additional costs.

**Self-distillation** We fine-tune the DeepSeekMath 7B base model on the above seed data to obtain the MCoTModel-initial. Recognizing the limited scope of our seed data on the MATH dataset, we have adopted a self-distillation approach to

substantially enhance the coverage and diversity of the dataset. We employ MCoTModel-initial due to its capability to generate MCoT paths, achieving accuracy rates of 77.10% and 53.48% on the GSM8K and MATH datasets, respectively. Given <Question, Answer> pairs from the training sets of GSM8K and MATH, the initial model can generate Markov reasoning paths and obtain answers. We will verify the answers to form a self-distillation dataset  $\mathcal{D}_{self}$ . Furthermore, by utilizing MCoTModel-initial with <Question, Answer> pairs from any dataset, we can create a self-distillation dataset. In the Appendix F.1, we provide a detailed analysis of the impact of selfdistillation.

Combining seed data  $\mathcal{D}_{seed}$  and self-distilled data  $\mathcal{D}_{self}$ , we remove duplicate entries to form the MCoTInstruct dataset, which is denoted as  $\mathcal{D} = \text{filter}(\{\mathcal{D}_{seed}, \mathcal{D}_{self}\})$ . The dataset comprises 82k Markov chains, totaling around 160k entries, data format is shown in Appendix D.2. Uniquely, in contrast to prior studies, each training instance corresponds to the step level rather than the solution level that may include multiple steps, while Table 6 in the Appendix D compares our dataset with recently proposed mathematical reasoning datasets.

## **3** Discussion

The insight of MCoT is Markov chain, which frames the question as a particular state and considers the derivation step as an associated action. Unlike Multi-Step Reasoning (MSR), the MCoT does not depend on historical derivation steps; Furthermore, while question decomposition reasoning requires aggregating partial answers from each subquestion, any reduction question within MCoT can directly yield the final answer.

The core of MCoT lies in the Markov property, which implies memorylessness, the future state depends only on the current state, not on the sequence of events that preceded it. On one hand, we utilize Markov property to ensure that any state (or question) within a Markov Chain of Thought can directly lead to the final answer, significantly boosting efficiency within MCoT. On the other hand, when an error arises in an intermediate state, the memoryless feature of MCoT might propagate it, leading to errors in subsequent states as well. In contrast, traditional MSR is capable of accessing all previous historical contexts, potentially allowing it to correct intermediate errors. However, in our experiments, we empirically observed that MSR does not necessarily correct more intermediate errors than our proposed MCoT approach.

The motivation of MCoT, which introduces the Markov property into natural language mathematical reasoning, is inspired by the successful application of the Markov property in formal language systems, such as the lean programming language (Moura and Ullrich, 2021). In formal language systems, a statement consists of conditions and a conclusion, e.g.,  $h_1, h_2, h_3 \rightarrow c$ . The proof process involves stepwise reductions, where each step simplifies the statement by eliminating old conditions and adding new ones, e.g.,  $h_3, h_4 \rightarrow c$ . This allows us to focus only on the updated statement, ensuring that if the new statement is proven or solved, the original one is verified as well.

While the Markov property is theoretically sound in formal language mathematical reasoning, formal languages like lean are not easily accessible to non-experts. Therefore, we explore applying Markov property to natural language mathematical reasoning, which is more user-friendly. Our future work will also investigate combining natural language and formal language to balance rigor and readability.

# 4 **Experiments**

#### 4.1 Experimental Setup

**Implementation Details** We fine-tune DeepSeekMath-Base (Shao et al., 2024), LLemma (Azerbayev et al., 2023), and LLama-3 (AI@Meta, 2024) series (ranging from 7B to 70B) on the MCoTInstruct to evaluate the efficacy and accuracy of our MCoT framework. The implementation details are described in Appendix E.3.

**Datasets** We have selected diversity evaluation datasets, encompassing both in-domain and outof-domain datasets from various mathematical fields, to assess the models' capabilities in mathematical reasoning. For the in-domain test sets, we choose GSM8K (Cobbe et al., 2021) and MATH (Hendrycks et al., 2021). For the outof-domain test sets, we choose the open-source OCWCourses (Lewkowycz et al., 2022) dataset and GaoKao2023-Math-En (Liao et al., 2024) dataset. A comprehensive overview of these datasets is presented in Appendix E.1. **Metrics** We evaluate from two perspectives: reasoning **efficiency** and reasoning **accuracy**. To ensure fairness when evaluating reasoning efficiency, we measure the average amount of cached GPU memory used per sample during inference and design a metric E to measure the decoding time of each token in the average step.

$$E = \frac{1}{T} \sum_{t=1}^{T} \frac{\operatorname{time}_{t}}{\#\{\mathbf{s}_{t}\}}$$
(4)

where T is the number of steps, time<sub>t</sub> is the decoding time for step t, and  $\#{s_t}$  is the number of tokens at step t. For assessing reasoning accuracy, we utilize the mathematics evaluation toolkit in Zhang et al. (2024).

**Baselines** We compared proprietary, opensource, and math-specific models fine-tuned on mathematical reasoning datasets. Details are in Appendix E.2.

#### 4.2 Main Results

Accuracy Table 1 demonstrates our models outperform other open-source competitive mathsolving models, exhibiting a clear advantage across both in-domain datasets and out-of-domain datasets. Our model MCoT-DeepSeek is finetuned from the DeepSeekMath-Base<sub>7B</sub> on the MCoTInstruct dataset. Compared to the base model, our model achieves substantial gains on the GSM8k and MATH datasets, with improvements of about 12% and 24%, respectively. MCoT-DeepSeek achieve state-of-the-art results across all datasets, in 7B models.

Moreover, our model MCoT-DeepSeek achieves 55.8% on MATH dataset, which surpasses all 34B and 70B models on MATH dataset without any extra strategies, such as majority voting (Wang et al., 2022b). Notably, during the training phase in MCoT, the model is exposed only to triplet data like  $(\mathbf{q}_{t-1}, \mathbf{s}_{t-1}, \mathbf{q}_t)$  or  $(\mathbf{q}_T, \mathbf{s}_T, \mathbf{a})$ . It has never been trained on the complete solution data. However, when a question is presented to the model during the inference stage, it first attempts a single-step solution before deciding whether to further reduce the problem or deliver the final answer. In the reasoning stage, the model leverages the fragmented knowledge acquired during training to construct a complete Markov chain reasoning process from question to final answer.

**Efficiency** To intuitively evaluate the efficiency of different reasoning methods, we compare the

Model	Size	Data	Tool	Zero	In-do			of-domain
		Size		Shot	GSM8K	MATH	OCW	GK2023
	Pro	prietary l	Models					
GPT-4	-	-	X	X	92.0	42.5	-	-
GPT-4-Code	-	-	1	×	92.9	69.7	30.1	43.6
ChatGPT	-	-	×	×	80.8	35.5	-	-
ChatGPT(PAL)	-	-	$\checkmark$	×	78.6	38.7	-	-
PaLM-2	540B	-	×	×	80.7	34.3	-	-
	Oper	n-Source	Models					
Llama-2	7B	-	×	X	13.3	4.1	3.7	-
Llama-2 SFT	7B	-	×	1	41.3	7.2	-	-
Llama-2 RFT	7B	-	×	1	51.2	-	-	-
Llemma	7B	-	×	×	36.4	18.0	7.7	-
Llemma(PAL)	7B	-	$\checkmark$	×	40.1	21.5	-	-
CodeLlama	7B	-	×	×	10.5	4.5	4.4	-
CodeLlama(PAL)	7B	-	1	×	27.1	17.2	-	-
DeepSeekMath-Base(PAL)	7B	-	1	×	66.9	31.4	-	-
Llama-3	8B	-	×	×	54.8	21.3	-	-
CodeLlama	34B	-	×	×	29.6	12.2	7.0	-
CodeLlama(PAL)	34B	-	1	×	53.3	23.9	-	-
Llemma	34B	-	×	×	51.5	25.0	11.8	-
Llemma(PAL)	34B	-	$\checkmark$	×	62.6	27.1	-	-
	Single-st	ep reason	ning Mo	dels				
WizardMath	Llama2-7B	96k	×	1	54.9	10.7	-	-
MAmmoTH-Coder	CodeLlama-7B	260k	1	×	59.4	33.4	11.0	15.3
WizardMath	Llama2-70B	96k	×	1	81.6	22.7	-	-
MAmmoTH	Llama2-70B	260k	$\checkmark$	×	76.9	41.8	11.8	24.7
	Multi-ste	ep reasor	ning Mo	dels				
MathCoder	CodeLlama-7B	80k	1	1	67.8	30.2	-	-
ToRA-Code	CodeLlama-7B	69k	1	1	72.6	44.6	4.8	23.9
MARIO	Llemma-7B	82k	1	1	70.1	47.0	21.7	34.5
MathGenie	Llemma-7B	250k	1	1	76.0	48.3	-	-
MathCoder	Llama2-70B	80k	1	1	83.9	45.1	-	-
ToRA	Llama2-70B	69k	1	1	84.3	49.7	9.6	30.9
MathGenie	Llama2-70B	250k	1	1	88.4	51.2	-	-
	МСоТ	reasoni	ng Mod	els				
MCoT-DeepSeek	DeepSeekMathBase-7B	$82k^{\dagger}$	1	1	78.8	55.8	31.6	41.3
MCoT-Llemma	Llemma-7B	$82k^{\dagger}$	1	1	69.3	48.1	18.0	33.3
	Llama3-8B	$82k^{\dagger}$	1	1	76.9	47.4	8.8	32.7
MCoT-Llama3	Llama3-70B	82k <sup>†</sup>	· /	· /	83.1	54.7	19.9	38.7

Table 1: Results on different datasets. The best results of 7B open-source models are bold. \*GK2023 represents Gaokao-2023-Math-En dataset.  $82k^{\dagger}$  represents the count of Markov chains, encompassing approximately 160k step-wise entries. Conversely, data size in prior methods are accounted for by enumerating the complete trajectories of multi-step reasoning.

performance of multi-step reasoning (MSR) and MCoT reasoning. To ensure a fair comparison, all reasoning approaches utilize an external tool - Python code interpreter. The MSR model is fine-tuned on our initial multi-step reasoning dataset,  $\mathcal{D}_{origin}$ . The MCoT model is fine-tuned on our MCoTInstruct dataset. The MCoTInstruct dataset is extended from  $\mathcal{D}_{origin}$ , with both the source data and solutions preserved as consistently as possible to minimize the impact of dataset variations. Moreover, the maximum number of reasoning steps is set to 8.

Table 2 presents the comparative results of MSR and MCoT regarding reasoning efficiency and accuracy. Our observations are as follows: (1) Compared to single-step reasoning in Table 1, MSR and MCoT indeed significantly enhance reasoning accuracy. (2) Compared to MSR, MCoT demonstrates notable improvements in reasoning accuracy and efficiency. For instance, in the Llemma<sub>7B</sub> model, MCoT achieves improvements over MSR on both the MATH (+2.1%) and GSM8K (+2.2%) datasets. Furthermore, MCoT's inference efficiency from *E* is 1.90 times greater than that of MSR.

**Different base models and model sizes** We evaluated the effectiveness of the MCoT approach using three base models: DeepSeek, Llemma, and the

Base Model	Methods	GSM8K(†)	MATH(↑)	$E^{\S}(\downarrow)$	Cache Memory (GB) <sup><math>\dagger</math></sup> ( $\downarrow$ )
DeepSeekMath-Base7B	MSR	77.3	54.9	1.12	48.7
	MCoT	<b>78.8</b>	<b>55.8</b>	<b>0.60</b>	<b>30.2</b>
Llemma <sub>7B</sub>	MSR	67.1	46.0	1.18	37.9
	MCoT	<b>69.3</b>	<b>48.1</b>	<b>0.62</b>	<b>25.7</b>
Llama3 <sub>8B</sub>	MSR	73.4	45.1	1.23	55.6
	MCoT	<b>76.9</b>	<b>47.4</b>	<b>0.69</b>	<b>37.9</b>

Table 2: The comparison between multi-step reasoning (MSR) and MCoT on Accuracy and Efficiency.  $E^{\$}$  means the metric defined in Eq. (4). <sup>†</sup> indicates the average amount of cached GPU memory used per sample.

llama3 series. Tables 1 and 2 show that MCoT outperforms multi-step reasoning in accuracy across all models, with significantly smaller cache memory usage. To investigate the effectiveness across varying model scales, we scale up the Llama3 model size from 8B to 70B, observing notable performance improvements on all benchmarks. Specifically, we found that the Llama3 series performs poorly overall on the OCW dataset. In our analysis of the OCW dataset, detailed in Appendix E.1, we found that its format causes Llama3 to mistakenly interpret it as in-context learning, even after fine-tuning with MCoTInstruct dataset.

# 4.3 Analysis 1: Efficiency

**Efficient Training** Figure 3a illustrates the distribution of token length for the MCoTInstruct dataset and the multi-step reasoning instruction dataset  $\mathcal{D}_{\text{origin}}$ . In comparison, the token length of MCoT is noticeably shorter than that of MSR, with an average reduction of 135.91 tokens. The underlying reason is that MCoT is only trained on the  $(\mathbf{q}_{t-1}, \mathbf{s}_{t-1}, \mathbf{q}_t)$  triplets, whereas MSR requires training on the entire trajectory.

**Efficient Inference** To investigate the efficiency of MCoT during inference, we compare the average prompt length of MCoT and MSR as the number of reasoning steps increases on the MATH test set, using DeepSeekMath-Base as the base model. As shown in Figure 3b, there is a stark contrast in the average prompt length between MCoT and MSR. MCoT maintains a stable prompt length, unaffected by the increasing reasoning steps, while MSR exhibits a growing prompt length.

In MCoT, the average token length during the derivation stage remains under 128 tokens, while in the reduction stage, it stays below 512 tokens. This indicates that MCoT can tackle complex mathematical reasoning problems, such as those in the MATH dataset, using only a 512-token context

window. This significantly reduces memory and computational demands. In contrast, the average prompt length surpasses 2048 tokens by the seventh step in MSR, indicating a substantial increase in memory and computational requirements as the reasoning process progresses.

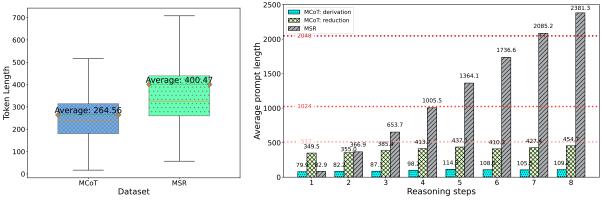
# 4.4 Analysis 2: Problem Solving

To assess MCoT's problem-solving capabilities, we analyze its performance on the MATH test set across various difficulty levels and subjects, calculating the success rate for each category. In Figure 4a, it is demonstrated that MCoT achieves a higher success rate in solving more challenging problems compared to MSR. We attribute this superior performance to MCoT's training method, which emphasizes derivation and reduction techniques rather than the complete reasoning path from question to answer. This approach enhances the model's generalization ability through autonomous and iterative problem-solving. Figure 4b shows that MCoT consistently excels in solving a broader range of problems across various subjects. More details and results w.r.t. other base models, such as Deepseek and Llama, are shown in Figure 8 and 9 in Appendix F.2.

## 4.5 Analysis 3: Hybrid training strategy

The MCoT approach notes that the model is not trained on full solution datasets, limiting its ability to generate complete solutions independently. To address this, we explore a hybrid training method that partially exposes the model to full solutions to assess performance improvements. We used the DeepSeekMath-Base-7B model, starting with a 2-epoch warm-up on a 27.4k multi-step reasoning dataset from GSM8K and MATH, followed by training on the MCoTInstruct dataset.

Table 3 shows that the hybrid training improves in-domain performance but performs worse on



(a) Token length distribution on training

(b) Average Prompt token Length on test set



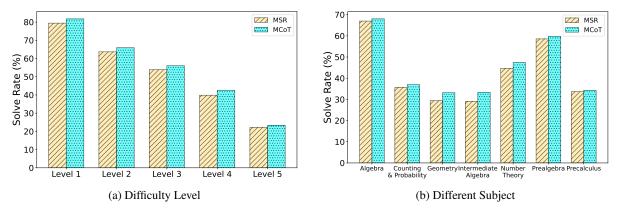


Figure 4: Comparison of problem solving between MCoT and MSR on MATH test set, with Llemma<sub>7B</sub> as base model.

OOD datasets compared to direct MCoT training. This may be due to overfitting caused by the inclusion of complete solution data, leading to weaker generalization. We will leave more exploration on how to train the LLM with mixed data as future work.

	GSM8K	MATH	OCW	GK2023
DeepSeekMath-Base	66.90	31.40	-	-
MSR-DeepSeek	77.30	54.90	27.94	38.96
MCoT-DeepSeek	78.80	55.80	31.60	41.30
Hybrid Training				
MSR-DeepSeekwarm-up	75.97	52.12	25.37	37.40
+ Continue <i>w.r.t.</i> MCoT	79.30	56.60	29.41	39.48

Table 3: The results on hybrid training strategy within DeepSeekMath-Base<sub>7B</sub> model.

# 4.6 Case study: Self-correction in MCoT

We provide a detailed case study in Appendix H to illustrate the reasoning process, highlighting MCoT's self-correction capabilities. Our experiments demonstrate that MCoT does not empirically propagate errors more significantly than traditional MSR frameworks. This is largely because MCoT incorporates a self-correction mechanism, as illustrated in Figure 10 and case study in Appendix H. Specifically, MCoT can summarize prior errors into the context of the next reasoning step and address them without needing to retain the full historical context.

# 5 Related Work

Chain of Reasoning LLMs have exhibited strong reasoning capabilities by utilizing Chain of Thought (Wei et al., 2022; Brown et al., 2020) prompting. Tree of Thoughts (ToT) (Yao et al., 2024) enables exploration over coherent units of thoughts that serve as intermediate steps toward problem-solving. Program of Thought (PoT) (Chen et al., 2022) enhances the capabilities of LLMs to use programs as thought processes. Several works (Zhou et al., 2022; Wang et al., 2022a; Li et al., 2023; Wang et al., 2023c,b) have developed CoT or PoT technology to employ LLMs to tackle reasoning tasks by allowing intermediate steps. It is important to note that in these methods, the intermediate steps are preserved as historical context, making them dependent. In contrast, our approach

leverages the inherent independence of the Markov chain to separate the intermediate steps.

Mathematical Reasoning Recent works (Wang et al., 2023a; Gou et al., 2023; Liao et al., 2024; Lu et al., 2024) have made significant advancements in enhancing reasoning capabilities within LLMs through the implementation of step-by-step natural language reasoning, achieving better results than single-step reasoning (Luo et al., 2023; Yu et al., 2023; Yue et al., 2023). In single-step reasoning, (Luo et al., 2023) and (Yu et al., 2023) utilize textual content as solutions, and (Yue et al., 2023) introduces a unique hybrid of CoT and PoT rationales. In multi-step reasoning, Wang et al. (2023a) and Gou et al. (2023) incorporate code snippets or tools within each step of the reasoning process, Liao et al. (2024) also adds text analysis based on the code snippets at each step. Nevertheless, as the number of reasoning steps increases, the multistep reasoning involves processing long contexts demands greater computational resources and a decline in reasoning drops (Levy et al., 2024). In our work, we utilize a process of derivation, then reduction in MCoT. This reduction step simplifies the historical questions and solutions into independent questions, enhancing clarity and efficiency.

# 6 Conclusion

This paper presents MCoT, an innovative Markov Chain of Thought framework for efficient multistep reasoning. Our framework leverages the independence of Markov chains, conceptualizing the solution process as a series of state transitions. This approach enables LLMs to address complex reasoning tasks more efficiently and intelligently. MCoT achieves superior performance on diverse mathematical reasoning tasks, substantially outperforming existing multi-step reasoning approaches in both efficiency and accuracy. Our work provides a new pathway for solving complex reasoning tasks.

# Limitations

The limitation of Markov Chain of Thought (MCoT) models primarily arises when an error occurs at an intermediate step, which can cascade and lead to failures in subsequent steps. This is due to the Markov property, which assumes that each step depends only on the current state, rather than on the sequence of events that preceded it. Consequently, errors are not corrected and may propagate through the chain, resulting in flawed conclusions. To address this limitation, integrating Monte Carlo Tree Search (MCTS) (Browne et al., 2012; Silver et al., 2016, 2017) could be a robust solution. By integrating MCTS with MCoT, we equip the reasoning models with the capacity for backtracking and learning from simulated explorations. This synergy not only addresses the original limitation of the MCoT concerning the independence assumption but also fortifies the model's ability to navigate complex problems more effectively. This potential direction is what we intend to explore in future work.

# **Ethical Considerations**

The MCoT framework introduces a novel paradigm for efficiently and intelligently handling complex reasoning tasks. Currently, our focus is on mathematical reasoning, Therefore, this work does not have direct negative social impacts. In our experiments, we used publicly available datasets widely employed in prior research, containing no sensitive information to the best of our knowledge. The authors have followed ACL ethical guidelines, and the application of this work poses no apparent ethical risks.

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# Appendix

A	Future Work	14
B	Real-world Applications	14
С	The reasoning process of Multi-step reasoning and MCoT	14
D	MCoTInstruct Dataset         D.1       Overview         D.2       Data Format	<b>14</b> 14 14
E	Experimental Details         E.1       Test Dataset	<b>14</b> 14 14 15
F	Additional Results and AnalysesF.1The Impact of Self-distillationF.2The Analysis on Problem-Solving	<b>15</b> 15 15
G	Dataset License	16
H	Case StudyH.1Case 1: Self-correctionH.2Case 2: Self-correctionH.3Case 3: Bad case	<b>19</b> 19 20 21
Ι	Prompt Template in GPT-4	23

# A Future Work

MCoT is a framework that empowers LLMs to more efficiently and intelligently in multi-step reasoning. MCoT framework can be applied to complex reasoning tasks, such as long context reasoning (Xiong et al., 2023; Caciularu et al., 2023; Chen et al., 2023). MCoT is capable of effectively reducing context information, thereby providing a practical and feasible approach for long context reasoning. This method filters and concentrates historical information, significantly improving the efficiency of processing and analyzing long context. Moreover, when integrated with the Retrieval-Augmented Generation (RAG) (Lewis et al., 2020; Gao et al., 2023b) technology, MCoT holds significant potential in understanding long context.

## **B** Real-world Applications

Inspired by the strict adherence to the Markov property in formal languages like lean, this work presents significant potential for real-world applications in formal reasoning processes. Our method aligns seamlessly with the detailed, stepby-step nature of formal proofs, such as the tactics used in lean. By generating natural language annotations for each step, our approach enhances the interpretability of complex formal arguments, showcasing its relevance to practical scenarios where both precision and human comprehension are paramount. In particular, this method could be applied in fields such as automated theorem proving, legal reasoning, and software verification, where clear, interpretable reasoning steps are crucial for both validation and decision-making.

# C The reasoning process of Multi-step reasoning and MCoT

Figure 5 illustrates the reasoning process using the Markov chain of thought and multi-step reasoning approaches. In multi-step reasoning, the KV cache is retained throughout, causing time and memory demands to increase linearly or quadratically with the number of steps. In contrast, MCoT clears the KV cache after each step, enabling longer chains of thought without a corresponding rise in resource usage. This makes MCoT more efficient, as its time and memory requirements do not scale with the number of reasoning steps.

# **D** MCoTInstruct Dataset

#### **D.1** Overview

Table 6 presents the detail information of different mathematical reasoning datasets. We list recently popular mathematical reasoning datasets. The **#An-notation Num** refers to the number of samples annotated during the dataset construction process. The **#Annotation Type** represents three categories: solution, trajectory, question. "solution" denotes the annotation of a solution, "trajectory" refers to the multi-step reasoning path, and "question" signifies the annotation of the reduced question.

Unlike previous works (Yue et al., 2023; Gou et al., 2023; Wang et al., 2023a; Liao et al., 2024), our approach requires only the use of GPT-4 for generating a new question, instead of crafting the complete solution that includes text analysis and code snippets. The number of questions that need to be generated is 29k.

# **D.2** Data Format

Figure 6 displays the format of Markov Chain of Thought reasoning. We decompose the Markov chain into tuples of  $(q_1, s_1, q_2)$  and  $(q_2, s_2, a)$  to form the MCoTInstruct dataset.

# **E** Experimental Details

## E.1 Test Dataset

We report the information of four test datasets in Table 4. Notably, the four datasets have obvious differences in difficulty and question types and MATH dataset has diverse categories, thereby ensuring the richness and diversity of the testsets. OCWCourses is a set of 272 STEM problems designed for college students, with most questions needing a few steps to solve. The GaoKao2023-Math-En dataset includes 385 math problems drawn from the 2023 Chinese National College Entrance Examination, the 2023 American Mathematics Competitions, and the 2023 American College Testing. These two OOD datasets are even more tricky to solve than the MATH dataset.

Notably, OCW dataset has a somewhat unique question format, which includes a premise, alongside sub problem and their respective solutions, as shown in Figure 7.

# E.2 Baselines

This comparison included notable models such as OpenAI's GPT-4 (Achiam et al., 2023) and

Markov Chain of	Thought Reasoning	Multi-step Reasoning
Question 1         If $Sf(x) = x^2s$ and $Sg(x) = 3x + 4s$ , what is $Sf(g(-3))s$ ?         To find $Sf(g(-3))s$ , we first need to calculate $Sg(-3)s$ and then the papely the result to the function $Sf(x)s$ . The function $Sg(x) = 3x + 4s$ will be evaluated at $8x = -3s$ , and then the result will be squared as per the definition of $Sf(x) = x^2s$ . "python def g(x): return $3^*x + 4$ Derivation 1 # Calculate g(-3) result g = g(-3) print(result g)	Clear KV cache of context         Question2         What is \$f(-5)\$ if \$f(x) = x^2\$?         To find \$f(-5)\$ when \$f(x) = x^2\$, we need to substitute \$-5\$ into the function \$f(x)\$ and calculate the result.         "python         T_s = lambda x: x**2         result = f_x(-5)         Derivation2         print(result)         "25"	Question 1         If $Sf(x) = x^2S$ and $Sg(x) = 3x + 4S$ , what is $Sf(g(-3))S$ ?         To find $Sf(g(-3))S$ , we first need to calculate $Sg(-3)S$ and then apply the result to the function $Sg(x) = 3x + 4S$ will be evaluated at $Sx = -3S$ ,         Derivation 1         To find $Sf(-5)S$ when $Sf(x) = x^2S$ and $Sg(x) = 3x + 4S$ , we need to substitute S-5S into the function $Sf(x)S$
Question2 What is \$f(-5)\$ if \$f(x) = x^2\$?	After executing the code, we observe that \$f(-5)\$ is equal to \$25\$. Final Answer: \$25\$ Answer	After executing the code, we observe that \$f(-5)\$ is equal to \$25\$. Final Answer: \$25\$ Answer

Figure 5: The reasoning process of two reasoning approachs for mathematical reasoning.

Dataset	#Training	#Test	Category	Domain
GSM8K	7473	1319	×	In-domain
MATH	7500	5000	$\checkmark$	In-domain
OCW	-	272	×	Out-of-domain
GaoKao2023	-	385	×	Out-of-domain

Table 4: The details of four datasets.

ChatGPT, Google's PaLM-2 (Anil et al., 2023), along with Llama3, Llama2 (Touvron et al., 2023), Llemma (Azerbayev et al., 2023), and CodeLlama (Roziere et al., 2023). To establish a fundamental reasoning method baseline, we initially considere Chain of Thought (CoT) prompts (Wei et al., 2022). Additionally, given our methodology's reliance on the Python code interpreter, we also evaluate the Program of Thought (PoT) (Chen et al., 2022) and Program-aided Language (PAL) model (Gao et al., 2023a).

For supervised fine-tuning (SFT) models, we categorize them into *single-step reasoning*: Mammoth (Yue et al., 2023), DeepSeekMath-Instruct (Shao et al., 2024) and *multi-step reasoning*: MathCoder (Wang et al., 2023a), ToRA (Gou et al., 2023), MARIO (Liao et al., 2024) and Math-Genie (Lu et al., 2024).

## E.3 Fine-tuning Details

In this work, we finetune all models using the LLaMA-Factory (Zheng et al., 2024) repository. During this optimization phase, we set the global batch size at 512, the learning rate at 2e-5, and used a cosine learning rate scheduler that included a warm-up phase constituting 3% of the total training duration, spread over 3 epochs. All models are optimized employing AdamW (Kingma and Ba, 2014). Training for all models was launched with the accelerate (Gugger et al., 2022) in Deep-

Speed ZeRO Stage2 (Rajbhandari et al., 2021) and Flash-Attention 2 (Dao, 2023) mechanism. The 7B/8B and 70B models are fine-tuned on 8 and 32 NVIDIA A100 80GB GPUs, respectively.

## F Additional Results and Analyses

#### F.1 The Impact of Self-distillation

Table 5 illustrates the impact of self-distillation. It can be observed that self-distillation enhances the coverage of the training sets and elevates the accuracy of the test sets. Specifically, the application of self-distillation led to a 5.5% increase in data coverage on the MATH training dataset. Furthermore, it achieved a notable 2.5% improvement in accuracy on the MATH test set and a 0.83% boost in accuracy on the GSM8K test set.

Methods	Trainset	Coverage	Testset A	Accuracy
Self-Distillation	GSM8K	MATH	GSM8K	MATH
w/o <sup>†</sup> w/ <sup>‡</sup>	99.75% <b>99.85%</b>	77.97% <b>83.46%</b>	77.94% <b>78.77%</b>	53.32% <b>55.78%</b>

Table 5: The impact of Self-distillation on trainset coverage and testset accuracy. Trainset coverage indicates the proportion of the dataset that encompasses questions from the original training sets of GSM8K and MATH, respectively. <sup>†</sup> denotes the stage in which self-distillation is not employed, signifying the utilization of seed data. <sup>‡</sup> represents the stage that employs self-distillation.

# F.2 The Analysis on Problem-Solving

Figure 8 and Figure 9 illustrate the problemsloving capabilities of MCoT-DeepSeek and MCoT-Llama3, respectively. In terms of difficulty levels as shown in 8a and 9a, MCoT outperforms MSR on levels 1 through 4 and is nearly on par with MSR at level 5. In terms of different subjects as shown in 8b and 9b, We discovered that, when using DeepSeek and Llama3 as base models, MCoT consistently outperforms MSR, particularly in the fields of Algebra, Counting & Probability, and Intermediate Algebra.

# G Dataset License

The MCoTInstruct dataset is built on GSM8K (Cobbe et al., 2021) and MATH (Hendrycks et al., 2021). We strictly abide by the corresponding data licenses.

Methods	#Annotation Num	#Annotation Type	Step	LLM Used	Source
MetaMATH (Yu et al., 2023)	395k	solution	Single	ChatGPT	MATH & GSM8K
WizardMath (Luo et al., 2023)	>96k	solution	Single	ChatGPT	MATH & GSM8K
MAmmoTH (Yue et al., 2023)	260k	solution	Single	GPT4	14 Datasets with MATH & GSM8K
MathCoder (Wang et al., 2023a)	49k	trajectory	Multi	GPT4	MATH & GSM8K
ToRA (Gou et al., 2023)	16k	trajectory	Multi	GPT4	MATH & GSM8K
MARIO (Liao et al., 2024)	27k	trajectory	Multi	GPT4	MATH & GSM8K
MathGenie (Lu et al., 2024)	80k	trajectory	Multi	GPT4	MATH & GSM8K
MCoTInstruct	29 <i>k</i>	question	Multi	GPT4	MATH & GSM8K

Table 6: Compared with mathematical reasoning datasets.Note that MCoTInstruct dataset instance corresponds to the step level rather than the solution level that may include multiple steps.

Find the constant \$t\$ such that $[(5x^2 - 6x + 7)(4x^2 + tx + 10) = 20x^4 - 54x^3 + 114x^2 - 102x + 70.]$	Question <sub>1</sub>
To find the constant \$t\$, we need to expand the product of the two quadratic expressions and compare the coefficients of resulting polynomial to the given polynomial \$20x^4 - 54x^3 + 114x^2 - 102x + 70\$. The coefficient of \$x^3\$ in the expan expression will give us the value of \$t\$. ```python from sympy import symbols, expand # Define the variable and the constant t x, t = symbols('x t') # Define the two quadratic expressions expr1 = 5*x**2 - 6*x + 7 expr2 = 4*x**2 + t*x + 10 # Expand the product of the two expressions expanded_expr = expand(expr1 * expr2) # Print the expanded expression print(expanded_expr) ``` Observation: 5*t*x**3 - 6*t*x**2 + 7*t*x + 20*x**4 - 24*x**3 + 78*x**2 - 60*x + 70	
Given the expanded expression $5tx^3 - 6tx^2 + 7tx + 20x^4 - 24x^3 + 78x^2 - 60x + 70$ , what value of $t$ will make t	
Given the expanded expression $55x^{-5}$ - $6x^{-2} + 7x + 20x^{-4} - 24x^{-5} + 78x^{-2} - 60x + 705$ , what value of \$t5 will make t coefficient of $x^{-3}$ equal to \$-54\$?	<sup>he</sup> <b>Question</b> <sub>2</sub>
	Question <sub>2</sub>

Figure 6: The format of Markov Chain of Thought reasoning.

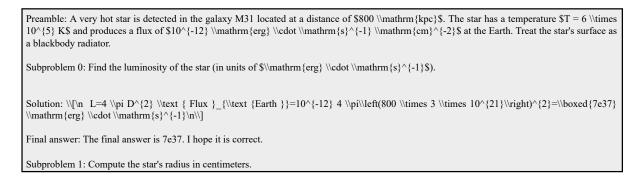


Figure 7: The data format of OCWCouses dataset.

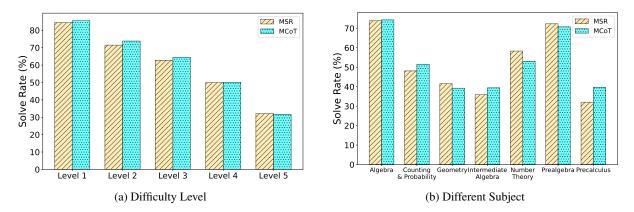


Figure 8: Comparison of problem-solving between MCoT and MSR on MATH test set, with DeepSeekMath-Base<sub>7B</sub> as base model.

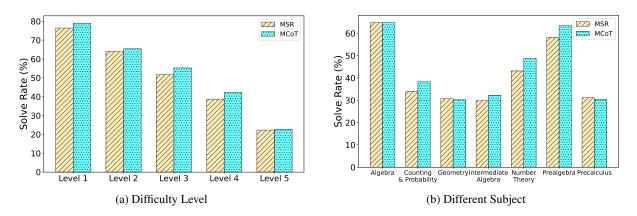


Figure 9: Comparison of problem-solving between MCoT and MSR on MATH test set, with Llama $3_{7B}$  as base model.

# H Case Study

To qualitatively analyze responses from Markov Chain of Thought reasoning, we report three cases with MCoT-DeepSeek. In cases 1 and 2, We observed that MCoT does possess some self-correction capabilities. In case 3, during the reduction process, MCoT lost some information, causing the reduced problem to no longer contain all the information of the original problem.

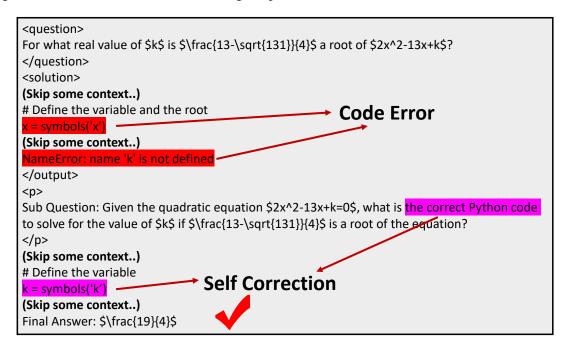


Figure 10: The illustration about MCoT's self-correction capability.

# H.1 Case 1: Self-correction

The Case 1 about MCoT's self-correcting capability

```
idx: "math_test_74" level: "Level 3" type: "Algebra" standard answer: "\frac{19}{4}"
<question>
For what real value of k is \frac{13-\sqrt{131}}{4} a root of 2x^2 - 13x + k?
</guestion>
<solution>
To find the value of k for which \frac{13-\sqrt{131}}{4} is a root of the quadratic equation 2x^2 - 13x + k = 0, we can substitute the
root into the equation and solve for \vec{k}.
<code>
from sympy import symbols, sqrt, solve
# Define the variable and the root
x = symbols('x')
root = (13 - sqrt(131)) / 4
# Define the quadratic equation
equation = 2*x**2 - 13*x + k
# Substitute the root into the equation and solve for k
k_value = solve(equation.subs(x, root), k)
print(k_value)
</code>
<output>
NameError: name 'k' is not defined
</output>
```

Sub Question: Given the quadratic equation  $2x^2 - 13x + k = 0$ , what is the correct Python code to solve for the value of k if  $\frac{13 - \sqrt{131}}{4}$  is a root of the equation?

#### <solution>

To find the value of k, we can use the fact that if  $\frac{13-\sqrt{131}}{4}$  is a root of the quadratic equation  $2x^2 - 13x + k = 0$ , then the other root must be  $\frac{13+\sqrt{131}}{4}$ . This is because the sum of the roots of a quadratic equation is given by  $-\frac{b}{a}$ , where a and b are the coefficients of  $x^2$  and x respectively. In our case,  $-\frac{b}{a} = \frac{13}{2}$ , so the sum of the roots is  $\frac{13}{2}$ . Therefore, we can find k by multiplying the roots.

from sympy import symbols, sqrt, simplify

```
# Define the variable
k = symbols('k')
```

# Define the roots
root1 = (13 - sqrt(131)) / 4
root2 = (13 + sqrt(131)) / 4

```
# Calculate the product of the roots (which gives us k)
product_of_roots = simplify(root1 * root2)
print(product_of_roots)
```

</code>

<output> 19/8 </output>

From the result, we can see that the product of the roots is  $\frac{19}{8}$ . Since the product of the roots is also equal to  $\frac{k}{a}$ , and a = 2 for our quadratic equation, we can find the value of k by multiplying the product of the roots by a. Since we have found that the product of the roots is  $\frac{19}{8}$  and a = 2, we can calculate k by multiplying the product of the roots of the roots by a. Final Answer:  $\frac{19}{4}$ 

#### H.2 Case 2: Self-correction

The Case 2 about MCoT's self-correcting capability

```
idx: "math_test_122" level: "Level 5" type: "Algebra" standard answer: "3"
```

#### <question>

For how many positive integral values of a is it true that x = 2 is the only positive integer solution of the system of inequalities:

 $\Big\{2x > 3x - 33x - a > -6\Big\}$ 

</question>

#### <solution>

To find the positive integral values of a for which x = 2 is the only positive integer solution to the system of inequalities, we need to solve the inequalities for x and then find the constraints on a.

The first inequality 2x > 3x - 3 simplifies to x < 3. This tells us that x must be less than 3.

The second inequality 3x - a > -6 can be simplified by adding *a* to both sides and then dividing by 3 to get  $x > \frac{a}{3} - 2$ . For x = 2 to be the only positive integer solution, *x* must be greater than or equal to 2 but less than 3. This means that  $2 \le x < 3$ .

Therefore, we need to find the range of a such that  $2 \le \frac{a}{3} - 2 < 3$ .

from sympy import symbols, solve, S

```
# Define the variable
a = symbols('a', real=True, positive=True)
```

```
# Inequality 1: 2 <= a/3 - 2
ineq1 = a/3 - 2 >= 2
```

```
# Inequality 2: a/3 - 2 < 3
```

```
ineq2 = a/3 - 2 < 3
# Solve the inequalities
solution1 = solve(ineq1, a)
solution2 = solve(ineq2, a)
# Find the intersection of the solutions
intersection = (S.Intersection(solution1, solution2)).evalf()
print(intersection)
</code>
```

#### <output>

AttributeError: Attribute 'Intersection' was not installed on SymPy registry S </output>

Sub Question: Given the inequalities  $2 \le \frac{a}{3} - 2 < 3$ , for how many positive integral values of a is a within the range found? </solution>

#### <solution>

The given inequalities are  $2 \le \frac{a}{3} - 2 < 3$ . To find the range of a, we need to solve these inequalities for a. <code>

from sympy import symbols, solve, S

```
# Define the variable
a = symbols('a')
```

```
# Define the inequalities
ineq1 = 2 <= a/3 - 2
ineq^2 = a/3 - 2 < 3
```

```
# Solve the inequalities
solution1 = solve(ineq1, a)
solution2 = solve(ineq2, a)
```

print(solution1, solution2)

</code>

#### <output>

 $(12 \le a) \& (a \le oo) (-oo \le a) \& (a \le 15)$ </output>

Sub Question: For how many positive integral values of a is a within the range  $12 \le a < 15$ ? </solution>

#### <solution>

The task is to determine the number of positive integral values of a that lie within the range  $12 \le a < 15$ . Since a must be an integer, we can simply list the integers within this range. The integers that satisfy  $12 \le a < 15$  are 12, 13, and 14. There are three such integers, so the answer is 3. Final Answer: 3 </solution>

#### H.3 Case 3: Bad case

#### The bad case

idx: "math\_test\_1601" level: "Level 4" type: "Counting & Probability" standard answer: "50" <question>

In how many ways can the letters of the word BANANA be rearranged such that the new word does not begin with a B? </question>

#### <solution>

To find the number of ways to rearrange the letters of the word BANANA such that the new word does not begin with a B, we can first find the total number of rearrangements of the word BANANA and then subtract the number of rearrangements that start with a B.

#### <code>

from math import factorial

```
# Total number of letters in BANANA is 6 (with A repeating 3 times)
# So the total number of rearrangements is 6! / (3!)
total_rearrangements = factorial(6) // factorial(3)
print(total_rearrangements)
```

</code>

#### <output> 120

</output>

Sub Question: Given that there are 120 ways to rearrange the letters of the word BANANA, how many of these rearrangements do not start with the letter B?

#### </solution>

#### <solution>

To find the number of rearrangements of the word BANANA that do not start with the letter B, we can first find the total number of rearrangements and then subtract the number of rearrangements that do start with the letter B. The total number of rearrangements of a word with repeated letters can be calculated using the formula for permutations of a multiset, which is

$$\frac{n!}{n_1! \cdot n_2! \cdot \ldots \cdot n_k!}$$

where n is the total number of letters, and  $n_1, n_2, ..., n_k$  are the frequencies of each distinct letter.

#### <code>

from math import factorial

```
# Total number of letters in BANANA
n = 6
# Frequency of each letter: A - 3 times, B - 1 time, N - 2 times
n_A = 3
n_B = 1
n_N = 2
# Total number of rearrangements
```

```
total_rearrangements = factorial(n) // (factorial(n_A) * factorial(n_B) * factorial(n_N))
print(total_rearrangements)
```

</code>

<output> 60 </output>

Sub Question: If there are 60 ways to rearrange the letters of the word BANANA, how many of these rearrangements start with the letter B? </ d>

#### ~solution>

#### <solution>

To find the number of rearrangements of the letters of the word BANANA that start with the letter B, we can consider the remaining 5 letters that can be arranged in any order after fixing the first letter B. Since the first letter is fixed as B, we have 5 remaining letters (A, N, A, N, A) to arrange. We need to calculate the number of unique arrangements of these 5 letters.

#### <code>

import math

```
# Calculate the number of unique arrangements of 5 letters
arrangements = math.factorial(5) // (math.factorial(2) * math.factorial(3))
print(arrangements)
```

#### </code>

<output> 10 </output>

From the result, we can see that there are 10 unique arrangements of the 5 remaining letters after fixing the first letter B.

Final Answer: 10 </solution>

# I Prompt Template in GPT-4

We provide prompts for generating simplified questions using GPT-4 on the MATH dataset and the GSM8K dataset, respectively.

Listing 1: Prompts of reduced question for GPT-4 on MATH dataset.

```
You will be provided with an original math problem and its intermediate thought, action and
observation. Please generate a sub question that should utilize the results of the intermediate
thought, action and observation to replace the related information of original problem and delete
redundant irrelevant information. The sub question should be wrapped by <subquestion> and </
subquestion>.
Here are some examples you may refer to:
The following are 2 demonstration examples.
<original problem>
Let f(x)=x^3+3 and g(x) = 2x^2 + 2x + 1. What is g(f(-2))?
</original problem>
<intermediate thought>
To find g(f(-2)), we first need to calculate f(-2) and then substitute this result into g(x).
</intermediate thought>
<intermediate action>
  `python
f_x = lambda x: x**3 + 3
result_f = f_x(-2)
result_f
</intermediate action>
<intermediate observation>
-5
</intermediate observation>
<subguestion>
what is g(-5) if g(x) = 2x^2 + 2x + 1?
</subquestion>
<original problem>
The perimeter of a rectangular garden is 60 feet. If the length of the field is twice the width, what
 is the area of the field, in square feet?
</original problem>
<intermediate thought>
he perimeter (P) of a rectangle is given by the formula P = 21 + 2w, where 1 is the length and
w is the width of the rectangle. We are given that the perimeter is 60 feet and the length is twice
 the width, which can be expressed as 1 = 2w. We need to find the area (A) of the rectangle, which
is given by the formula A = 1 \times w.
</intermediate thought>
<intermediate action>
  ``python
from sympy import symbols, Eq, solve
# Define symbols
1, w = symbols('1 w')
# Given perimeter
P = 60
# Length is twice the width
length_eq = Eq(1, 2*w)
```

# Perimeter equation perimeter\_eq = Eq(2\*1 + 2\*w, P)# Solve the system of equations for 1 and w solution = solve((length\_eq, perimeter\_eq), (l, w)) print(solution) </intermediate action> <intermediate observation> {l: 20, w: 10} </intermediate observation> <subauestion> Given that the length of a rectangle is 20 feet and the width is 10 feet, what is the area of the rectangle, in square feet? </subquestion> Now! It's your turn. <original problem> A rectangular band formation is a formation with m band members in each of r rows, where m and \$r\$ are integers. A particular band has less than 100 band members. The director arranges them in a rectangular formation and finds that he has two members left over. If he increases the number of members in each row by 1 and reduces the number of rows by 2, there are exactly enough places in the new formation for each band member. What is the largest number of members the band could have? </original problem> <intermediate thought> The problem describes two different rectangular formations. In the first formation, there are \$m\$ members in each of \$r\$ rows with 2 members left over. In the second formation, there are \$m+1\$ members in each of \$r-2\$ rows, and there are no members left over. This means that the total number of band members can be expressed in two ways: 1. \$mr + 2\$ (first formation) 2. \$(m+1)(r-2)\$ (second formation) Since these two expressions represent the same total number of band members, we can set them equal to each other and solve for one variable in terms of the other. We also know that the total number of band members is less than 100. </intermediate thought> <intermediate action> ```python from sympy import symbols, Eq, solve m, r = symbols('m r', integer=True) eq = Eq(m\*r + 2, (m+1)\*(r-2))solution = solve(eq, m) print(solution) </intermediate action> <intermediate observation> [r/2 - 2]</intermediate observation>

#### Listing 2: Prompts of reduced question for GPT-4 on GSM8K dataset.

You will be provided with an original math problem and its intermediate thought, action and observation. Please generate a sub question that should utilize the results of the intermediate thought, action and observation to replace the related information of original problem and delete redundant irrelevant information. The sub question should be wrapped by <subquestion> and </ subquestion>.

Here are some examples you may refer to:

The following are 2 demonstration examples.

<original problem>

Alexis is applying for a new job and bought a new set of business clothes to wear to the interview. She went to a department store with a budget of \$200 and spent \$30 on a button-up shirt, \$46 on suit pants, \$38 on a suit coat, \$11 on socks, and \$18 on a belt. She also purchased a pair of shoes, but lost the receipt for them. She has \$16 left from her budget. How much did Alexis pay for the shoes? </original problem>

<intermediate thought> To find out how much Alexis paid for the shoes, I need to calculate the total amount spent on the other items she bought and subtract this from her initial budget. The initial budget is \$200, and she has \$16 left after all her purchases. The equation for this calculation is: \[ \text{Cost of shoes} = \text{Initial budget} - (\text{Cost of shirt} + \text{Cost of pants} + \ text{Cost of coat} + \text{Cost of socks} + \text{Cost of belt} + \text{Money left}) \] </intermediate thought> <intermediate action> `python initial\_budget = 200  $cost_shirt = 30$  $cost_pants = 46$  $cost_coat = 38$ cost\_socks = 11 cost\_belt = 18  $money_left = 16$ other\_items = cost\_shirt + cost\_pants + cost\_coat + cost\_socks + cost\_belt + money\_left print(other\_items) </intermediate action> <intermediate observation> 143 </intermediate observation> <subauestion> Alexis had a budget of \$200 for her business attire and after purchasing several items, she was left with \$16. If the total cost of the other items was \$143, how much did she spend on the pair of shoes? </subquestion> <original problem> James creates a media empire. He creates a movie for \$2000. Each DVD cost \$6 to make. He sells it for 2.5 times that much. He sells 500 movies a day for 5 days a week. How much profit does he make in 20 weeks? </original problem> <intermediate thought> To calculate the profit James makes, we need to consider the initial cost of creating the movie, the cost of producing each DVD, the selling price of each DVD, the number of DVDs sold per day, the number of days he sells per week, and the total number of weeks. The profit for each DVD sold is the selling price minus the cost to make it. The total profit is the sum of the profit from each DVD sold minus the initial cost of creating the movie. The profit per DVD can be calculated as follows: Profit per DVD = Selling price per DVD - Cost to make per DVD The total profit can be calculated as follows: Total profit = (Profit per DVD \* Number of DVDs sold per day \* Number of days per week \* Number of weeks) - Initial cost of creating the movie Let's calculate the profit per DVD first. </intermediate thought> <intermediate action> ```python  $cost_per_dvd = 6$ selling\_price\_per\_dvd = 2.5 \* cost\_per\_dvd profit\_per\_dvd = selling\_price\_per\_dvd - cost\_per\_dvd print(profit\_per\_dvd) </intermediate action> <intermediate observation> 90 </intermediate observation> <subauestion> Given that James makes a profit of \$9.0 per DVD, sells 500 DVDs a day for 5 days a week, and the initial cost of creating the movie was \$2000, how much total profit does he make in 20 weeks? </subquestion> Now! It's your turn.

James creates a media empire. He creates a movie for \$2000. Each DVD cost \$6 to make. He sells it for 2.5 times that much. He sells 500 movies a day for 5 days a week. How much profit does he make in 20 weeks? </original problem> <intermediate thought> To calculate the profit James makes, we need to consider the initial cost of creating the movie, the cost of producing each DVD, the selling price of each DVD, the number of DVDs sold per day, the number of days he sells per week, and the total number of weeks. The profit for each DVD sold is the selling price minus the cost to make it. The total profit is the sum of the profit from each DVD sold minus the initial cost of creating the movie. The profit per DVD can be calculated as follows: Profit per DVD = Selling price per DVD - Cost to make per DVD The total profit can be calculated as follows: Total profit = (Profit per DVD \* Number of DVDs sold per day \* Number of days per week \* Number of weeks) - Initial cost of creating the movie Let's calculate the profit per DVD first. </intermediate thought> <intermediate action> ``python  $cost_per_dvd = 6$ selling\_price\_per\_dvd = 2.5 \* cost\_per\_dvd profit\_per\_dvd = selling\_price\_per\_dvd - cost\_per\_dvd print(profit\_per\_dvd) </intermediate action> <intermediate observation> 9.0 </intermediate observation>