RATIONAL METAREASONING FOR LARGE LANGUAGE MODELS

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ABSTRACT

Being prompted to engage in reasoning has emerged as a core technique for using large language models (LLMs), deploying additional inference-time compute to improve task performance. However, as LLMs increase in both size and adoption, inference costs are correspondingly becoming increasingly burdensome. How, then, might we optimize reasoning's cost-performance tradeoff? This work introduces a novel approach based on computational models of metareasoning used in cognitive science, training LLMs to selectively use intermediate reasoning steps only when necessary. We first develop a reward function that incorporates the Value of Computation by penalizing unnecessary reasoning, then use this reward function with Expert Iteration to train the LLM. Compared to few-shot chain-of-thought prompting and STaR, our method significantly reduces inference costs (20-37% fewer tokens generated across three models) while maintaining task performance across diverse datasets.

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1 INTRODUCTION

027 Large language models (LLMs) rely on substantial computational power to handle complex problems (OpenAI et al., 2024; Chowdhery et al., 2022; de Vries, 2023). While initial studies mostly focused on the 029 cost of training (Verdecchia et al., 2023), LLMs' widespread deployment has made inference-time costs an increasingly important factor. Model compression techniques such as quantization, pruning, and knowledge 030 distillation can lower post-training costs (Wan et al., 2024). However, there is a fundamental tension between 031 inference cost and task performance: while many of these methods reduce costs at the expense of performance, others, such as chain-of-thought prompting (CoT; Wei et al., 2023; Kojima et al., 2023), do the opposite, 033 raising inference costs to enhance task performance (Snell et al., 2024). It is worth noting that none of the previous approaches are *adaptive*: model compression modifications and existing CoT methods tend to raise 035 or lower the inference cost on *all* queries, regardless of task complexity. 036

In stark contrast to this static tradeoff, humans are able to adaptively allocate computational resources based 037 on task difficulty (Krämer, 2014; Russell, 1997; Lieder & Griffiths, 2017). In this work, we draw inspiration 038 from rational metareasoning – literally, reasoning about reasoning – a concept originally from the artificial intelligence literature (Russell & Wefald, 1991) that has been used to explain how humans adaptively manage 040 computational resources (Lieder & Griffiths, 2017; Lieder et al., 2018; Griffiths et al., 2019a). Building 041 on this, we develop a novel reward function based on the Value of Computation (VOC; Russell & Wefald, 1991), which formalizes the trade-off between inference cost and task performance. We adopt an iterative 043 reinforcement learning process inspired by the Expert Iteration algorithm (Anthony et al., 2017). In each iteration, we generate multiple reasoning chains for each question. These reasoning chains are ranked using 045 the reward function, and the dataset is filtered to retain only the best reasoning chain for each question. The model is then fine-tuned using this filtered dataset. However, unlike previous applications of Expert Iteration

to LLMs (Zelikman et al., 2022), which filter generated examples based on correctness, our method optimizes for both the correctness *and the cost* of the reasoning process.

We evaluated the effectiveness of our solution across a diverse set of tasks, from science knowledge (ARC; Clark et al., 2018) to commonsense reasoning (CommonsenseQA; Talmor et al., 2019), mathematical problem solving (GSM8K; Cobbe et al., 2021), and logical deductive reasoning (ProofWriter; Tafjord et al., 2021). Additionally, we assess the out-of-domain generalization on MMLU (Hendrycks et al., 2021), a multitask benchmark. Our approach achieves a substantial reduction in generated tokens (35.6-37.4% compared to few-shot prompting and 20.1-27.3% compared to STaR; Zelikman et al. 2022) while retaining comparable performance. Thus, we make the following contributions:

- 1. We introduce the idea of using rational metareasoning to optimize the tradeoff between inference cost and performance of LLMs.
- 2. We formalize a novel reward function inspired by the Value of Computation (VOC) and integrate it into LLM training.
- 3. We empirically demonstrate that rational metareasoning achieves the same task performance at lower inference costs (20-37% fewer tokens on average) across various datasets and reasoning tasks.

2 RATIONAL METAREASONING

069 Unlike artificial intelligence, humans have limited time and cognitive resources (Griffiths et al., 2019b; 070 Griffiths, 2020). We face diverse challenges requiring different approaches: avoiding a sudden obstacle when 071 driving needs quick, intuitive thinking, whereas selecting a retirement investment strategy requires slow, 072 deliberate reasoning (Krämer, 2014). Rational metareasoning (Russell & Wefald, 1991) suggests agents 073 should adapt their reasoning based on the problem at hand. Intuitively, while reasoning solves a problem, 074 metareasoning solves the problem of *how* to solve a problem: deciding which computations to perform 075 while problem-solving. The essence of rational metareasoning is calculating the value of computation (VOC; Russell & Wefald, 1991) for each potential computation. The VOC balances the benefit of computation c 076 (characterized by the expected increase in the agent's eventual utility) against its cost (usually time or energy). 077

To formalize this, agents are assumed to have some internal belief state $b \in \mathcal{B}$, which determines their expectation about the value of each action $a \in \mathcal{A}$: $\mathbb{E}[U(a)|b]$. A rational agent would simply choose the highest-value action: $a^* = \arg \max_{a \in \mathcal{A}} [U(a)|b]$. In contrast, a meta-rational agent can perform computation to change their belief state before choosing an action. Each computation $c \in \mathcal{C}$ updates the agent belief to b' with probability P(b'|c), which in turn affects their beliefs about the value of actions. However, each computation has an associated cost (cost(c)). The VOC then quantifies the value of performing computation c given a starting belief state b,

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$$VOC(c,b) = \mathbb{E}_{P(b'|c)}[\max_{a'} \mathbb{E}[U(a')|b'] - \max_{a} \mathbb{E}[U(a)|b]] - \operatorname{cost}(c).$$
(1)

Thus, a meta-rational agent should pursue the computation c^* with the highest VOC: $c^* = \arg \max_{c \in C} VOC(c, b)$. If no computation has positive VOC, the agent should stop thinking and act in the world. Rational meta-reasoning can explain how humans allocate cognitive resources in various tasks (Lieder & Griffiths, 2017; Lieder et al., 2018; Callaway et al., 2018; 2021; 2022; Russek et al., 2022).

3 RATIONAL METAREASONING WITH LARGE LANGUAGE MODELS

To achieve an optimal balance between performance and efficiency, our approach introduces a new VOCinspired reward function (Eq. 2) into an Expert Iteration training loop (Anthony et al., 2017; Zelikman et al., 2022), fine-tuning a LLM to produce reasoning chains adaptively depending on task difficulty.

3.1 REWARD MODELING

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Chain-of-thought prompting is a technique in which a language model is encouraged to generate an intermediate output – a "chain of thought" – prior to producing the answer to a question (Wei et al., 2023; Kojima et al., 2023) We define the reward of a chain of thought as the difference between its utility and its cost,

$$\mathcal{R}_{\pi}(x, y, z) = \mathcal{U}_{\pi}(z|x, y) - \mathcal{C}(z) \tag{2}$$

where x denotes the input for the task, z represents the chain of thought, and y is the target solution. The utility of the chain of thought is represented by $\mathcal{U}_{\pi}(z|x, y)$, and the cost of the intermediate computations is denoted by $\mathcal{C}(z)$. Equation 2 mirrors the VOC Equation 1: here, individual reasoning tokens correspond to intermediate computations c, making the reasoning chain z a sequence of computations c, while the actions $a \in \mathcal{A}$ map to the potential outputs $y \in \mathcal{Y}$ of the language model. In the context of LLMs, utility quantifies the increase in the likelihood of generating the target sequence y when the chain of thought z is added to the input x, under the policy π :

$$\mathcal{U}_{\pi}(z|x,y) = \log \pi_{\theta}(y|z,x) - \log \pi_{\theta}(y|x).$$
(3)

115 Specifically, $\pi_{\theta}(y|z, x)$ indicates the probability of generating the target sequence y given both the chain of 116 thought z and the input x, while $\pi_{\theta}(y|x)$ denotes the probability of generating y with only the input x. With 117 respect to Equation 1, the language model's initial belief about the value of actions or outputs is described by 118 $\pi_{\theta}(y \mid x)$ (from Equation 3), whereas its final belief after generating a sequence of computations or tokens 119 (a chain of thought z) is described by $\pi_{\theta}(y \mid z, x)$. The cost is directly proportional to the logarithm of the 120 number of tokens in the chain of thought l(z):

$$\mathcal{C}(z) = \gamma \cdot \log l(z). \tag{4}$$

The hyperparameter γ scales the cost and utility to the same magnitude. We found that both linear and logarithmic cost functions perform adequately in our training algorithm, but the latter was better at balancing utility and cost, especially with higher sequence-length variance. A key benefit of this reward function is that it is parameterized by the same weights θ as the generative policy π_{θ} , eliminating the need for an external reward model. This allows for direct estimation of the utility of a reasoning chain using the policy itself.

3.2 COT GENERATION

We begin with a pretrained language model π_{θ} and an initial dataset of problems x along with their corre-130 sponding correct final answers $y: \mathcal{D} = \{(x_i, y_i)\}_{i=1}^{D}$. Following prior work in online RL (Tang et al., 2024), 131 we utilize the model itself to generate the reasoning chains, with few-shot prompting as a guide. Specifically, 132 we concatenate a small set of examples, denoted as \mathcal{P} , each containing intermediate reasoning chains z, to 133 each example in \mathcal{D} . For each task $\tau_i = (x_i, y_i)$ in the original dataset \mathcal{D} , we generate K reasoning chains: 134 $\hat{\tau}_i = \{(x_i, z_{k,i}, y_i)\}_{k=1}^K$. If none of the K generated reasoning chains for a task τ_i leads to the correct answer, 135 we discard all samples. To minimize the likelihood of this outcome, we adopt the rationalization approach 136 introduced by STaR (Zelikman et al., 2022): if the model fails to generate the correct answer, we generate a 137 new reasoning chain by supplying the model with the correct answer in the prompt. Intuitively, rationalization 138 increases the sample size, providing more options when selecting the $\arg \max$ of the VoC reward. We found that it provided marginal reduction in length with no effect on performance. Finally, we assess each reasoning 139 140 chain using the Rational Metareasoning reward function (Equation 2).

141 3.3 METAREASONING TRAINING

We demonstrate the effectiveness of our reward using a variation of the Expert Iteration algorithm (EI, Anthony et al., 2017). EI is known for its sample efficiency and strong performance on reasoning tasks (Havrilla et al., 2024; Zelikman et al., 2022). As an example of an online reinforcement learning (RL) algorithm, EI involves both exploration and policy improvement phases, with the policy π_{θ} being updated using data from the exploration phase. STaR (Zelikman et al., 2022) applies EI to LLMs by iteratively generating reasoning chains via few-shot prompting and compiling them into a fine-tuning dataset to refine the model. We build on this framework for our rational metareasoning training process, described in Algorithm 1.

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Algorithm 1 Rational Metareasoning Training 151 **Input** π : a pretrained LLM; dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{D}$ 152 1: $\pi_0 \leftarrow \pi$ ▷ Copy the original model 153 2: $\mathcal{D}_0 \leftarrow \emptyset$ 154 3: for *n* in 1...*N* do ▷ Iterations 155 $\mathcal{D}_n \leftarrow \{\mathcal{T} \subseteq \mathcal{D} \mid |\mathcal{T}| = T\} \cup \mathcal{D}_{n-1}$ ▷ Sample batch from dataset 4: 156 for k in 1...K do ▷ Perform reasoning chain generation 5: 157 $(z_{i,k}, y_{i,k}) \leftarrow \pi_{n-1}(x_i) \quad \forall i \in [1, D_i]$ 6: 158 $(z_{i,k}, y_{i,k}) \leftarrow \pi_{n-1}(\operatorname{add_hint}(x_i)) \quad \forall i \in [1, D_i] \land y_{i,k} \neq y_i$ 7: ▷ Compute rationalization 159 8: end for 160 $r_{i,k} \leftarrow \mathcal{R}_{\pi_{n-1}}(x_i, y_i, z_{i,k}) \quad \forall i, k (i \in [1, D_i] \land y_{i,k} = y_i)$ ▷ Compute reward 9: 161 $\hat{z}_i \leftarrow \arg\max_k \{r_{i,k}\}_{k=1}^K \\ \mathcal{D}_n^* \leftarrow \{(x_i, \hat{z}_i, y_i) \in [1, D_i]\}$ \triangleright Select best reasoning chain for each task *i* 10: 162 11: ▷ Create the optimal dataset 163 12: $\pi_n \leftarrow \operatorname{train}(\pi, \mathcal{D}_n^*)$ ▷ Finetune the original model on the optimal solutions 164 13: end for

Initially, in the exploration phase, we approximate the optimal policy $\hat{\pi}^*$ (whose computations maximize 166 the VoC reward) by using rejection sampling on our student policy π_{θ} . After generating K intermediate 167 reasoning chains z_1, \ldots, z_K for a given question x (Section 3.2), we evaluate them using our reward function 168 \mathcal{R}_{π} (Section 3.1). We then construct $\mathcal{D}_{1}^{*} = \{(x_{i}, z_{i}, y_{i})\}_{i=1}^{N}$ by setting the rejection sampling threshold dynamically to the highest reward for each task *i*, therefore increasing robustness to hyperparameter choices : 169 170 $z_i = \arg \max_k \{\mathcal{R}_{\pi}(x, z_k, y)\}_{k=1}^K$. These rollouts are distilled into a policy π_1 using standard cross-entropy 171 loss. This process can be iteratively repeated to refine the policy π_n on the dataset \mathcal{D}_n^* . Finally, similar to 172 STaR (Zelikman et al., 2024), instead of utilizing the entire training dataset at each iteration, as is typical 173 in standard EI algorithms (Anthony et al., 2017; Gulcehre et al., 2023), we begin with a batch of T steps 174 during the first iteration and progressively increase the number of fine-tuning training steps by T with each 175 subsequent iteration. This approach allows the model to encounter new examples gradually, resulting in 176 slower training initially, which ultimately enhances model performance. 177

4 EXPERIMENTS

We now detail the datasets (Sec. 4.1), baselines (Sec. 4.2), and training (Sec 4.3) used to evaluate our method.

4.1 DATASETS

In our efforts to develop a general-purpose reasoning model, we applied our training process and assessed its effectiveness across a diverse range of datasets and reasoning tasks. We constructed our training set by combining the training sets from these datasets into one dataset \mathcal{D} and then evaluated the model on all corresponding test sets \mathcal{T} . Below is a detailed description of the datasets used:

• ARC (Clark et al., 2018). The AI2 Reasoning Challenge (ARC) dataset comprises grade-schoo	1
science questions, designed to evaluate a model's capability to apply scientific knowledge.	

- **CommonsenseQA** (Talmor et al., 2019). This dataset is centered on commonsense question answering. It leverages implicit human knowledge that is commonly known and sensible, testing the model's ability to provide answers based on everyday reasoning.
- **GSM8K** (Cobbe et al., 2021). This dataset includes a variety of linguistically diverse grade school math word problems. It assesses the model's proficiency in solving mathematical problems that require comprehension and application of arithmetic reasoning.
 - **ProofWriter** (Tafjord et al., 2021). This dataset assesses logical deductive reasoning by asking the model to determine if a conclusion can be inferred from premises presented in natural language.

These datasets have very different train split sizes. To ensure fairness and balance between the datasets, and to manage computational costs, we composed our training mixture by sampling 1,024 random samples from each of the training sets. We then evaluated the model on the public test set of each dataset. To further assess the generalization of our approach, we conducted out-of-distribution testing on **MMLU** (Hendrycks et al., 2021), a massive multitask benchmark consisting of multiple-choice questions from various branches of knowledge. Again, to limit computational costs, we conducted the test on the first 100 samples of each subject within the MMLU benchmark, giving us a total of 5700 questions across 57 subjects.

4.2 BASELINES

209 We illustrate the advantages of our model by comparing its performance to two types of prompting strategies: 210 Direct prompting, where the model is required to provide an immediate answer, and Chain of Thought 211 prompting (CoT), where the model is encouraged to reason through the problem step-by-step before arriving 212 at a solution. Since we are using pretrained models which are not specifically trained for instruction following, 213 we provide five few-shot examples for each task from the unused portion of the training dataset. These 214 examples are carefully chosen to ensure that the length of the reasoning chain matches the perceived difficulty 215 of the question. In addition to these prompting methods, we adopt a finetuning baseline, comparing our 216 method to STaR (Self-Taught Reasoner; Zelikman et al. 2022), which also uses the expert iteration algorithm. 217 While CoT prompting may not yield optimal trajectories, more advanced methods (Yao et al., 2023a; Zheng et al., 2024; Madaan et al., 2023) often increase sequence lengths. Focusing on efficiency, we find CoT's 218 simplicity ideal for testing our method. Reducing reasoning tokens without performance loss here suggests 219 similar gains in more complex approaches. 220

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4.3 TRAINING DETAILS

For our experiments, we use Microsoft Phi-2 (Javaheripi et al., 2023), Meta Llama-3-8B (Dubey et al., 2024), 224 and Mistral-7B-v0.3 (Jiang et al., 2023) as the pretrained base models. We have chosen $\gamma = 0.1$ to align 225 the distributions of costs and rewards more closely, although we have found the method to be robust to 226 small variations in the choice of this hyperparameter. We sample K = 4 reasoning chains for each question, 227 using a temperature t of 0.5 and a top_p value of 0.9. These parameters are chosen to balance the exploration 228 and exploitation trade-off, allowing us to generate diverse yet relevant reasoning chains. For each iteration 229 n, we sample a dataset \mathcal{D}_n of size 512 from the union of four training datasets \mathcal{D} described in 4.1. In the 230 self-supervised fine-tuning step, we use a batch size of 16 and a learning rate of 1e-6. We believe that 231 further improvements are possible through a more comprehensive hyperparameter search; however, due 232 to computational constraints, we leave this for future work. Finally, we evaluate all models using greedy 233 decoding to ensure consistent and deterministic output generation. We use pattern matching techniques to extract the answers; an exact match between the generated answer and the ground truth is considered correct.

	Model	Method	Accuracy (%) ↑	# Input Tokens \downarrow	# Output Tokens↓
		Direct Few-Shot	50.7 (± 1.3)	441.6 (± 0.9)	$0.0 (\pm 0.0)$
	mhi J	CoT Few-Shot	56.6 (± 1.3)	$1047.3 (\pm 0.9)$	$193.9 (\pm 4.3)$
	phi-2	STaR	63.2 (± 1.5)	75.1 (± 0.9)	$156.9 (\pm 2.4)$
		Metareasoning	64.7 (± 1.4)	75.1 (± 0.9)	123.1 (± 2.1)
		Direct Few-Shot	55.5 (± 1.3)	421.3 (± 0.9)	$0.0 (\pm 0.0)$
	Mata Llama 2 0D	CoT Few-Shot	63.7 (± 1.4)	$995.0 (\pm 0.9)$	$148.4 (\pm 3.1)$
	Meta-Llama-3-8B	STaR	63.9 (± 1.3)	73.3 (± 0.8)	119.7 (± 2.0)
		Metareasoning	64.4 (± 1.4)	73.3 (± 0.9)	95.6 (± 2.2)
		Direct Few-Shot	52.7 (± 1.4)	498.2 (± 1.0)	$0.0 (\pm 0.0)$
	Mistral-7B-v0.3	CoT Few-Shot	57.5 (± 1.5)	$1180.9 (\pm 1.1)$	$182.7 (\pm 4.3)$
		STaR	60.1 (± 1.3)	83.2 (± 0.9)	$157.4 (\pm 2.0)$
		Metareasoning	60.5 (± 1.5)	83.2 (± 1.0)	114.4 (± 2.2)

Table 1: Comparison of different methods based on accuracy and length metrics, averaged across datasets (means with 95% confidence intervals; bold indicates best performing approaches with overlapping 95% intervals; see Tables 4 and 5 for per-dataset results). Metareasoning achieves comparable performance while using significantly fewer input and output tokens compared to STaR or CoT Few-Shot prompting.

5 Results

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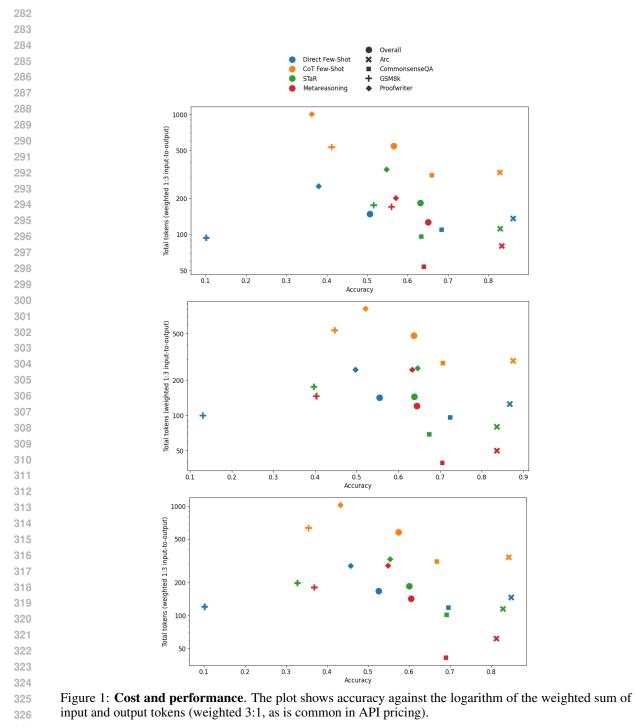
5.1 PERFORMANCE VS COST

258 We first evaluate our approach against baselines (Sec. 4.2) across several datasets (Sec. 4.1). Our key criteria 259 are *performance* (measured by accuracy) and *cost* (measured by the number of input and output tokens). 260 Our experiments confirm that across all three models and four datasets, our training approach reduces cost while matching or improving performance (see Table 1 for results averaged across datasets; Tables 4 and 5 261 for per-dataset results; and Appendix E for example reasoning chains). Fig. 1 shows these results for all 262 three models: the y axis compares cost across different baselines and datasets, while the x axis compares 263 performance. We first consider the performance of our baselines: CoT Few-Shot prompting uses a large 264 number of input and output tokens, but yields reasonable performance. In contrast, Direct Few-Shot prompting 265 uses fewer input (and far fewer output) tokens, but yields poor performance on reasoning-intensive datasets 266 (GSM8K and Proofwriter, see Table 4). STaR improves on all of these approaches, using significantly fewer 267 tokens, while achieving comparable or superior performance. Finally, Metareasoning further improves the 268 cost-performance tradeoff by matching STaR's accuracy while generating 20-37% fewer tokens on average. 269

5.2 ADAPTIVE COMPUTATION

272 Section 5.1 demonstrates that our method reduces computational costs on average. But does it actually 273 teach models to reason *adaptively* (by adjusting reasoning to match task complexity), or just to reason *less*? To address this question, we first divided our test set \mathcal{T} based on whether or not reasoning was needed to 274 obtain the correct answer. We split the data based on whether Direct Few-Shot on Phi-2 obtained the correct 275 answer. This yielded a split of 4412 "easy" and 2700 "hard" examples. Adaptive methods should use less 276 computation to solve the easy problems. We can empirically compare the results across methods for these 277 two data splits. As shown in Table 2, all models and methods are able to differentiate between hard and 278 easy problems, generating fewer tokens on easier problems.¹ Intriguingly, STaR decreases the difference 279

¹We note that we specifically chose CoT few shot examples that demonstrated adaptive reasoning length; we expect the effects here to be dependent on the chosen examples.



Model	Method	Hard Split	Easy Split	Length Reduction (%)
	CoT Few-Shot	$145.0 (\pm 4.0)$	86.0 (± 2.0)	40.7
Phi-2	STaR	135.0 (± 4.0)	91.0 (± 1.0)	32.6
Phi-2	Metareasoning	$122.0 (\pm 4.0)$	57.0 (± 3.0)	53.3
	CoT Few-Shot	132.0 (± 3.0)	57.0 (± 1.0)	56.8
Mata Ilama 2.0D	STaR	126.0 (± 3.0)	$64.0 (\pm 2.0)$	49.2
Meta-Llama-3-8B	Metareasoning	99.5 (± 2.5)	$27.0 (\pm 1.0)$	72.9
	CoT Few-Shot	$144.0 (\pm 4.0)$	77.0 (± 3.0)	46.5
Misture 1 7D 0 2	STaR	$149.0 (\pm 6.0)$	98.0 (± 1.0)	34.2
Mistral-7B-v0.3	Metareasoning	125.0 (± 3.0)	32.0 (± 1.0)	74.4

Table 2: The length of generated reasoning chains across models and methods (mean number of tokens with 95% confidence intervals). Adaptive methods should maximize the difference in length between the two distributions. Our method (Metareasoning) reduces the overall length and increases the difference in the length distribution between the Hard and Easy splits (as seen in column Length Reduction), demonstrating an improvement in the model's ability to adapt the reasoning length to the complexity of the task.

Model	Method	Accuracy (%) \uparrow	# Output Tokens ↓
Phi-2	STaR Metareasoning	$\begin{array}{c} 47.9 \ (\pm \ 1.3) \\ 48.1 \ (\pm \ 1.3) \end{array}$	110.5 (± 1.5) 78.7 (± 1.5)
Meta-Llama-3-8B	STaR Metareasoning	$56.3 (\pm 1.1) \\ 54.5 (\pm 1.4)$	75.4 (± 1.4) 48.8 (± 2.1)
Mistral-7B-v0.3	STaR Metareasoning	$54.5 (\pm 1.3) \\ 54.0 (\pm 1.4)$	112.0 (± 1.6) 50.6 (± 1.5)

Table 3: Comparison of different methods based on accuracy and length metrics in an out-of-distribution setting on the MMLU benchmark. We report the mean with 95% confidence intervals. Metareasoning achieves comparable performance while generating significantly fewer output tokens compared to STaR.

in reasoning length between hard and easy problems, suggesting that it trains out this adaptive tendency, biasing the model towards using reasoning on all problems. In contrast, Rational Metareasoning *increases* the difference in reasoning between hard and easy problems, achieving a length reduction of up to 74.4% on Mistral 7B. This indicates that our approach trains models to reason adaptively, helping them recognize when detailed reasoning is necessary and when a shorter response is sufficient.

5.3 GENERALIZATION

We assess the out-of-distribution generalization of our method using the MMLU benchmark (Hendrycks et al., 2021, see Section 4.1). As presented in Table 3, our approach achieves comparable performance while generating 28.8% to 54.8% fewer tokens compared to STaR. Among the 57 subcategories of MMLU, Fig. 2 highlights four—high school chemistry, mathematics, U.S. history, and macroeconomics—that effectively showcase the strengths of our model. We specifically chose two subjects (U.S. history and macroeconomics) where the use of chain-of-thought (CoT) reasoning appears to be counterproductive compared to Direct Few-Shot prompting, as well as two subjects (mathematics and chemistry) where the benefits of CoT are more pronounced. Consistent with our findings from the four in-domain datasets, we observe that the reduction in output length achieved by our method is inversely related to the benefits gained from intermediate reasoning

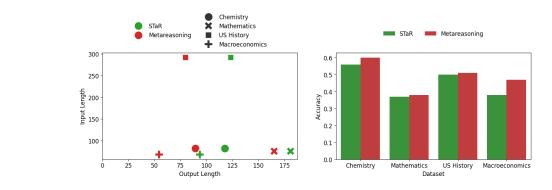


Figure 2: Cost and Performance for Phi-2 Across Selected MMLU Domains. Left panel: Input and output token distributions for different methods and domains. Right panel: While CoT improves performance in subjects like mathematics and chemistry, it appears less effective in history and macroeconomics. The latter domains show a greater reduction in output tokens (35% for history and 37% for macroeconomics), compared to the smaller reductions seen in chemistry (20%) and mathematics (12%), where intermediate reasoning chains provide more substantial benefits.

chains. In the cases of U.S. history and macroeconomics, our method results in a substantial reduction in generated tokens. In contrast, in mathematics and chemistry, the reduction in token count is smaller.

6 RELATED WORK

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6.1 REDUCING INFERENCE COSTS

402 The rising cost of deploying large language models (LLMs) has driven efforts to reduce inference costs. 403 Techniques such as Speculative Decoding (Leviathan et al., 2023) and Medusa (Cai et al., 2024) improve 404 efficiency through parallelization, while Mixture of Experts (Jacobs et al., 1991; Zhou et al., 2022) activates 405 only a subset of LLM parameters during decoding. Though effective, these methods require significant 406 architectural changes and don't adapt computation based on task difficulty. Other approaches have developed 407 neural architectures that enable adaptive computation (Graves, 2017; Banino et al., 2021; Dehghani et al., 2019; Mohtashami et al., 2023; Schuster et al., 2022) but involve new architectures or training methods. In 408 contrast, our approach uses existing architectures and pretrained models, modifying only the fine-tuning 409 process. More similar to our approach, model routing (Ong et al., 2024; Jiang et al., 2024) optimizes resource 410 utilization based on query complexity by routing easier queries to smaller models and harder queries to larger 411 ones. However, this necessitates multiple models and a router, while our approach trains a single model to 412 adaptively adjust its own outputs to match task complexity. 413

414 415 6.2 REASONING IN LLMS

Techniques such as Chain of Thought (CoT) and related methodologies (Wei et al., 2023; Yao et al., 2023a; Yasunaga et al., 2024; Madaan et al., 2023; Zheng et al., 2024) have proven effective at enhancing LLM
performance across a wide range of tasks. CoT boosts LLMs' performance on complex reasoning by guiding them through a series of intermediate reasoning steps, increasing inference costs to improve task performance. This method can be implemented through in-context learning (Wei et al., 2023), prompting (Kojima et al., 2023), or training (Li et al., 2023). The benefits of CoT can be attributed to both a greater computation depth (Goyal et al., 2024; Pfau et al., 2024) and the semantic values of the thought tokens, which function as

423 intermediate variables in the computation of the answer (Prystawski et al., 2023). However, recent studies 424 have raised concerns regarding the meaningfulness of such reasoning chains in reaching the target solution, 425 and whether models effectively utilize them to solve tasks (Turpin et al., 2023; Paul et al., 2024; Sprague et al., 426 2024). We further demonstrate that standard prompting and training methods fail to teach the model to use 427 CoT purposefully, resulting in inefficient inference. Reasoning can also be used to bootstrap language models. 428 Self-improving techniques (Huang et al., 2022; Zelikman et al., 2022) consist of generating reasoning chainaugmented answers for unlabeled questions and fine-tuning the LLM using those self-generated solutions 429 as target outputs. Similar techniques, such as ReST (Gulcehre et al., 2023), can also be used to better 430 align LLMs with human preferences and needs. Our approach builds on these techniques to optimize the 431 inference cost of reasoning chains in addition to their task performance. Another related work, Quiet-STaR 432 (Zelikman et al., 2024), has improved LLM reasoning performance by modifying pretraining to generate 433 intermediate s between tokens. While effective for downstream tasks, it increases computational costs by 434 generating reasoning chains at every step, even when unnecessary. More recently, chat models that "think 435 before answering" have been developed (OpenAI, 2024), using inference-time computation to enhance their 436 outputs. Although these models outperform others, they expend more computational resources on all tasks, 437 even when it may not be necessary. Our method could be incorporated into their training process to help the 438 model determine when this additional computation is genuinely beneficial.

7 CONCLUSION

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In this work, we introduced a novel method inspired by previous research in AI and cognitive science aimed at reducing inference costs in LLMs. We operationalize the concept of rational metareasoning – which formalizes humans' adaptive use of cognitive resources – with a novel reward function based on the Value of Computation (VOC). This reward function trains the LLM to optimize the use of intermediate reasoning steps in task execution, enabling it to balance task performance with computational efficiency. Empirically, we find that this approach significantly reduces the number of generated tokens and input context length while maintaining comparable performance across diverse datasets.

449 However, we note some limitations to our approach. First, the focus of our work here is enhancing the 450 efficiency of large language models in reasoning tasks, rather than the overall performance of such systems. 451 Thus, we aimed to reduce unnecessary intermediate reasoning steps, rather than improve the quality of 452 reasoning per se. It remains to be seen whether our approach can be extended to enhance task performance in 453 addition to computational efficiency. Additionally, we tested our approach on well-established datasets in science, commonsense reasoning, and math, but it remains untested in more specialized domains. Notably, 454 one of these untested settings is the agentic one, where LLMs act as agents to perform complex tasks in digital 455 environments (Yao et al., 2023b; Schick et al., 2023). Our method could be adapted by including the number 456 of LLM API calls to such tools in the cost section of our reward function, ideally encouraging the model to 457 minimize unnecessary tool calls. Broader testing could help assess its generalizability and effectiveness across 458 diverse contexts. Additionally, the VoC reward function is highly adaptable and can be used with various 459 algorithms. For instance, it can provide numerical rewards for PPO or guide DPO by training on samples 460 with the highest and lowest rewards. In this work, we focused on EI, the most sample-efficient algorithm 461 for reasoning tasks Havrilla et al. (2024), to demonstrate its generalization across models and benchmarks. 462 Exploring its application to other algorithms is an exciting direction for future research.

Most excitingly, our work demonstrates how cognitively-inspired reward functions can endow LLMs with desirable inference-time properties, opening a broad avenue of future work. Given its flexibility, this method could be integrated into instruction tuning to potentially enhance performance, even in scenarios where verifying the correctness of answers is challenging. Since the utility measure within the reward function can be tailored to prioritize any desired, measurable property, this approach offers the potential to guide models toward achieving these enhanced qualities while still benefiting from the reduced computational costs.

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А FULL RESULTS TABLES

Model	Method	ARC	Commonsenseqa	GSM8K	Proofwriter
	Direct Few Shot	86.1 (± 1.1)	68.4 (± 2.6)	$10.2 (\pm 1.6)$	38.0 (± 3.0)
Phi-2	Cot Few Shot	82.8 (± 1.2)	$66.0 (\pm 2.6)$	$41.2 (\pm 2.8)$	36.3 (± 3.1)
F 111-2	STaR	$82.9 (\pm 1.1)$	63.4 (± 2.9)	51.6 (± 2.8)	54.8 (± 2.8)
	Metareasoning	83.9 (± 1.3)	$61.6~(\pm 2.7)$	$54.9 (\pm 2.6)$	58.2 (± 2.9)
	Direct Few Shot	86.7 (± 1.0)	72.4 (± 2.5)	$13.1 (\pm 1.8)$	49.7 (± 3.1)
Meta-Llama-3-8B	Cot Few Shot	87.5 (± 1.2)	$70.6~(\pm 2.5)$	$44.7 (\pm 2.6)$	52.1 (± 3.0)
Meta-Liaina-3-0D	STaR	83.6 (± 1.2)	$67.4 (\pm 2.7)$	39.7 (± 2.5)	$64.6 (\pm 2.7)$
	Metareasoning	83.6 (± 1.2)	$70.5~(\pm 2.7)$	40.3 (± 2.8)	63.3 (± 2.8)
	Direct Few Shot	84.9 (± 1.3)	69.6 (± 2.6)	$10.2 (\pm 1.6)$	45.8 (± 2.9)
Mistral-7B-v0.3	Cot Few Shot	84.3 (± 1.2)	$66.8 (\pm 2.7)$	35.5 (± 2.4)	43.3 (± 2.9)
Mistral-/B-V0.3	STaR	$82.9 (\pm 1.4)$	$69.2 (\pm 2.5)$	32.8 (± 2.4)	55.4 (± 3.0)
	Metareasoning	81.3 (± 1.2)	$69.0 (\pm 2.3)$	$36.9 (\pm 2.8)$	54.9 (± 3.2)

Table 4: Comparison of accuracy of different methods across datasets and models. We report the mean with 95% confidence scores.

Model	Method	ARC	Commonsenseqa	GSM8K	Proofwriter
	Direct Few Shot	$0.0 (\pm 0.0)$	$0.0~(\pm 0.0)$	$0.0~(\pm 0.0)$	$0.0 (\pm 0.0)$
Phi-2	Cot Few Shot	$74.6 (\pm 1.4)$	$80.4 (\pm 2.2)$	$161.0 (\pm 2.9)$	459.6 (± 16.5)
F III-2	STaR	$91.4 (\pm 1.0)$	$80.6 (\pm 1.5)$	155.7 (± 3.1)	299.9 (± 7.2)
	Metareasoning	55.2 (± 1.2)	$53.0 (\pm 1.7)$	$143.8 (\pm 2.6)$	$240.4~(\pm 6.8)$
	Direct Few Shot	$0.0 (\pm 0.0)$	$0.0~(\pm 0.0)$	$0.0~(\pm 0.0)$	$0.0 (\pm 0.0)$
Meta-Llama-3-8B	Cot Few Shot	$59.5 (\pm 0.9)$	$69.9 (\pm 2.0)$	$157.1 (\pm 2.8)$	307.1 (± 11.4)
Wieta-Liaina-J-0D	STaR	61.3 (± 1.2)	55.7 (± 1.9)	$155.3 (\pm 2.8)$	$206.4 (\pm 6.2)$
	Metareasoning	$31.4 (\pm 0.7)$	$26.1 (\pm 0.7)$	$125.8 (\pm 4.7)$	$199.2~(\pm 8.2)$
	Direct Few Shot	$0.0~(\pm 0.0)$	$0.0~(\pm 0.0)$	$0.0~(\pm 0.0)$	$0.0 (\pm 0.0)$
Mistral-7B-v0.3	Cot Few Shot	$71.0 (\pm 1.4)$	$66.2 (\pm 2.3)$	174.8 (± 3.6)	418.8 (± 16.9)
	STaR	93.1 (± 1.3)	$85.0 (\pm 1.9)$	175.7 (± 3.8)	275.9 (± 5.7)
	Metareasoning	39.7 (± 1.0)	$25.0 (\pm 0.7)$	158.6 (± 3.6)	234.3 (± 7.2)

Table 5: Comparison of mean output length of different methods across datasets and models. We report the mean with 95% confidence scores.

В ALTERNATIVE PLOT OF ACCURACY VS COST

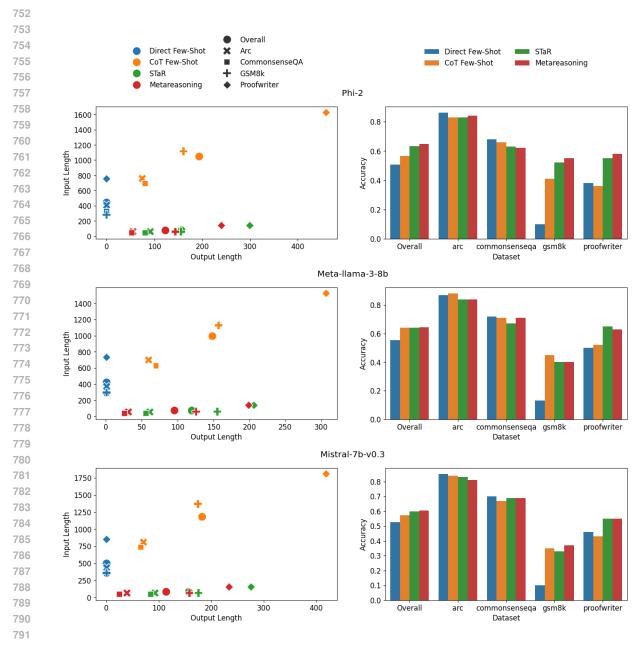


Figure 3: Cost and performance. Left panel: the distribution of input and output tokens across various methods and datasets. Our method, Metareasoning, eliminates the need for few-shot prompting (reducing input tokens) and trains the model to use fewer reasoning tokens compared to STaR. Right panel: Metareasoning matches or improves accuracy relative to other methods, despite substantially reducing inference costs. Across datasets, the reduction in token count (left) is inversely related to the effectiveness of the CoT (right): the model learns that CoT is essential in GSM8K and Proofwriter, but less necessary in CommonsenseQA.

Dataset	Method	Accuracy (%) \uparrow	# Input Tokens	# Output Tokens
MMLU	Direct Few-Shot CoT Few-Shot STaR Metareasoning	$\begin{array}{c} 34.1 (\pm 1.1) \\ 50.7 (\pm 1.3) \\ 48.2 (\pm 1.3) \\ 48.3 (\pm 1.4) \end{array}$	$\begin{array}{c} 495.7 (\pm 2.1) \\ 1050.7 (\pm 2.2) \\ 94.7 (\pm 2.1) \\ 94.7 (\pm 2.2) \end{array}$	$\begin{array}{c} 0.0 \ (\pm \ 0.0) \\ 99.1 \ (\pm \ 2.2) \\ 110.5 \ (\pm \ 1.5) \\ 78.7 \ (\pm \ 1.6) \end{array}$
Aqua-Rat	Direct Few-Shot CoT Few-Shot STaR Metareasoning	$\begin{array}{c} 22.4 (\pm 5.1) \\ 38.6 (\pm 5.5) \\ 42.9 (\pm 5.9) \\ 36.6 (\pm 5.9) \end{array}$	$\begin{array}{c} 477.9 (\pm 2.5) \\ 1032.9 (\pm 2.6) \\ 76.9 (\pm 2.5) \\ 76.9 (\pm 2.4) \end{array}$	$\begin{array}{c} 0.0 \ (\pm \ 0.0) \\ 152.6 \ (\pm \ 11.3) \\ 138.8 \ (\pm \ 11.5) \\ 111.2 \ (\pm \ 7.7) \end{array}$

Table 6: Additional OOD testing on Phi-2. This table compares the performance of our method against STaR, CoT and Direct Few-Shot across two out-of-domain benchmarks: MMLU and AQUA-RAT. The results highlight that our method achieves comparable accuracy while requiring fewer output tokens, demonstrating both efficiency and robustness in diverse reasoning tasks.

C ADDITIONAL OUT OF DOMAIN TESTING

To further evaluate the out-of-domain generalization capabilities of our method, we conducted additional assessments on AQUA-RAT (Ling et al., 2017) and MMLU Hendrycks et al. (2021) using the Phi-2 model. For MMLU, we incorporated a few-shot prompting baseline with examples drawn from datasets used during training and compared the results to STaR and Metareasoning. AQUA-RAT was tested under the same conditions. The results indicate that our method performs comparably to few-shot prompting and STaR on both datasets, while requiring fewer output tokens. This analysis highlights the strength of our approach in achieving a balance between computational efficiency and accuracy in OOD scenarios. Comprehensive results for MMLU and AQUA-RAT are provided in Table 6.

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D COMPARISON TO INSTRUCTION TUNED MODELS

It is reasonable to question whether instruction-tuned models can dynamically adjust the length of their reasoning chains based on task complexity. To explore this, we tested Meta-Llama-3-8B-Instruct using the following prompt:

Answer the following question, thinking step by step to get to the
answer. You can think however long you need, but answer as soon as
you're ready. Keep you response concise and use the minimum number of
steps to get to the answer. Once you're finished thinking, write your
answer after the 'Answer: ' prompt.

Unfortunately, this method did not effectively adapt response lengths to align with task complexity in our
experiments, as shown in Tables 7 and 8 and Fig. 4. While the observed performance drop might partially
result from deviations from the expected input format, it is evident that the length of the reasoning chains was
generally much higher and not meaningfully adaptive to the complexity of the task.

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E QUALITATIVE EXAMPLES

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Below we show one example of question, reasoning chain and answer per dataset, generated with each method:
CoT Few Shots (Yellow), STaR (green) and Metareasoning (Red). The following examples were generated
by Phi-2 (Javaheripi et al., 2023). The reasoning chains shown here serve as intermediate computations

Model	Method	Accuracy (%) \uparrow	# Input Tokens	# Output Tokens
	Direct Few-Shot	55.5 (± 1.2)	421.3 (± 1.0)	$1.0 (\pm 0.0)$
	CoT Few-Shot	$63.7 (\pm 1.4)$	$995.0 (\pm 0.9)$	$148.4 (\pm 3.0)$
Meta-Llama-3-8B	CoT Instruct	$57.7 (\pm 1.3)$	$73.3 (\pm 0.9)$	$190.4 (\pm 2.5)$
	STaR	$63.9 (\pm 1.5)$	$73.3 (\pm 1.0)$	$119.7 (\pm 1.9)$
	Metareasoning	64.4 (± 1.4)	73.3 (± 0.9)	95.6 (± 2.3)

Table 7: Llama Instruct results. The table shows accuracy (in %), average number of input tokens, and average number of output tokens for each method. Despite the instruction, reasoning chains remain lengthy.

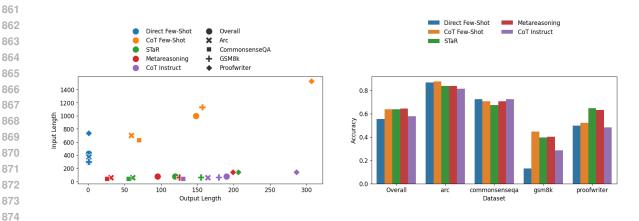
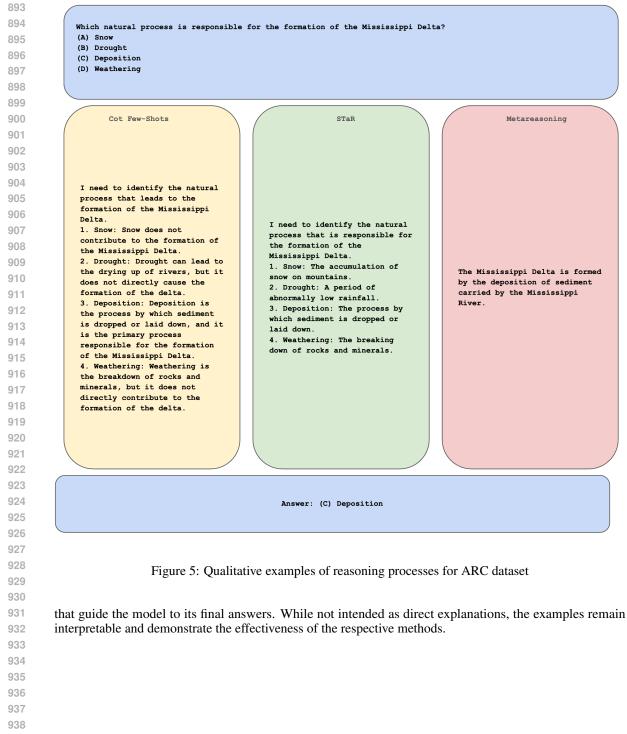
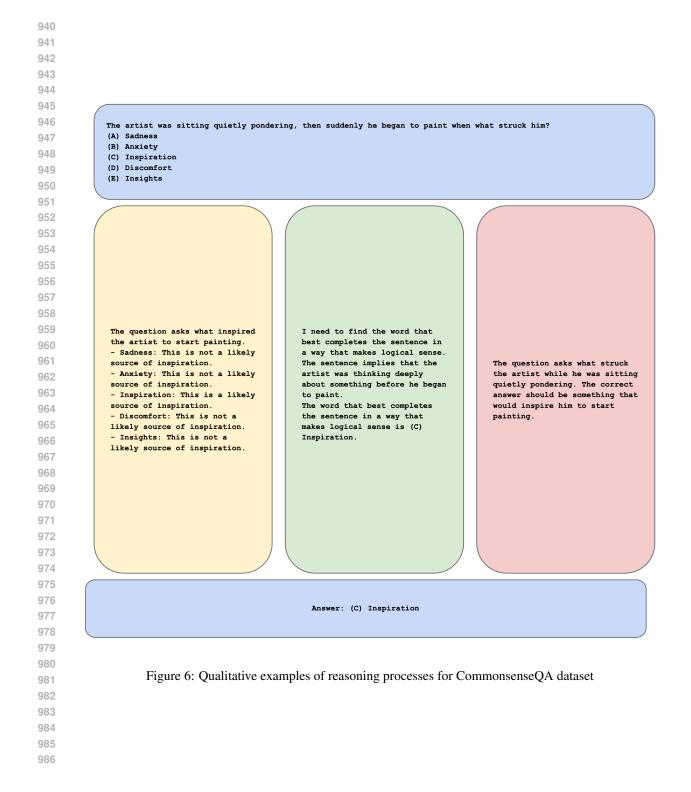


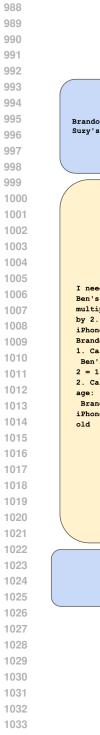
Figure 4: Llama Instruct plot. Left panel: the distribution of input and output tokens across various methods and datasets. Right panel: Comparison of performance across datasets.

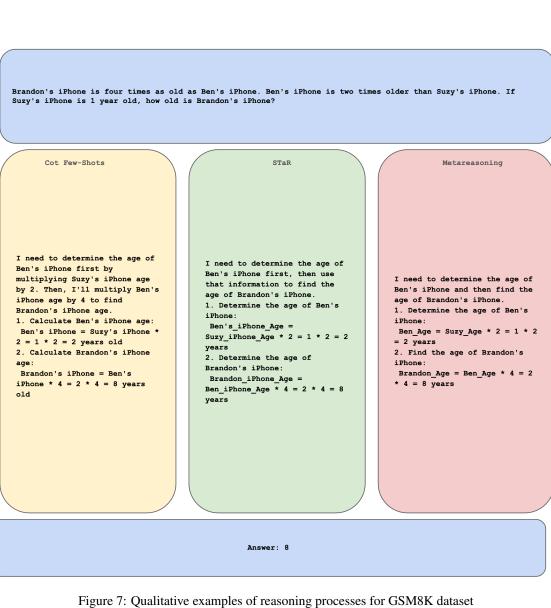
Model	Method	Hard Split	Easy Split	Length Reduction (%) ↑
Meta-Llama-3-8B	CoT Few-Shot	132.0 (± 3.0)	57.0 (± 1.0)	56.8
	CoT Instruct	$181.0 (\pm 4.0)$	$150.0 (\pm 2.0)$	17.1
	STaR	$126.0 (\pm 3.0)$	$64.0 (\pm 2.0)$	49.2
	Metareasoning	99.5 (± 2.5)	27.0 (± 1.0)	72.9

Table 8: The length of generated reasoning chains across models and methods (mean number of tokens with 95% confidence intervals). Adaptive methods should maximize the difference in length between the two distributions. Our method (Metareasoning) reduces the overall length and increases the difference in the length distribution between the Hard and Easy splits (as seen in column Length Reduction), demonstrating an improvement in the model's ability to adapt the reasoning length to the complexity of the task.







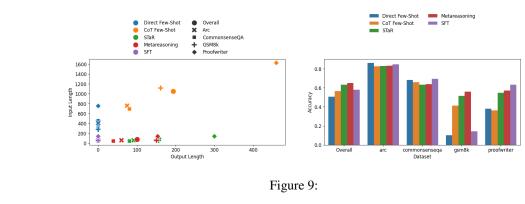




young. All rough people are furry. If someone is white and not young then they are cold. Smart people are rough. Conclusion: Erin is not furry. Is the conclusion True, False or Unknown based on the premises? Let's analyze the premises step by step to determine if Erin is furry. 1. Anne is furry: IsFurry(Anne). 2. Bob is smart: IsSmart(Bob). 3. Bob is white: IsWhite(Bob). 4. Dave is quiet: IsQuiet(Dave). 5. Erin is rough: IsRough(Erin). 6. Erin is not smart: ~IsSmart(Erin). 7. Erin is young: IsYoung(Erin). 8. All rough people are furry: Let's analyze the premises step IsRough(x) -> IsFurry(x). by step to determine if Erin is 9. If someone is white and not furry. young then they are cold: 1. Anne is furry: IsFurry(Anne). Let's analyze the premises step IsWhite(x) and ~IsYoung(x) -> 2. Bob is smart: IsSmart(Bob). by step to determine if Erin is IsCold(x). 3. Bob is white: IsWhite(Bob). furry. 10. Smart people are rough: 4. Dave is quiet: IsQuiet(Dave). 1. Erin is rough: IsRough(Erin). IsSmart(x) -> IsRough(x). 5. Erin is rough: IsRough(Erin). 2. All rough people are furry: From the premises, I know that 6. Erin is not smart: IsRough(x) -> IsFurry(x). Since ~IsSmart(Erin). Erin is rough: Erin is rough, Erin is furry: IsRough(Erin).Let's look at the 7. Erin is young: IsYoung(Erin). IsFurry (Erin) . rules: 8. All rough people are furry: Hence, the conclusion that Erin IsRough(x) -> IsFurry(x). Since 1. All rough people are furry: is not furry is False. IsRough(x) -> IsFurry(x). Since Erin is rough, Erin is furry: Erin is rough, Erin is furry: IsFurry (Erin) . IsFurry (Erin) . Hence, the conclusion that Erin 2. If someone is white and not is not furry is False. young then they are cold: IsWhite(x) and ~IsYoung(x) -> IsCold(x). Since Erin is not young, Erin is cold: IsCold(Erin). 3. Smart people are rough: IsSmart(x) -> IsRough(x). Since Erin is smart, Erin is rough: IsRough (Erin) . Therefore, the conclusion that Erin is not furry is False. Answer: False

Premises: Anne is furry. Bob is smart. Bob is white. Dave is quiet. Erin is rough. Erin is not smart. Erin is

Figure 8: Qualitative examples of reasoning processes for Proofwriter dataset



F DIRECT FINETUNING BASELINE

We also tested our method against a direct finetuning baseline. It can be seen that while this method provides an even bigger efficiency gain, the performance is less consistent.

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