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LANGUAGE MODELS ARE HIDDEN REASONERS: UNLOCKING LATENT REASONING CAPABILITIES VIA SELF-REWARDING

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Abstract

Large language models (LLMs) have shown impressive capabilities, but still struggle with complex reasoning tasks requiring multiple steps. While prompt-based methods like Chain-of-Thought (CoT) can improve LLM reasoning at inference time, optimizing reasoning capabilities during training remains challenging. We introduce LaT ent Reasoning Optimization (LaTRO), a principled framework that formulates reasoning as sampling from a latent distribution and optimizes it via variational approaches. LaTRO enables LLMs to concurrently improve both their reasoning process and ability to evaluate reasoning quality, without requiring external feedback or reward models. We validate LaTRO through experiments on GSM8K and ARC-Challenge datasets using multiple model architectures. On GSM8K, LaTRO improves zero-shot accuracy by an average of 12.5% over base models and 9.6% over supervised fine-tuning across Phi-3.5-mini, Mistral-7B, and Llama-3.1-8B. Our findings suggest that pre-trained LLMs possess latent reasoning capabilities that can be unlocked and enhanced through our proposed optimization approach in a self-improvement manner.

1 INTRODUCTION

The development of large language models (LLMs) with enhanced reasoning capabilities has emerged 031 as a crucial area of research. Despite their impressive advances, the inherent next-token prediction 032 mechanism of LLMs makes it challenging for these models to solve complex problems requiring 033 multiple reasoning steps (Wang et al., 2022; Huang et al., 2023). For instance, LLMs often struggle 034 to directly provide accurate solutions to mathematical problems or even simple puzzles like counting specific letters in a word. Consequently, researchers have explored various prompting strategies that guide LLMs to generate reasoning trajectories or rationales-sequences of tokens that build a 037 step-by-step progression toward an answer. Techniques such as Chain-of-Thought (CoT) (Wei et al., 038 2022), Tree-of-Thought (ToT) (Yao et al., 2024), and Program-of-Thought (PoT) (Chen et al., 2023) prompting methods exemplify this approach.

⁰⁴⁰ Recent progress has also focused on inference-time techniques to enhance the reasoning abilities of 041 LLMs (Wu et al., 2024; Brown et al., 2024), as observed in the OpenAI o1 model (OpenAI, 2024). 042 These methods have demonstrated remarkable performance in diverse reasoning tasks, including 043 mathematics (Cobbe et al., 2021b; Trinh et al., 2024; Luo et al., 2024), coding (Jimenez et al., 2023; 044 Guo et al., 2024; Zhang et al., 2024), and scientific problem-solving (Rein et al., 2023). Notable inference-time methods, such as CoT with Self-Consistency (CoT-SC) (Wang et al., 2023) and CoT-Decoding (Wang & Zhou, 2024), extend the CoT approach by generating multiple reasoning 046 paths and selecting the most consistent one. Additionally, techniques like ReAct (Yao et al., 2023a) 047 and Reflexion (Shinn et al., 2023) integrate reasoning into LLM agent loops, further enhancing their 048 problem-solving capabilities. 049

Despite the promising results at inference time, improving the reasoning abilities of LLMs during their
 training phase remains a challenging problem. Several obstacles impede progress in this area. Firstly,
 there is a scarcity of high-quality reasoning data for complex problems, limiting the applicability
 of traditional supervised fine-tuning (SFT) approaches (Zelikman et al., 2022). Moreover, when
 such data is available, SFT on deterministic reasoning paths may result in a lack of diversity in



108 2 RELATED WORK

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110 **Prompt-based LLM Reasoning** Prompt-based reasoning methods prove to be effective across 111 various domains, such as math problem-solving (Polu & Sutskever, 2020; Hendrycks et al., 2021; 112 Cobbe et al., 2021a), logical reasoning (Sprague et al., 2024) and agentic tasks (Yao et al., 2023a; 113 Shinn et al., 2023; Yao et al., 2023b), Chain-of-Thoughts or CoT (Wei et al., 2022) is the pioneering 114 work that prompts LLMs to decompose challenging tasks into smaller reasoning steps. After that, two primary research directions further improved reasoning capabilities during inference. One direction 115 searched over the reasoning trajectories against a process-based verifier, or reward model (Yao et al., 116 2024; Besta et al., 2024; Lightman et al., 2023). For example, tree-of-thoughts (Yao et al., 2024) 117 explored over thoughts by depth-first search (DFS), breadth-first search (BFS) or beam search. The 118 other approach used a critic model to provide verbal feedback, iteratively refining the responses with 119 that feedback (Saunders et al., 2022; Shinn et al., 2023; Yao et al., 2023b; Madaan et al., 2023). 120

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Self-Rewarding for LLM Reasoning Reasoning capabilities in LLMs can be enhanced in post-122 training through self-rewarding and reinforcement learning. The Self-Taught Reasoner, or STaR (Ze-123 likman et al., 2022) introduced a bootstrapping technique that allows LLMs to generate rationales 124 and fine-tune itself with self-generated reasoning paths. Quiet-STaR (Zelikman et al., 2024) extended 125 this by training LLMs to infer implicit rationales across arbitrary text, enhancing both reasoning 126 and predictive abilities without task-specific fine-tuning, Reinforced Fine-Tuning, or ReFT (Trung 127 et al., 2024) took this further by leveraging reinforcement learning to improve generalization in 128 reasoning tasks like math problem-solving, enabling LLMs to learn from multiple reasoning paths. Self-correction capabilities in LLMs can also be reinforced through self-generated data (Kumar et al., 129 2024). Lastly, Hoffman et al. (2024); Hu et al. (2023) formulated the reasoning process as latent 130 variable models, aligning LLMs towards more accurate reasoning with fewer annotated data. 131

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140 141 142 **3** BACKGROUND AND MOTIVATION

We start by briefly introducing reasoning techniques (*e.g.*, chain-of-thought (Wei et al., 2022), ReAct (Yao et al., 2023a), *etc*). Given a user query \boldsymbol{x} , the standard procedure to sample the response \boldsymbol{y} is to leverage an autoregressive pretrained LLMs π_{θ} (parameterized by θ): $\boldsymbol{y} \sim \pi_{\theta}(\cdot | \boldsymbol{x})$. As for prompt-based reasoning techniques such as chain-of-thought (Wei et al., 2022), the LLM π_{θ} is firstly asked to generate thoughts (*a.k.a* reasoning rationale) before generating the answers to the response:

$$oldsymbol{x}' := \operatorname{Reason}(oldsymbol{x}) = oldsymbol{x} \oplus \operatorname{Prompt}$$
 Template of Thought $oldsymbol{z} \sim \pi_{ heta}(\cdot \mid oldsymbol{x}'), \quad oldsymbol{y} \sim \pi_{ heta}(\cdot \mid oldsymbol{x}' \oplus oldsymbol{z}),$

where z is the thought or the reasoning rationale path, \oplus indicates the concatenate operator, and the prompt template of the thought can be some hint prompt such as "Let's think s tep by step" ¹.Empirically, people observe that there is a higher chance for the LLM π_{θ} to generate the desired answer y following the above procedure than directly sampling the response $y \sim \pi_{\theta}(\cdot | x)$. From a statistical perspective, we hypothesize that good reasoning rationales can significantly improve the probability of generating good answers y: $\exists z$, s.t. $\pi_{\theta}(y | x \oplus z) \gg \pi_{\theta}(y | x)$.

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150 To validate the hypothesis, we check the probability of the correct answers y on pretrained LLMs with or with-151 out reasoning rationales. In Figure 2, we visualize the 152 negative log probability of the correct answers on three 153 different LLMs on GSM8K dataset (Cobbe et al., 2021b). 154 We have observed that when the LLMs are conditioned 155 on the reasoning rationales, the probability of the correct 156 answer is remarkably larger than without reasoning ratio-157 nales. This suggests that good reasoning rationales help 158 the LLMs generate desired answers for complex tasks by 159 increasing their probability, giving them a higher chance 160 of generating the correct answers.



Figure 2: Average negative log probabilities of LLMs to generate correct responses.

¹We omit the difference between x' and x for convenience in the latter notation.

The above observation inspires us that we can potentially further improve the reasoning ability of existing LLMs. One may find some surrogate objective to enhance the quality of the reasoning rationales or improve the ability of LLMs to leverage good reasoning rationales. In the following Proposition 1, we show that *Self-Consistency* Chain-of-Thought (CoT-SC) (Wang et al., 2023), which takes a majority vote of multiple reasoning rationales to improve the reasoning ability, approximates some surrogate objective.

Proposition 1. Denote the user query, model response, and reasoning rationale by $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$, respectively. The distribution of the majority vote answer of the K reasoning rationales obtained by CoT-SC approximates $p_M(\boldsymbol{y}|\boldsymbol{x}) := \mathbb{E}_{\boldsymbol{z} \sim \pi_{\theta}(\cdot|\boldsymbol{x})}[\pi_{\theta}(\boldsymbol{y}|\boldsymbol{x} \oplus \boldsymbol{z})]$, as $K \to \infty$.

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182 183 *Proof.* Given a user query \boldsymbol{x} , CoT-SC essentially follows the procedure: 1) Sample K *i.i.d* reasoning rationales together with model responses: $(\boldsymbol{z}_k, \boldsymbol{y}_k) \sim \pi_{\theta}(\cdot | \boldsymbol{x}), \ 1 \leq k \leq K$. 2) Take the majority vote of $(\boldsymbol{y}_1, \dots, \boldsymbol{y}_K)$. For a specific response \boldsymbol{y} , its frequency can be calculated as $F(\boldsymbol{y}) := \frac{1}{K} \sum_{k=1}^{K} \mathbb{1}\{\boldsymbol{y}_k = \boldsymbol{y}\}$, where $\mathbb{1}$ is the indicator function. Then the expectation of $F(\boldsymbol{y})$ is

$$\mathbb{E}_{\boldsymbol{y}_{1},\ldots,\boldsymbol{y}_{K}}F(\boldsymbol{y}) = \frac{1}{K}\sum_{k=1}^{K}\mathbb{E}_{\boldsymbol{y}_{i}}\mathbb{1}\{\boldsymbol{y}_{i}=\boldsymbol{y}\} = \frac{1}{K}\sum_{i=1}^{K}\mathbb{P}_{\boldsymbol{y}_{i}\sim\pi_{\theta}(\cdot|\boldsymbol{x}\oplus\boldsymbol{z}_{i})}[\boldsymbol{y}_{i}=\boldsymbol{y}]$$
$$= \frac{1}{K}\sum_{i=1}^{K}\pi_{\theta}(\boldsymbol{y}|\boldsymbol{x}\oplus\boldsymbol{z}_{i}) \xrightarrow{K\to\infty} \mathbb{E}_{\boldsymbol{z}\sim\pi_{\theta}(\cdot|\boldsymbol{x})}\pi_{\theta}(\boldsymbol{y}|\boldsymbol{x}\oplus\boldsymbol{z}).$$

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CoT-SC essentially leverages $p_M(\boldsymbol{y}|\boldsymbol{x}) := \int \pi_{\theta}(\boldsymbol{z}|\boldsymbol{x}) \pi_{\theta}(\cdot|\boldsymbol{x} \oplus \boldsymbol{z}) d\boldsymbol{z}$ to obtain reasoning rationales 187 and produces final correct answers. Inspired by the conclusion, we could leverage surrogate objectives 188 like $\mathbb{E}_{\boldsymbol{z} \sim \pi_{\theta}(\cdot | \boldsymbol{x})}[\phi(\pi_{\theta}(\boldsymbol{y} | \boldsymbol{x} \oplus \boldsymbol{z}))]$ to further enhance the reasoning ability of LLMs, where ϕ is some 189 monotonic transform such as logarithm $(\log(\cdot))$. Further, we could also optimize the parameters of 190 LLMs to enhance the reasoning abilities of existing LLMs during the training, so we can obtain 191 LLMs with better reasoning abilities with the same inference time budget. In the following sections, 192 we introduce the idea of optimizing LLMs to improve reasoning abilities without external feedback, 193 by proposing a principled framework containing the surrogate objective. 194

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4 OPTIMIZING THE REASONING PROCESS

In this section, we describe how to optimize the reasoning rationale without external feedback. Specifically, we introduce the objective for optimizing the reasoning rationale in Section 4.1 from a variational perspective of LLM training; we derive the gradient estimation for the new objective in Section 4.2, and discuss the sampling procedure together with reward shaping in Section 4.3. We summarize the proposed algorithm, <u>LaT</u>ent <u>Reasoning Optimization (LaTRO)</u> in Algorithm 1, and illustrate the overall procedure in Figure 1.

4.1 LATENT REASONING OPTIMIZATION: A VARIATIONAL APPROACH

Suppose we are given a golden dataset $\mathcal{D}_{Gold} := \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^N$ consisting of N query and answer pairs, where $(\boldsymbol{x}, \boldsymbol{y})$ denotes the query and the answer respectively. A standard finetuning procedure to fit the LLM π_{θ} to the dataset \mathcal{D}_{Gold} is by likelihood maximization:

$$\max_{\theta} \mathbb{E}_{(\boldsymbol{x},\boldsymbol{y}) \sim \mathcal{D}_{\text{Gold}}} \left[\log \pi_{\theta}(\boldsymbol{y} \mid \boldsymbol{x}) \right], \qquad (1)$$

where θ are the parameters of the LLM π_{θ} to optimize. Based on the discussion in Section 3, it is more feasible to optimize π_{θ} with additional reasoning rationale path z, compared with standard finetuning objective in Equation (1). Hence, we can introduce another "reasoner" q(z|z) to sample the latent reasoning rationales that can help the optimization procedure of π_{θ} . This is achievable by optimizing the following lower bound:

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$$\log \pi_{\theta}(\boldsymbol{y}|\boldsymbol{x}) = \log \int \pi_{\theta}(\boldsymbol{y} \mid \boldsymbol{x} \oplus \boldsymbol{z}) \pi_{0}(\boldsymbol{z} \mid \boldsymbol{x}) d\boldsymbol{z}$$

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234 235 236 $= \log \int \pi_{\theta}(\boldsymbol{y} \mid \boldsymbol{x} \oplus \boldsymbol{z}) \frac{q(\boldsymbol{z} \mid \boldsymbol{x})}{q(\boldsymbol{z} \mid \boldsymbol{x})} \pi_{0}(\boldsymbol{z} \mid \boldsymbol{x}) d\boldsymbol{z}$ $\geq \max_{q(\boldsymbol{z} \mid \boldsymbol{x})} \mathbb{E}_{q(\boldsymbol{z} \mid \boldsymbol{x})} \left[\log \pi_{\theta}(\boldsymbol{y} \mid \boldsymbol{x} \oplus \boldsymbol{z}) \right] - D_{\mathrm{KL}} [q(\boldsymbol{z} \mid \boldsymbol{x}) || \pi_{0}(\boldsymbol{z} \mid \boldsymbol{x})], \qquad (2)$

where π_0 is a prior reference LLM that regularizes the "reasoner" $q(\boldsymbol{z}|\boldsymbol{x})$, and the lower bound is achieved via Jensen's inequality (Higgins et al., 2017). Based on the literature of variational Bayes (Kingma, 2013), one can either learn and optimize $q(\boldsymbol{z}|\boldsymbol{x})$ via variational Expectation Maximization (EM) (Abdolmaleki et al., 2018; Liu et al., 2022), or introduce another parameterized LLM $q_{\phi}(\boldsymbol{z}|\boldsymbol{x})$ and optimize ϕ to amortize the cost. Additionally, from the discussion in Section 3, we know π_{θ} itself can also serve as a naive "reasoner", since π_{θ} is an autoregressive LLM.

To simplify the learning procedure, we propose to use π_{θ} as the "reasoner" $q(\boldsymbol{z}|\boldsymbol{x})$. As a result, we can jointly learn one single LLM π_{θ} , that is capable of generating good reasoning rationale together with providing correct answers given the query and its own generated reasoning rationale. To be more specific, we can define the learning objective as follows:

$$\max_{\theta} J(\theta) := \mathbb{E}_{(\boldsymbol{x},\boldsymbol{y})\sim\mathcal{D}_{\text{Gold}}} \left[\mathbb{E}_{\boldsymbol{z}\sim\pi_{\theta}}(\cdot|\boldsymbol{x}) \left[\underbrace{\log \pi_{\theta}(\boldsymbol{y}||\boldsymbol{x}\oplus\boldsymbol{z})}_{R_{\theta}(\boldsymbol{z},\boldsymbol{y},\boldsymbol{x})} \right] - D_{\text{KL}}[\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})||\pi_{0}(\boldsymbol{z}|\boldsymbol{x})] \right], \quad (3)$$

where we specify the reference LLM π_0 to be the original π_{θ} before the optimization. Furthermore, log $\pi_{\theta}(\boldsymbol{y} | \boldsymbol{x} \oplus \boldsymbol{z})$ in Equation (3) can be viewed as the reward function $R_{\theta}(\boldsymbol{z}, \boldsymbol{y}, \boldsymbol{x})$ to evaluate the quality of the rationale \boldsymbol{z} given the pair $(\boldsymbol{x}, \boldsymbol{y})$, since the reasoning rationale \boldsymbol{z} with higher likelihood log $\pi_{\theta}(\boldsymbol{y} | \boldsymbol{x} \oplus \boldsymbol{z})$ indicates that it would provide a higher probability for the model to answer the question correctly.

Remark By substituting $\log \pi_{\theta}(\boldsymbol{y} \mid \boldsymbol{x} \oplus \boldsymbol{z})$ with $R_{\theta}(\boldsymbol{z}, \boldsymbol{y}, \boldsymbol{x})$, Equation (3) exactly recovers the 242 standard optimization objective defined in offline RL (Levine et al., 2020), RLHF (Ouyang et al., 243 2022; Rafailov et al., 2024) literature. Though Equation (3) unifies the learning procedure of the 244 "reasoner" $\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})$ and the "reward" function $R_{\theta}(\boldsymbol{z}, \boldsymbol{y}, \boldsymbol{x}) := \log \pi_{\theta}(\boldsymbol{y}||\boldsymbol{x} \oplus \boldsymbol{z})$, we can break down 245 these two procedures to analyze them separately. When we fix $R_{\theta}(\boldsymbol{z}, \boldsymbol{y}, \boldsymbol{x})$ and optimize the "reasoner" 246 $\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})$, the procedure can be interpreted as *self-improvement* learning, where we improve $\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})$ 247 on self-generated synthetic reasoning rationale. When we fix $\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})$ and optimize $R_{\theta}(\boldsymbol{z},\boldsymbol{y},\boldsymbol{x})$, 248 the procedure can be interpreted as *self-reward* learning, where we learn the self-reward function 249 $\log \pi_{\theta}(\boldsymbol{y} \mid \boldsymbol{x} \oplus \boldsymbol{z})$. The procedure can also be considered finetuning optimization given the learned 250 reasoning rationale and query. Fortunately, we can naturally enjoy the benefits of these two self-251 learning procedures with the new reasoning finetuning objective.

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4.2 GRADIENT ESTIMATION FOR LATRO

From previous RL literature, we know that estimating $\nabla_{\theta} J(\theta)$ in Equation (3) involves the use of policy gradient methods, which usually suffers from high variances with the naive REINFORCE estimators (Williams, 1992). Inspired by the recent work on policy gradient for LLMs (Ahmadian et al., 2024), we also leverage the REINFORCE Leave-One-Out (RLOO) (Kool et al., 2019) to optimize the "reasoner" $\pi_{\theta}(z|x)$, where we can achieve lower variances of gradient estimation by sampling multiple rationales. We summarize the empirical gradient estimation for solving LaTRO in Proposition 2.

Proposition 2. (LaTRO Gradient Estimation) Suppose we are given a set of training data \mathcal{D}_{Gold} := $\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$, we sample K i.i.d reasoning rationales $\boldsymbol{z}_1^{(i)}, \boldsymbol{z}_2^{(i)}, \dots, \boldsymbol{z}_K^{(i)} \sim \pi_{\theta}(\cdot|\boldsymbol{x}_i)$ for each query and answer pair $(\boldsymbol{x}_i, \boldsymbol{y}_i)$. The empirical gradient estimator for $\nabla_{\theta} J(\theta)$ is expressed as

$$\nabla_{\theta} \widehat{J}(\theta) := \frac{1}{NK} \sum_{i=1}^{N} \sum_{k=1}^{K} \left(\nabla_{\theta} \log \pi_{\theta}(\boldsymbol{x}_{i} \mid \boldsymbol{z}_{k}^{(i)}) \cdot A_{k}^{(i)} + \nabla_{\theta} \log \pi_{\theta}(\boldsymbol{y}_{i} \mid \boldsymbol{z}_{k}^{(i)} \oplus \boldsymbol{x}_{i}) \right),$$
(4)

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$$\text{ with } A_k^{(i)} = r(\boldsymbol{z}_k^{(i)}) - \frac{1}{K-1} \sum_{j \neq k}^K r(\boldsymbol{z}_j^{(i)}) \,, r(\boldsymbol{z}_k^{(i)}) := \log \pi_{\theta}(\boldsymbol{y}_i \mid \boldsymbol{x}_i \oplus \boldsymbol{z}_k^{(i)}) - \beta \log \frac{\pi_{\theta}(\boldsymbol{x}_i \mid \boldsymbol{z}_k^{(i)})}{\pi_0(\boldsymbol{x}_i \mid \boldsymbol{z}_k^{(i)})} \,,$$

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Algorithm 1: LaTent Reasoning Optimization (LaTRO)

Input: Language model π_{θ} , learning rate η , KL penalty factor β , MC sample size K, maximum generation length L, sample temperature T, number of epochs M, training dataset \mathcal{D}_{Gold} . **Output:** An optimized language model π_{θ} .

def generate $(\pi, \boldsymbol{x}, K, L, T)$:

Given an autoregressive language model π , input x, sample K sequences of length L from the distribution $\pi(\cdot | \boldsymbol{x})$ at temperature T. **return** K sampled sequences Intialize reference language model π_0 as π_{θ} for epoch in range(M): for $\boldsymbol{x}_i, \boldsymbol{y}_i$ in \mathcal{D}_{Gold} : $[\boldsymbol{z}_1^{(i)}, \dots, \boldsymbol{z}_K^{(i)} \leftarrow \texttt{generate}(\pi_{\theta}, \boldsymbol{x}_i, K, L, T)]$ Estimate $\nabla_{\theta} \widehat{J}(\theta)$ with Proposition 2 $\theta \leftarrow \theta + \eta \nabla_{\theta} \widehat{J}(\theta)$ return π_{θ}

where $\beta \geq 0$ is the coefficient to control the KL penalty. The proof can be found in Appendix A.1.

The first gradient term in Equation (4) serves as policy gradient to improve the ability of the LLM π_{θ} to generate high-quality reasoning rationales, and $\log \pi_{\theta}(\boldsymbol{y}|\boldsymbol{x} \oplus \boldsymbol{z})$ can be viewed as the evaluator for reasoning rationale, which is further used to calculate the advantages. The second gradient term in Equation (4), which is the gradient of supervised finetuning loss, essentially helps the LLM π_{θ} to leverage the reasoning rationales to produce correct answers.

4.3 PRACTICAL CONSIDERATIONS

298 To reduce computation overhead and better control the sampling of reasoning rationales during 299 training, we limit their maximum token length to L. The rationale ends either at the EOS token or at the start of a predefined answer template (e.g., "The answer is"). We then use the truncated rationale 300 z, along with the query x and the answer z, for further computation. 301

302 We also encourage the LLM to finish its reasoning process with L tokens. Inspired by the implementa-303 tion of the RLOO trainer in the TRL library (von Werra et al., 2020), we introduce a constant penalty 304 for rationales truncated by the maximum token length L. This penalty encourages the generation of 305 rationales that fit within the specified token limit.

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5 **EXPERIMENTS**

5.1 Setup

We evaluate the performance of the proposed method across two datasets: a mathematical reasoning dataset (GSM8K, Cobbe et al. (2021b)) and a logical reasoning dataset (ARC-Challenge, Talmor et al. (2019)). The sizes of the datasets are listed in Table 1.

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315 Training. For each dataset, we fine-tune three 316 base models: Phi-3.5-mini-instruct (Abdin et al., 317 2024), Mistral-7B-Instruct-v0.3 (Jiang et al., 2023), 318 and Meta-Llama-3.1-8B-Instruct (Dubey et al., 319 2024), abbreviated as Phi-3.5, Mistral-7B, and 320 Llama-3.1-8B, respectively. We provide two base-321 line comparisons: the base model and the super-

Table 1: Size of the datasets

Name	Training	Evaluation
GSM8K	7473	1319
ARC-Challenge	1119	1172

vised fine-tuned (SFT) model. For GSM8K, LaTRO fine-tuning excludes golden rationales from 322 the solutions in the training set, while the SFT model is trained using golden rationales. For ARC-323 Challenge, as suggested in (Zheng et al., 2024), the model is trained to generate answers to the text of multiple-choice questions rather than selecting labels. Since no golden rationales are available for
 ARC-Challenge, the SFT model is trained to directly generate answers.

Evaluation. For GSM8K, we evaluate all models with CoT prompting, and for ARC-Challenge, we evaluate the SFT baseline with direct answer generation, while the base model and the LaTRO fine-tuned model with CoT prompting. All evaluations are conducted with zero-shot prompts. We report both greedy decoding (GD) results and self-consistency (with temperature T = 1) results. We choose a self-consistency sample size k = 8 (maj@8) in Table 2 after observing that more than 8 samples did not bring further performance improvement (see Figure 3 (b) for details).

Implementation. LaTRO is implemented on the high level as in Algorithm 1, with additional engineering techniques as discussed in section 4.3. LaTRO is implemented using the widely recognized transformers (Wolf et al., 2020) and TRL (von Werra et al., 2020) libraries, with PyTorch (Ansel et al., 2024) as backend. DeepSpeed ZeRO (Rasley et al., 2020) is used in stage 3, along with Flash Attention 2 (Dao et al., 2022) to enhance training efficiency. The models were trained on a machine equipped with 8xH100 80GB GPUs, using bfloat16 precision.

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340 **Hyperparameters.** AdamW optimizer with a learning rate of 5×10^{-7} , no warm-up steps, and a 341 linear decay strategy is used. The Monte Carlo (MC) sample size K = 16 and the batch size of the 342 data loader 3 are predetermined, resulting in an effective batch size of 48. Gradient accumulation 343 steps and training batch size are subsequently adjusted to prevent out-of-memory errors during 344 training. A temperature of T = 1 is used for MC sampling, and a penalty factor $\gamma = 2$ is applied for incomplete rationales. The KL penalty is set at $\beta = 0.05$ for GSM8K and 0.25 for ARC-Challenge. 345 Except for the results presented in Section 5.3, the maximum generation length is maintained at 346 L = 500. We train all models up to six epochs for GSM8K, and 12 epochs for ARC-Challenge. The 347 checkpoint with best test accuracy is chosen. 348

For the SFT baseline experiments, we use a batch size of 32 and adjust the learning rate to ensure that the evaluation loss decreases and finally converges. All SFT baselines are trained for a maximum of 12 epochs. The checkpoint with the best test accuracy is selected.

In addition to the main quantitative results, we conduct ablation studies on two factors: 1. The maximum generation length L, where we study the effects of tuning L in both training and inference times; 2. The self-consistency samples k, where we explore to what extent LaTRO can still benefit from inference-time scaling.

The main quantitative results, qualitative analysis of sample responses, and results of the ablation study are presented in Sections 5.2 to 5.4, respectively. Additional details on our prompt templates and more samples can be found in Appendices B and C.

360 5.2 RESULTS

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In this subsection, we present evaluation results that demonstrate how effectively LaTRO enhances the reasoning abilities of LLMs on downstream datasets. The detailed results are provided inTable 2.

364 For the GSM8K dataset, LaTRO fine-tuned models outperform all base models by up to 19.5%365 (Mistral-7B, $47.8\% \rightarrow 67.3\%$) and show an average improvement of 12.5% across the three models 366 examined with greedy decoding. The greatest improvement margin is observed for Mistral-7B, 367 while the smallest is seen for Llama-3.1-8B, consistent with our initial findings in Figure 2, where 368 Mistral-7B exhibited the lowest log probability for directly answering questions and Llama-3.1-8B exhibited the highest. With self-consistency, the improvements are by up to 16.5% (Phi-3.5, 369 $74.0\% \rightarrow 90.5\%$) and the average improvement is 13.1%. Furthermore, LaTRO models demonstrate 370 superior performance relative to SFT baselines, with an average improvement of 9.6% for greedy 371 decoding and 13.2% for self-consistency. It is worth noting that for the SFT baseline of Llama-3.1-8B, 372 overfitting on the test set is still observed after tuning the learning rate. 373

For ARC-Challenge, LaTRO fine-tuned models still outperform the baselines, though with a smaller margin. When using greedy decoding, the improvements over the base models are up to 1.6% with an average increase of 1%. We see more increment with self-consistency, where the improvement margins are on average 2.4%. Comparing to SFT baslines, we find that all three models are very sensitive when fine-tuning to directly generate the answer of ARC-Challenge questions. They perform

378	Table 2: Zero-shot accuracy (%) comparison between LaTRO and the baselines on GSM8K and
379	ARC-Challenge datasets. The models are fine-tuned on corresponding training datasets. The base
380	model are marked with "N/A" in the training method. GD stands for greedy decoding at inference
381	time and maj@8 stands for self-consistency with 8 samples. The models are evaluated by default
382	using CoT, except that † indicates the direct answer generation is applied during evaluation.

Base Model	Training Method	Inference Method	GSM8K	ARC-Challenge
	N/A	GD	72.9	85.1
		maj@8	74.0	86.0
Dh; 25	SFT	GD	75.8	81.0^{\dagger}
Phi-3.5 Mistral-7B Llama-3.1-8B		maj@8	77.1	80.5^{\dagger}
	LaTRO	GD	87.6	86.4
		maj@8	90.5	87.5
	N/A	GD	47.8	74.1
		maj@8	58.2	74.1
	SFT	GD	57.2	70.0^{\dagger}
		maj@8	59.9	70.6^{\dagger}
	LaTRO	GD	67.3	74.3
		maj@8	73.8	78.9
	N/A	GD	76.8	81.4
		maj@8	79.7	84.4
	SFT	GD	73.2	77.0^{\dagger}
		maj@8	74.7	76.4^{\dagger}
	LaTRO	GD	80.1	83.0
		maj@8	87.0	85.3

even inferior to the unoptimized base models. When using greedy decoding, the improvements of
LaTRO fine-tuned models over the SFT baselines are on an average of 5.2%, and by up to 6%
(Llama-3.1-8B). In the case of self-consistency, LaTRO performs better than the base models by
an average of 2.4%, and surpasses the SFT models by an average of 8.1%. On the less surprising
results compared to GSM8K, we conjecture that for ARC-Challenge, the models are already good at
producing the answer either directly or through CoT prompting. Hence, further optimization of the
reasoning process did not yield significant improvement.

418 5.3 ABLATION STUDY

In this subsection, we present our ablation study on the effect of different parameters in LaTRO. For consistency, we fix the base model to Phi-3.5 and the dataset to GSM8K throughout the ablation experiments.

How many tokens are enough? Liu et al. (2024) demonstrated that when the input length is n, a transformer model with a hidden size of $O(\log n)$ can solve problems equivalent to Boolean circuits of size m, using m CoT steps. However, the empirical determination of sufficient CoT tokens for optimal performance remains underexplored. In this section, we report zero-shot accuracy with generation length L ranging from 200 to 1000 tokens at inference time. Additionally, a Phi-3.5 model is fine-tuned with L = 200 for comparison. We distinguish two LaTRO fine-tuned models, referred to as LaTRO and LaTRO₂₀₀. As shown in Figure 3(a) accuracy gains plateau when $L \ge 500$, suggesting 500 tokens might suffice for grade school math problems. In contrast, limiting L to 200 reduces accuracy, unless the model is trained accordingly. Interestingly, LaTRO significantly improves performance under this constraint by training the model to generate more concise rationales.



Figure 3: Ablation study results on GSM8K with base model Phi-3.5. In (a), the x-axis represents various maximum token length L of reasoning rationales, y-axis is the accuracy, and the plot shows the zero-shot performance v.s. various maximum token lengths for different methods. In (b), the x-axis represents the # of sampled reasoning rationales, the y-axis is the accuracy, and the plot shows the zero-shot performance v.s. the # of reasoning rationales used in the majority vote.

This finding implies LaTRO can also train LLMs to condense rationales for limited inference-time compute. A sample from LaTRO₂₀₀ is provided in Appendix C for qualitative analysis.

Is inference-time scaling still beneficial? While LaTRO shifts much of the reasoning computation to training time, it can still benefit from the inference-time scaling. To explore this, We evaluate the models again using self-consistency with the number of samples k ranging from 1 to 32. As shown in Figure 3 (b), with k = 8 rationales and majority voting, LaTRO achieves 90% accuracy on GSM8K. This indicates that LaTRO equipped with self-consistency can further enhance performance, even with LaTRO's focus on training-time optimization.

Question: Frankie and Binkie went bowling together. Frankie's score was 15 better more than twice as high as Binkie's. If Binkie bowled a score of 90, what was Frankie's score? Let's think step by step.
 Response (Base model): Let's break this problem down into steps:

1. We know that the difference between Frankie's score (F) and Binkie's score (B) is 15. So we can express Frankie's score as F = B + 15

2. We also know that Frankie's score is twice as high as Binkie's score. So we can write another equation: F = 2B

4693. Now, we have two equations with two unknowns. Let's solve for Frankie's score (F) by470setting the two equations equal to each other: -2B = B + 15 - Multiply both sides by 1 to get471rid of the fraction: 2B - B = 15 - Simplify: B = 15 (since subtracting B from 2B results in 15)4724. Now that we know Binkie's score, we can find Frankie's score using either of the equations473we created earlier. Let's use the first one (F = B + 15): -F = 15 + 15 - Frankie's score is 30474more than Binkie's score, which is 15 in this case. So Frankie's score is 15 + 15 = 30 + 15 = 45

The final answer is that Frankie's score was 45.

Reponse (SFT): Twice as many as Binkie's 90 score is equal to 2*90= «2*90=180»180. Therefore, 180-(180-15)=165 was the number Frankie bowled. The answer is 165

Response (LaTRO): Here's how to solve the problem: 1. We know that Binkie's score is 90. 2. The problem states that Frankie's score was 15 better more than twice as high as Binkie's score. This means that Frankie's score is 15 + (2 * 90) = 15 + 180 = 195.

Figure 4: Sample responses of a GSM8K question from Mistral-7B models, the errors are highlighted in red.

486 5.4 CASE STUDY

488 We take a closer look at the responses generated by the LaTRO fine-tuned models. We select a question from GSM8K and compare the responses from the base, the SFT model, and the LaTRO 489 finetuned model. We choose the set of responses from the Mistral-7B models that we evaluated. As 490 can be seen in Figure 4, the base model not only generates a lengthy response, it also makes a logical 491 mistake at the first step, where the correct equation to establish here is "F = 2B + 15". The SFT model 492 simplifies the answer and makes the first step correct. However, in the second step it first makes a 493 wrong equation, then makes an arithmetic error when evaluating this equation. Further, LaTRO can 494 give a concise and correct answer. We include more sample responses in Appendix C. 495

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6 CONCLUSION

In conclusion, this work introduces LaTRO, a principled framework for optimizing language models' 499 reasoning capabilities without external feedback or reward models. By formulating reasoning as 500 sampling from a latent distribution and leveraging self-rewarding, LaTRO enables models to concur-501 rently improve both their reasoning process and ability to evaluate reasoning quality. Our extensive 502 experiments across multiple model architectures and tasks demonstrate significant performance gains, 503 with LaTRO outperforming baseline models and supervised fine-tuning approaches. These findings 504 suggest that pre-trained LLMs possess latent reasoning capabilities that can be unlocked through our 505 proposed optimization approach, representing a significant step towards creating more intelligent 506 systems that can self-evolve their problem-solving capabilities. 507

While LaTRO shows promising results, there are some limitations to consider. The computational 508 cost of sampling multiple rationales during training could be prohibitive for very large models. Future 509 work could explore ways to reduce this computational overhead, such as using more efficient sampling 510 techniques or adaptive rationale generation. Other promising directions include investigating the 511 applicability of LaTRO to a wider range of reasoning tasks beyond math and science problems, and 512 exploring how to conduct multi-step reasoning learning to to enhance reasoning capabilities further. 513 Despite these limitations, our contributions advance both the state-of-the-art in LLM reasoning 514 capabilities and provide valuable insights into the nature of LLM alignment and its potential for 515 self-improvement.

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ADDITIONAL DETAILS ON OUR THEORETICAL FRAMEWORK А

A.1 PROOF OF PROPOSITION 2

Proof. We restate the objective as follows:

$$J(\theta) := \mathbb{E}_{(\boldsymbol{x},\boldsymbol{y})\sim\mathcal{D}_{\text{Gold}}} \left[\mathbb{E}_{\boldsymbol{z}\sim\pi_{\theta}(\cdot|\boldsymbol{x})} \left[\log \pi_{\theta}(\boldsymbol{y}|\boldsymbol{x}\oplus\boldsymbol{z}) \right] - \beta D_{\text{KL}} [\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})||\pi_{0}(\boldsymbol{z}|\boldsymbol{x})] \right],$$

$$= \mathbb{E}_{(\boldsymbol{x},\boldsymbol{y})\sim\mathcal{D}_{\text{Gold}}} \left[\mathbb{E}_{\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})} [\log \pi_{\theta}(\boldsymbol{y}|\boldsymbol{x}\oplus\boldsymbol{z}) - \log \pi_{\theta}(\boldsymbol{z}|\boldsymbol{x}) + \log \pi_{0}(\boldsymbol{z}|\boldsymbol{x})] \right],$$

where $\beta > 0$ is a positive coefficient to control the regularization strength. We take the gradient w.r.t θ at each sample pair $(\boldsymbol{x}, \boldsymbol{y})$, and we get

$$\begin{aligned} \nabla_{\theta} J(\theta; \boldsymbol{x}, \boldsymbol{y}) &:= \nabla_{\theta} \int (\pi_{\theta}(\boldsymbol{z} | \boldsymbol{x})) (\log \pi_{\theta}(\boldsymbol{y} | \boldsymbol{x} \oplus \boldsymbol{z}) - \beta \log \pi_{\theta}(\boldsymbol{z} | \boldsymbol{x}) + \beta \log \pi_{0}(\boldsymbol{z} | \boldsymbol{x})) d\boldsymbol{z} \\ &= \mathbb{E}_{\pi_{\theta}(\boldsymbol{z} | \boldsymbol{x})} \left[\nabla_{\theta} \log \pi_{\theta}(\boldsymbol{z} | \boldsymbol{x}) \left(\log \pi_{\theta}(\boldsymbol{y} | \boldsymbol{x} \oplus \boldsymbol{z}) - \beta \log \frac{\pi_{\theta}(\boldsymbol{z} | \boldsymbol{x})}{\pi_{0}(\boldsymbol{z} | \boldsymbol{x})} \right) \right] \\ &+ \mathbb{E}_{\pi_{\theta}(\boldsymbol{z} | \boldsymbol{x})} \left[\nabla_{\theta} \log \pi_{\theta}(\boldsymbol{y} | \boldsymbol{x} \oplus \boldsymbol{z}) - \beta \nabla_{\theta} \log \pi_{\theta}(\boldsymbol{z} | \boldsymbol{x}) \right]. \end{aligned}$$

We further define $r(z) := \log \pi_{\theta}(y|x \oplus z) - \beta \log \frac{\pi_{\theta}(x|z)}{\pi_0(x|z)}$, and use the fact that $\mathbb{E}_{\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})}[\nabla_{\theta}\log \pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})] = \int \pi_{\theta}(\boldsymbol{z}|\boldsymbol{x}) \frac{\nabla_{\theta}\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})}{\pi_{\theta}(\boldsymbol{z}|\boldsymbol{x})} d\boldsymbol{z} = \nabla_{\theta} \int \pi_{\theta}(\boldsymbol{z}|\boldsymbol{x}) d\boldsymbol{z} = 0.$ we obtain the final gradient as

$$\nabla_{\theta} J(\theta; \boldsymbol{x}, \boldsymbol{y}) = \mathbb{E}_{\pi(\boldsymbol{z}|\boldsymbol{x})} \left[\nabla_{\theta} \log \pi_{\theta}(\boldsymbol{z}|\boldsymbol{x}) \cdot r(\boldsymbol{z}) + \nabla_{\theta} \log \pi_{\theta}(\boldsymbol{y}|\boldsymbol{z}, \boldsymbol{x}) \right]$$

And when we use RLOO estimator with empirical samples, we can replace above gradient estimation with empirical samples, which gives us the following result:

$$\nabla_{\theta} \widehat{J}(\theta) := \frac{1}{NK} \sum_{i=1}^{N} \sum_{k=1}^{K} \left(\nabla_{\theta} \log \pi_{\theta}(\boldsymbol{x}_{i} \mid \boldsymbol{z}_{k}^{(i)}) \cdot A_{k}^{(i)} + \nabla_{\theta} \log \pi_{\theta}(\boldsymbol{y}_{i} \mid \boldsymbol{z}_{k}^{(i)} \oplus \boldsymbol{x}_{i}) \right),$$

with
$$A_k^{(i)} = r(\boldsymbol{z}_k^{(i)}) - \frac{1}{K-1} \sum_{j \neq k}^K r(\boldsymbol{z}_j^{(i)}), r(\boldsymbol{z}_k^{(i)}) := \log \pi_{\theta}(\boldsymbol{y}_i \mid \boldsymbol{x}_i \oplus \boldsymbol{z}_k^{(i)}) - \beta \log \frac{\pi_{\theta}(\boldsymbol{x}_i \mid \boldsymbol{z}_k^{(i)})}{\pi_0(\boldsymbol{x}_i \mid \boldsymbol{z}_k^{(i)})},$$

which completes the proof.

PROMPT TEMPLATES В

In this section, we list all prompt templates used in our experiments. For the GSM8K dataset, we used a minimum prompt template. For the ARC-Challenge dataset, we use a CoT template for the base model and LaTRO fine-tuning, and another template direct answer generation in SFT.

{question} Let's think step by step.

Figure 5: CoT template for GSM8K

Question: {question} Options: {choices["text"] } Let's think step by step first then print your answer like 'The answer is (one of the options)'.""",

Figure 6: CoT template for ARC-Challenge

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865	The output MUST strictly follow the structure and format described below:
866	1. The answer should be strictly one of the options given in the question
867	2. Do not include any text after you choose an option.
868	**Example:**
869	Question: (question here)
870	Options: [option1, option2, option3]
871	The answer is: (one of the options).
872	Question: {question}
873	Options: {choices["text"]}
874	

Figure 7: Direct answer generation template for ARC-Challenge

C SAMPLE RESPONSES

Question: 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 for them? Let's think step by step.

Response (Base model):

Step 1: Determine the cost of one regular glass and one discounted glass. One regular glass costs \$5. Every second glass costs 60% of the price of a regular glass, so: 60% of 5 = 0.60*5 = \$3

Step 2: Calculate the total number of regular and discounted glasses. Kylar wants to buy 16 glasses in total. Since every second glass is discounted, we can divide the total number of glasses by 2 to find the number of discounted glasses: 16 glasses / 2 = 8 discounted glasses Now, subtract the number of discounted glasses from the total number of glasses to find the number of regular glasses: 16 glasses - 8 discounted glasses = 8 regular glasses Step (did not finish)

Response (LaTRO₂₀₀): Let's break it down:

1. Kylar needs to buy 16 glasses.

2. Every second glass costs 60% of the original price (\$5), which is \$3.

3. So, for every pair of glasses (one full price and one discounted), Kylar pays 5 + 3 = 8.

4. Since he needs 16 glasses, he buys 8 pairs. 5. Therefore, Kylar needs to pay 8 pairs * \$8

per pair = \$64. So, Kylar needs to pay \$64 for the 16 glasses. The answer is 64.

Figure 8: Sample responses of a GSM8K question, from Phi-3.5 models, maximum generation length L = 200. The base model does not finish the generation, while the LaTRO model generates a short and correct answer.

Question: Water, ice, and steam all have different temperatures. What is the order from
coldest to hottest?
Options : ['ice, water, steam', 'ice, steam, water', 'steam, ice, water', 'steam, water, ice']
Response (Base model) : To determine the order from coldest to hottest, let's evaluate each
option.
- Ice: It is the solid form of water and is typically around $0^{\circ}C$ (32°F).
- Water: It is the liquid form of water and is usually around 100°C (212°F) or 0°C (32°F) a
standard pressure and temperature conditions, respectively.
- Steam: It is the gaseous form of water and is typically at a temperature equal to or greate
than 100°C (212°F) at standard pressure conditions, depending on the pressure and othe
factors.
Option 1: 'ice, water, steam' - This order seems incorrect since steam is typically hotter that
water at standard conditions.
Option 2: 'ice, steam, water' - This order is incorrect because ice is the coldest, but the relativ
order of water and steam is opposite of what we know.
Option 3:'steam, ice, water' - This order is incorrect since ice is colder than steam.
Option 4:'steam, water, ice' - This order seems the most plausible, considering that steam i
hotter than water and water is hotter than ice.
The answer is 'steam, water, ice'.
Response (SFT): water, ice, steam
Response (LaTRO): To determine the order from coldest to hottest, let's analyze each option
1. Ice has a solid form and a fixed temperature, which is typically around 0°C (32°F) a
standard pressure.
2. Water is liquid and exists at a temperature of 0°C (32°F) at standard pressure, melting poir
of ice.
3. Steam is the gaseous state of water and is typically around 100°C (212°F) at standard
pressure.
Based on this information, we can now order them from coldest to hottest:
First, we have ice, as it is the coldest. Then, we have water at 0°C, which is the middl
temperature. Lastly, we have steam, which is the hottest.
So, the order from coldest to hottest is 'ice, water, steam'.
The answer is ['ice, water, steam'].