Improve Student's Reasoning Generalizability through Cascading Decomposed CoTs Distillation

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Abstract

001 Large language models (LLMs) exhibit enhanced reasoning at larger scales, driving efforts to distill these capabilities into smaller 004 models via teacher-student learning. Previ-005 ous works simply fine-tune student models on teachers' generated Chain-of-Thoughts (CoTs) 007 data. Although these methods enhance indomain (IND) reasoning performance, they struggle to generalize to out-of-domain (OOD) tasks. We believe that the widespread spurious correlations between questions and answers may lead the model to preset a specific 012 answer which restricts the diversity and generalizability of its reasoning process. In this paper, we propose Cascading Decomposed CoTs Distillation (CasCoD) to address these issues by decomposing the traditional single-step 017 learning process into two cascaded learning steps. Specifically, by restructuring the training objectives-removing the answer from outputs and concatenating the question with the ra-022 tionale as input—CasCoD's two-step learning process ensures that students focus on learning 024 rationales without interference from the preset answers, thus improving reasoning generalizability. Extensive experiments demonstrate the effectiveness of CasCoD on both IND and OOD benchmark reasoning datasets¹.

1 Introduction

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Recent developments in LLMs have brought remarkable improvements in reasoning tasks via CoT prompting (Wei et al., 2022b). However, these great reasoning capabilities are often associated with more parameters (Wei et al., 2022a), which is not practical to emergent in smaller language models (SLMs). Existing works (Magister et al., 2023; Ho et al., 2023; Fu et al., 2023; Zhou and Ai, 2024) try to make the reasoning capabilities isolated and distilled to student SLMs by simply fine-tuning



Answer: (A) To swim in a heated pool.

(D) To participate in a polar bear plunge event.

(b) A case of spurious correlation between questions and answers.

Figure 1: (a) Empirical results of standard CoT distillation (Std-CoT) and directly fine-tuning on answer labels without CoTs (Answer SFT) on one in-domain (BBH-test) and the other four out-of-domain benchmark reasoning datasets. (b) In the given example, the semantic similarity between "swimsuit" in the question and "swim" in the answer demonstrates a high level of match, which could allow the model to predict the answer using simple keyword matching or certain rules.

on teacher LLMs generated CoTs data, known as standard CoTs distillation (Std-CoT). Although the method effectively leverages the LLMs' CoTs to boost the reasoning performance of student models on seen tasks, it does not ensure effective reasoning in OOD settings, leading to weak generalization on unseen tasks. Our pioneer study demonstrates that, as shown in Figure 1 (a), when using the same IND training dataset, student models developed via the method Std-CoT perform better on IND tasks but significantly worse on OOD tasks compared

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¹Code can be found at https://anonymous.4open. science/r/ef334sf-FB92

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to models fine-tuned directly with question-answer pairs. The surprising findings indicate that students' CoTs do not effectively transfer to new domains and these SLMs seem to be more adept at learning to predict answers directly from questions.

We attribute these issues to the spurious correlations between questions and answers that are commonly found in implicit reasoning tasks (Gururangan et al., 2018; Zellers et al., 2019; Blodgett et al., 2020), as illustrated in Figure 1 (b). The Std-CoT approach requires models to learn both the rationale and the answer in a single step, where the learned spurious correlations in training stage can adversely affect the quality of rationale generation during inference. That is to say, upon reading a question, student models may fastly, unconsciously, and automatically formulate a "preset answer" (Hagendorff et al., 2022), which in turn may lead them to implicitly reduce the token generation space when producing CoT. This results in diminished diversity and generalizability of their rationales.

In this paper, we propose **Cas**cading decomposed CoTs Distillation (CasCoD), a straightforward yet effective method to address these issues. Specifically, we decompose the traditional singlestep learning process of Std-CoT into two cascaded learning steps: a rationale learning step and an answer learning step. In the rationale learning step, the training objective, with the answer removed, is defined as ²: $q \rightarrow r$. In the answer learning step, we concatenate the question with the target output from the rationale learning step and use this combined input for the answer learning step, setting the training objective as $q, r \rightarrow a$. This cascading two-step learning configuration mitigates the capture of spurious correlations between questions and answers during the training phase, ensuring that students focus on learning rationales without interference from the preset answers. Furthermore, the inference phase execution pipeline is aligned with the training phase; the model first generates a rationale when given a question, and then, based on the question-rationale pair, predicts the final answer, further alleviating potential reasoning biases caused by spurious correlations.

Extensive experiments demonstrate that CasCoD outperforms the baselines on both IND and OOD benchmark reasoning datasets (§4.3). Besides, we validate the generalizability of CasCoD across different models, model sizes, and training data sizes

 ^{2}q : the question, r: the rationale, a: the answers.

(§4.4). Further analyses validate our hypothesis (§5.1) and confirm the significant impact of the two-step cascading learning process (§5.2) and the robustness of CasCoD (§5.3). The experiments on reasoning faithfulness (§5.4) and case studies (§5.5) indicate that models distilled by CasCoD can reason more consistently and demonstrate better generalization than baselines, effectively addressing interference from question-answer spurious correlations. Our contributions are as follows:

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- We find that standard CoT distillation methods exhibit limited generalizability on OOD tasks, almost performing worse than methods finetuned directly with question-answer pairs.
- We decompose the traditional single-step learning process into two cascading learning steps to alleviate the impact of spurious correlations between questions and answers.
- Extensive experiments confirm the effectiveness of our method across both IND and OOD datasets, showing that CasCoD can generate more generalizable CoTs.

2 Related Works

CoT Capability of Language Models. LLMs have demonstrated a wide array of capabilities in numerous natural language processing tasks, underscored by various studies (Chowdhery et al., 2023; Wei et al., 2022a). One notable manifestation of this is the CoT prompting technique (Wei et al., 2022b), which facilitates models in articulating a series of deductive reasoning steps. This method has substantially enhanced LLMs' problem-solving abilities, as evidenced in several works (Kojima et al., 2022a; Wang et al., 2023b; Huang et al., 2023). Despite these advancements, the effectiveness of CoT prompting notably diminishes in smaller models (Wei et al., 2022a). Research by Chung et al. (2022) indicates that with targeted training on CoT data via instruction tuning, SLMs can unlock CoT capabilities. In our study, we show that SLMs' CoT performance can be further enhanced by decomposing the standard CoT distillation process into two cascaded learning steps.

Distilling Knowledge from LLMs. Numerous studies (Taori et al., 2023; Chiang et al., 2023; Peng et al., 2023) have explored the knowledge distillation from advanced LLMs like ChatGPT (OpenAI, 2023). These efforts typically focus on



Figure 2: Overview of our proposed method **Cascading Decomposed CoTs Distillation (CasCoD)**. Different from the standard CoTs distillation, we decompose the single CoT learning step into two comprehensive learning steps including the rationale learning step and the answer learning step, and then learn them in a cascaded way.

distilling a broad range of abilities via instruction 149 tuning on extensive and varied datasets (Xu et al., 150 2023; Wu et al., 2023; Jiang et al., 2023b; Li et al., 151 2024). However, our work is aimed at distilling 152 the CoT reasoning capabilities from LLMs, in line 153 with Magister et al. (2023); Ho et al. (2023), who 154 propose standard CoTs distillation by directly fine-155 tuning SLMs on teacher LLMs' CoTs. Fu et al. 156 (2023) expands on this by using various reason-157 ing data formats for specializing domain-specific 158 SLMs. Wang et al. (2023c) distill SLMs via learn-159 ing from self-reflection and feedback in an inter-160 active, multi-round paradigm with teacher LLMs. Hsieh et al. (2023) propose to learn the rationale 162 and answers as separate goals for optimizing. Li et al. (2022) propose learning the entire CoTs and the single answers to enhance the reasoning of stu-165 dents. Based on these, Liu et al. (2023) introduce 166 an additional distillation objective, self-evaluation, 167 aiming for SLMs to assess the accuracy of their CoTs akin to LLMs' evaluative processes. And Chen et al. (2024) maximize the mutual informa-170 tion between objectives. Ranaldi and Freitas (2024) use in-family and out-family teachers to gener-172 ate more CoTs for fine-tuning students. However, these methods are affected by the spurious correla-174 tions due to their isolated optimization objectives. 175 In contrast, we reorganize the training objectives 176 to effectively mitigate this issue. 177

3 Methodology

In this section, we introduce our new distillation method that decomposes the single-step leanring process of standard CoTs distillation into two cascaded learning steps, as illustrated in Figure 2. Formally, the standard CoTs distillation objective $q \rightarrow CoT$ is split into two learning processes, rationale step learning with the objective $q \rightarrow r$ and answer step learning with the objective $q, r \rightarrow a$. Below we first describe how to extract CoTs from teacher LLMs in §3.1. Then we describe the standard CoTs distillation method and discuss its limitations in §3.2. Finally, we provide a detailed presentation of our method in §3.3. 178

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3.1 Extract CoTs From Teacher LLMs

The initial phase of the distillation is to extract CoTs from teacher LLMs for each question-answer pair $\{q, a\}$ in a raw dataset. This involves employing the CoT prompting technique (Wei et al., 2022b), which guides the teacher LLMs to generate CoTs that follow a prescribed format with multiple reasoning steps. The prompt template is shown in Appendix C.1. Note that CoTs produced by LLMs may not always be correct. To maintain CoTs quality, following the previous work (Magister et al., 2023; Hsieh et al., 2023), we retain only those that match the ground truth answer in the dataset, build205ing a CoT dataset $\mathcal{D} = \{q, CoT\}$ for training the206student model. Additionally, to facilitate the intro-207duction of CasCoD, we explicitly split the extracted208CoTs into two parts based on predefined rules in209CoT prompting, formalizing this as $CoT = r \oplus a$.210For instance, we use the phrase "Therefore, the211answer is" to divide the CoT, categorizing the text212before this delimiter as the rationale r and the text213after it as the answer a.

3.2 Preliminaries for CoTs Distillation

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Previous standard CoTs distillation (Magister et al., 2023; Ho et al., 2023), referred to as single-step learning, is to teach SLMs to generate the CoT in one time as follows:

$$\mathcal{L}_{\text{Std-CoT}} = \mathbb{E}_{q,CoT \sim \mathcal{D}} \left[\ell \left(q, CoT \right) \right]$$
(1)

where ℓ signifies the negative log-likelihood loss function, expressed as:

$$\ell(x, y) = -\sum_{y_t \in y} \log P\left(y_t \mid x, y_{< t}\right) \qquad (2)$$

However, this method requires the model to simultaneously learn both rationales and answers in a single step, readily leading to the capture of question-answer spurious correlations in widespread implicit reasoning datasets (Blodgett et al., 2020). These correlations degrade the quality of CoT generation during inference, resulting in weak reasoning generalization. In other words, this implicit learning of correlations might lead student models to preset answers after reading the questions, potentially causing a state reduction in the token generation space when producing CoTs.

3.3 Cascading Decomposed CoTs Distillation

Different from the training strategy in standard CoTs distillation, our method decomposes its single-step learning process into two cascaded learning steps, one for the rationale learning step and the other for the answer learning step.

For the rationale learning step, each question is combined with a rationale learning delimiter "Rationale:" as the input q, with the rationale rproduced by the teacher serving as the label for distilling the rationale. With the answer objective removed, this training strategy allows models to engage in learning rationales without the interference of spurious correlations. The loss function of rationale step learning is as follows:

$$\mathcal{L}_{\text{rationale}} = \mathbb{E}_{q,r,a\sim\mathcal{D}}\left[\ell\left(q,r\right)\right] \tag{3}$$

For the answer learning step, we concatenate both the input and output of the rationale learning step with an answer learning delimiter "Therefore, the answer is" as the input, and the answer *a* serves as the label for distilling the answer. This strategy helps students learn to reason consistently from the question-rationale pair rather than merely presetting spurious answers based solely on the question. The loss function of answer learning step is thus: 251

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$$\mathcal{L}_{\text{answer}} = \mathbb{E}_{q,r,a\sim\mathcal{D}}\left[\ell\left(q\oplus r,a\right)\right]$$
(4)

Due to the inherent tight connection between rationale learning and answer learning, for each instance in the dataset, we optimize both learning objectives simultaneously for the CoTs distillation:

$$\mathcal{L}_{\text{CasCoD}} = (1 - \alpha)\mathcal{L}_{\text{rationale}} + \alpha \mathcal{L}_{\text{answer}} \quad (5)$$

where α is a hyperparameter used to weight the loss in the two learning steps.

During inference, student models follow the same pipeline as in training: first, generate a rationale based on the question, and then predict the final answer using the question-rationale pair. The cascading training objectives reduce the probability of student models capturing spurious correlations between questions and answers in the training phase, thereby alleviating potential reasoning biases caused by spurious correlations in the inference stage, thus enhancing CoTs generalizability.

4 Experiments

In this section, we conduct extensive experiments and analysis to evaluate the effectiveness of our method across both IND and OOD datasets.

4.1 Datasets

In-domain Dataset: BIG-Bench Hard (BBH) (Suzgun et al., 2023) comprises 27 challenging tasks covering arithmetic, symbolic reasoning et al. from BIG-Bench (BB) (Guo et al., 2023). The majority of the data involve multiple-choice questions, with a few being open-ended. To underscore the superiority of our approach, we chose to perform distillation on this most challenging dataset. We randomly divide the BBH dataset into a training set (BBH-train) for distillation and a test set (BBH-test) for IND evaluation, in a 4:1 ratio.

Out-of-domain Datasets: (1) **BIG-Bench Sub** (**BB-sub**). BB is a popular benchmark consisting of 203 tasks covering a wide range of topics, including

mathematics, common-sense reasoning, and vari-297 ous other domains. For ease of evaluation, we filter 298 the subtasks within BB based on subtask keywords, focusing on tasks related to "multiple-choice" and "reasoning", and ensure that tasks from BBH were 301 excluded, resulting in 61 subtasks. Then we randomly sample up to 100 instances for each subtask, resulting in BB-sub. (2) AGIEval (Zhong et al., 2023) is a renowned human-centric benchmark used to assess LMs' reasoning abilities, whose tasks span various domains, including college en-307 trance exams (English / Math / Law), logic tests et al. We evaluate our method on the subtasks that are related to multiple-choice questions in the English 310 language. (3) AI2 Reasoning Challenge (ARC) 311 (Clark et al., 2018) consists of ARC-Easy (ARC-E) and ARC-Challenge (ARC-C). The distinction lies 313 in ARC-E consisting of relatively simpler questions 314 from middle and high school science exams, while 315 ARC-C comprises more complex and challenging questions. We utilize the testing set of the ARC 317 dataset for evaluation. The statistics of all above datasets can be found in Appendix B.1. 319

4.2 Models & Baselines & Setup

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Models. We employ the popular open-source language model LLaMA2-7B (Touvron et al., 2023) as the student SLM in the main experiment and also explore different student models in §4.4. Considering the pricing and capabilities, we utilize OpenAI's powerful black-box LLM, gpt-3.5-turbo-0613, as teacher LLMs to extract CoTs with the same manual prompt used in the previous work (Suzgun et al., 2023).

Baselines. We compare our method with the following baselines: (1) Teacher & Vanilla Student 331 under various settings, e.g., Zero-shot (+CoT) or Few-shot (+CoT), for showing the impact of dis-334 tilling reasoning ability from LLMs. (2) Std-CoT (Magister et al., 2023; Ho et al., 2023), which is the standard CoTs distillation method that directly finetune student models on the CoTs data. (3) Step-bystep (Hsieh et al., 2023) is a multi-task CoTs distil-338 lation method that distills rationales and answers separately. (4) MT-CoT (Li et al., 2022) is also 340 a multi-task CoTs distillation method, but unlike 341 Step-by-step, it simultaneously optimizes the objec-342 tives of answer prediction and entire CoTs learning. (5) **SCOTT** (Wang et al., 2023a) that enhances 344 the reasoning consistency of the student model by introducing additional counterfactual data.

Setup. We employ LoRA (Hu et al., 2022) for parameter-efficient fine-tuning of the student SLMs. In §5.3, our empirical results indicate that the optimal weight is set α at 0.3. However, to mitigate the effects of unbalanced weighting, we include an additional method setup for comparison against the baselines in Table 1, labeled CasCoD ($\alpha = 0.5$). All experiments are conducted using a mixed-precision training strategy on 4 × A100 GPUs. For the inference stage, vLLM³(Kwon et al., 2023) is utilized to accelerate inference, employing a greedy decoding strategy to generate text on one single A100 GPU. More details on training and hyperparameters can be found in Appendix B.2. 347

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4.3 Main Results

Table 1 presents the automatic evaluation results of our proposed CasCoD and baselines.

CoTs distillation enhances the reasoning performance of students. Comparing with the Zero-shot-CoT and Few-shot-CoT settings of student models, the performance of those with distillation is significantly improved by learning CoTs. Except for BB-sub, the student model has 3-4 times improvement compared to vanilla ones across all datasets.

CasCoD overcomes limitations of distillation baselines in OOD performance. From the Table 1, we can find that Answer-SFT on the OOD datasets outperforms all the distillation baselines by an average of 5%, which indicates that it seems student models' performance decreases when learning the CoTs. This pattern is also noticeable in models without distillation, as evidenced by the comparison between Zero-shot and Zero-shot-CoT (or Few-shot and Few-shot-CoT) settings. We attribute this to spurious correlations between questions and answers as introduced in Figure 1 (b), which students can easily learn. The distillation baselines that require students to consider predicting answers while generating the rationale, inadvertently make the simpler task of answer prediction interfere with the rationale learning, thus reducing the generalization of CoTs. In contrast, CasCoD* not only surpasses Answer-SFT by 7.9% in IND datasets but also achieves comparable results in OOD scenarios. This underscores the effectiveness of our cascade two step learning strategy, which restructures training objectives to mitigate the impact of spurious correlations, in enhancing reasoning capabilities across diverse datasets.

³https://github.com/vllm-project/vllm

Method	Distill?	Gen CoT?	BBH-test	BB-sub	AGIEval	ARC-E	ARC-C	AVG
In-domain?			 ✓ 	×	×	×	×	
		Teacher: Ch	atGPT (gpt	-3.5-turbo)			
Zero-shot-CoT	X	\checkmark	42.7	44.1	49.5	91.9	81.1	61.9
Few-shot-CoT	×	\checkmark	73.1	-	-	-	-	-
		Stude	nt: LLaMA	2-7B				
Zero-shot	X	×	14.8	15.5	6.9	18.2	13.9	13.9
Zero-shot-CoT	×	\checkmark	10.6	7.7	7.1	18.4	14.8	11.7
Few-shot	×	×	15.1	28.5	25.5	25.5	25.4	24.0
Few-shot-CoT	×	\checkmark	16.3	25.3	9.9	17.2	17.2	17.2
Answer-SFT	×	×	51.5	33.2	31.2	71.6	53.7	48.2
Std-CoT (Magister et al., 2023)	 ✓ 	\checkmark	54.2	28.7	21.6	59.6	45.1	41.8
SCOTT (Wang et al., 2023a)	\checkmark	\checkmark	42.4	18.8	13.0	45.7	34.1	30.8
MT-CoT (Li et al., 2022)	\checkmark	\checkmark	<u>56.8</u>	30.3	22.0	49.4	38.2	39.3
Step-by-step (Hsieh et al., 2023)	\checkmark	\checkmark	42.4	27.7	28.8	68.5	48.6	43.2
CasCoD (ours, $\alpha = 0.5$)	\checkmark	\checkmark	52.5	36.4	28.1	71.8	54.7	48.7
CasCoD* (ours, $\alpha = 0.3$)	✓	\checkmark	59.4	37.0	<u>28.3</u>	<u>70.6</u>	<u>52.7</u>	49.6

Table 1: Accuracy (%) on in-domain and out-of-domain datasets with different methods. We employ "Let's think step by step" (Kojima et al., 2022b) for Zero-shot-CoT settings and the manually curated prompt (Suzgun et al., 2023) for Few-shot-CoT settings. The best performance among distilled student models is marked in **bold**, and the second-best performance is indicated by an <u>underline</u>.

CasCoD significantly outperforms the distillation baselines across IND and OOD datasets. From Table 1, it can be observed that CasCoD significantly outperforms baselines on both IND and OOD datasets in most cases, regardless of whether the loss is weighted. Specifically, CasCoD* secures an average in-domain improvement of 5.2% and an out-of-domain enhancement of 8.4% over the Std-CoT, along with an overall 6.4% improvement compared to the multi-task learning (Step-by-step) approach. Impressively, CasCoD* achieves 80.1% of the teacher LLM's performance in Zero-shot-CoT settings. These results underscore the efficacy of CasCoD, significantly boosting the generative capabilities of CoTs on unseen tasks.

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4.4 Ablation Study on Model & Data Sizes

CasCoD is universally applicable to models of varying sizes. We perform model distillation on TinyLLaMA-1.1B⁴ (Zhang et al., 2024), LLaMA2-7B, and LLaMA2-13B, respectively and compare with standard CoTs distillation (Std-CoT) and multi-task distillation (MT-CoT & Step-by-step). In Figure 3 and 7, we can find that CasCoD consistently outperforms the baselines on both IND and OOD datasets across various sizes of student models. Notably, the performance improvement of our method is the most obvious in the BB-sub, where the performance of the 13B student model reaches 92.7% of the teacher LLM's performance. Furthermore, as model sizes increase, the performance gap between CasCoD and the baselines widens on OOD datasets, highlighting CasCoD's superior efficiency in distilling CoTs for larger models. 423

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CasCoD is universally applicable to models of different architectures. We perform model distillation on CodeLLaMA-7B (Touvron et al., 2023), LLaMA3-8B (AI@Meta, 2024) and Mistral-7B-v0.2 (Jiang et al., 2023a), respectively, and compare with Std-CoT and Step-by-step. From the Table 3, we can see that regardless of whether it's CodeLLaMA, LLaMA3, or Mistral, CasCoD significantly outperforms the baselines on OOD tasks, demonstrating its high effectiveness and scalability. Particularly, on the powerful base model Mistral, the superiority of our method is further amplified.

CasCoD significantly outperforms standard CoTs distillation on OOD with much less training data. In Figure 6, CasCoD achieves a 6.3% improvement over Std-CoT on the BB-sub dataset, using only 25% of the full BBH-train data. In the case of other OOD datasets, CasCoD requires merely 12.5% of the full training data to surpass the Std-CoT trained with the full dataset by 5% to 7% in performance. These results demonstrate the efficiency of CasCoD, capable of enhancing CoTs generalization with a smaller amount of CoTs data.

⁴https://huggingface.co/TinyLlama/TinyLlama-1. 1B-intermediate-step-1431k-3T



Figure 3: Ablation study on model size for four OOD datasets. The dotted line indicates the performance of the teacher LLM under the Zero-shot-CoT setting. The results in IND dataset can be found in Appendix A.2.1.

5 Analysis

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5.1 Hypothesis Validation

In this subsection, we aim to validate our hypothesis that student learning of spurious correlations affects the quality of their generated rationales. Due to the nature of causal language modelsautoregression, we incorporate "The answer is" into input prompts to directly prompt models to provide the answer immediately (which we treat as the "preset answer" referred to $\S1$) after reading the question, rather than generating rationales before providing an answer. We define the following metrics to assist the validation: (1) A: The proportion of incorrect CoT reasoning when the preset answer is wrong. A higher ratio indicates a greater negative impact of the preset answer on CoT reasoning; (2) **B**: The proportion of correct CoT reasoning when the preset answer is correct. A higher ratio indicates a greater positive impact of the preset answer; (3) C = A - B (combine A and B). We compare CasCoD with Std-CoT using these metrics on four OOD tasks. The results are shown in Table 2. We observe that Std-CoT significantly outperforms CasCoD in metrics 'A' and 'C', while significantly underperforms CasCoD in metric 'B' on all four OOD tasks. This indicates that our method can selectively utilize spurious correlations to some extent, suppressing the negative effects of incorrect preset answers on reasoning and reinforcing the positive effects of correct preset answers on reasoning, thereby enhancing performance on OOD tasks, which experimentally validate our hypothesis.

484 5.2 Two-Step vs. Single-Step Implementation

In this subsection, we explore whether CasCoD's two-step training objectives can be achieved in a single-step computation. Upon analysis of the two

Method & Metric	BB-sub	AGIEval	ARC-E	ARC-C
Std-CoT (A) \downarrow	79.7	82.2	63.7	50.8
Std-CoT (\mathbf{B}) \uparrow	47.5	30.6	58.1	69.7
Std-CoT (C) \downarrow	32.2	51.6	5.6	-18.9
$CasCoD\left(\mathbf{A}\right) \downarrow$	73.3	77.9	61.8	50.9
CasCoD (B) \uparrow	57.4	36.7	71.4	83.9
CasCoD (C) \downarrow	15.9	41.2	-9.6	-33.0

Table 2: Hypothesis validation results (%) on four OOD tasks. The hypothesis is better supported when ' \mathbf{A} ' is lower, ' \mathbf{B} ' is higher, and ' \mathbf{C} ' is lower.

cascaded learning steps, we find that under teacherforcing (Goodfellow et al., 2016), CasCoD closely mirrors Std-CoT, with key distinctions including adjustable token-level weights and the omission of delimiters in loss calculations. Each sample in CasCoD's original framework undergoes two forward calculation, raising the question of whether a similar outcome is possible with only one. To investigate this, we introduce a variant, CasCoD-single, which is designed to fulfill the two-step training objectives through a single forward computation. Figure 4 indicates that the two-step CasCoD consistently surpasses the single-step variant across all



Figure 4: Comparison between two-step and single-step training implementations of CasCoD.



Figure 5: Ablation study on task weights α . The results are reported by IND-AVG and OOD-AVG that respectively denote averge accuracy on IND and OOD datasets. The best performance among weights are marked with "\$\phi".

datasets. This underscores that a single forward calculation does not suffice to meet CasCoD's training objectives, emphasizing the critical importance of the cascading two-step learning process.

Impact of Weights 5.3

In this subsection, we explore how variations in weights affect the performance of models with different parameter sizes on both IND and OOD datasets, as shown in Figure 5.

Students' performance is not sensitive to weights 510 on OOD datasets. From the figure, we observe 512 that regardless of weight changes, CasCoD consistently outperforms Std-CoT in OOD by average, 513 even at $\alpha = 0.9$ (meaning the model allocated only 514 10% of its attention to rationales generation). This 515 demonstrates that CasCoD exhibits robust general-516 ization in OOD and also underscores the effective-517 ness of decomposing CoTs for distillation. 518

CasCoD is more robust for smaller student mod-519 520 els. We observe that the 1.1B model shows less variation in performance compared to the 7B and 13B models in IND. Notably, the performance of the 13B model drops sharply as α changes from 0.5 to 0.9, indicating that larger models are more sus-524 ceptible to weight adjustments in the IND dataset.

Prioritizing the rationale over the answer yields better results. It is evident that across different model sizes, the optimal weights on both IND and OOD datasets range approximately from 0.01 to 0.3, indicating that focusing on the rationale help improve the generalizability of CoTs.

5.4 Faithfulness of Students

To ensure that the rationale provided by students supports their predicted answers, another metric for evaluating CoTs distillation is the faithfulness of students. Following the previous work (Wang et al., 2023a), we use the LAS metric (Hase et al., 2020), whose core idea is to measure the extent that the rationales r' aid a simulator in predicting the answers a', defined as:

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$$LAS = Acc (q, r' \to a') - Acc (q \to a') \quad (6)$$

where we employ ChatGPT and GPT4 as the simulator, respectively. The results are shown in Table 4. CasCoD is observed to generate rationales that are more consistent with answers than baselines. This suggests that despite CasCoD's multi-step learning process, the introduction of cascading learning ensures that students can faithfully reason.

5.5 **Case Study**

Due to page limitations, we provide a systematic case study in Appendix D to illustrate our hypothesis and the improvement in CoT generalizability.

6 Conclusion

We propose a simple yet effective CoTs distillation method CasCoD to address the issue of questionanswer spurious correlations that previous CoTs distillation methods suffer from. Specifically, we decompose the traditional single-step learning process into two cascaded learning steps and restructure their training objectives. Extensive experiments show that CasCoD significantly outperforms the baselines across both IND and OOD datasets. Further analysis reveals that CasCoD is robust to model size, training data size, different models, and weights and can lead to faithful student models.

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Limitations

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In our study, we explore distilling CoTs into two cascading steps, which is an initial step toward un-568 derstanding finer decompositions. Research (Scha-569 effer et al., 2023a) suggests that the emergent abili-570 ties of LLMs result from managing multiple sub-571 tasks simultaneously, hinting at the potential for more intricate cascading steps in CoTs. Our current 573 work does not yet define the precise rules for such 574 more steps decomposition, nor the optimal timing and methods for focusing learning on specific steps. We hope our work can inspire the community and leave these aspects for future exploration, intended 578 to refine and extend the CoT reasoning capabilities of SLMs as suggested by our findings.

Ethics Statement

Our work utilizes CoT data extracted from Chat-GPT for distillation, which may result in inheriting the social biases (Schaeffer et al., 2023b) and hallucination (Zhang et al., 2023) present in LLMs. However, we are optimistic that future advancements in resolving these issues in LLMs will naturally lead to the development of student models with reduced toxicity.

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A Additional Experimental Results

A.1 Detailed Results on Mathematical Reasoning Tasks

Given the community's focus on mathematical reasoning, we present detailed experimental results for math-related subtasks from our evaluation datasets in Table 5. It should be noted that the subtasks in the datasets we utilized involve mathematical reasoning tasks. We list as follows:

- 1. BB-sub: includes subtasks like 'elementary_math_qa' and 'identify_math_theorems', as detailed in Table 9.
- 2. BBH: includes subtasks such as 'DateUnderstanding' and 'Multi-StepArithmetic', as detailed in Table 8.
- 3. AGIEval: includes subtasks like 'AQuA-RAT' and 'SAT-Math', as detailed in Table 6.

While ARC does not specifically feature tasks for mathematical computation, we identify a number of scientific questions within this dataset that involve mathematical calculations. From the Table 5, We can observe that CasCoD has achieved performance improvements on mathematical reasoning tasks as well.

A.2 Ablation Study on In-domain Dataset

A.2.1 W.R.T. Model Size

The results of the model size ablation study on IND datasets are presented in Figure 7. We observe that CasCoD outperforms the baselines on both the 7B and 13B model and significantly surpasses the teacher LLMs in the Zero-shot CoT setting.

A.2.2 W.R.T. Training Data Size

The results of the training data ablation study on IND datasets, as shown in Figure 8, indicate that CasCoD outperforms standard CoTs distillation across various sizes of training data. This demonstrates the efficiency of our proposed method.

Models & Methods	BBH-test	BB-sub	AGIEval	ARC-E	ARC-C	AVG
In-domain?	\checkmark	×	×	×	×	
CodeLLaMA-7B + Std-CoT	56.2	<u>29.7</u>	19.2	<u>42.0</u>	<u>32.2</u>	35.9
CodeLLaMA-7B + Step-by-step	40.7	29.0	<u>23.9</u>	41.5	32.8	33.6
CodeLLaMA-7B + CasCoD	<u>54.8</u>	35.4	25.8	42.9	31.7	38.1
LLaMA3-8B + Std-CoT	66.9	33.9	32.7	69.8	60.2	52.7
LLaMA3-8B + Step-by-step	44.2	<u>35.5</u>	<u>38.8</u>	<u>83.7</u>	<u>70.7</u>	<u>54.5</u>
LLaMA3-8B + CasCoD	<u>65.2</u>	42.9	40.1	87.2	74.0	61.9
Mistral-7B-v0.2 + Std-CoT	72.2	37.6	<u>32.0</u>	68.8	57.9	<u>53.7</u>
Mistral-7B-v0.2 + Step-by-step	56.4	<u>38.9</u>	20.1	<u>76.4</u>	<u>62.3</u>	50.8
Mistral-7B-v0.2 + CasCoD	<u>71.7</u>	42.5	40.1	83.9	74.2	62.5

Table 3: Accuracy (%) on IND and OOD datasets with different student models distilled by different methods.



Figure 6: Ablation study on training data size for four OOD datasets. The dotted line indicates the performance of fine-tuning the student models by standard CoTs distillation using the full set (100% of) BBH-train dataset. The results in IND dataset can be found in Appendix A.2.2.

Method	ChatGPT	GPT4	AVG
Teacher	41.1	36.3	38.7
Std-CoT	40.8	29.8	35.3
SCOTT	36.2	29.4	32.8
MT-CoT	36.2	25.8	31
Step-by-step	6.6	-0.1	3.25
CasCoD (ours)	40.8	31.6	36.2

Table 4: Faithfulness (LAS, %) of the compared methods with different LLM evaluators on the IND dataset. The prompt templates can be found in Appendix C.2

B Details of Experiment

B.1 Dataset Statistics

Table 6, Table 7, Table 8 and Table 9 show the data statistics of AGIEval, ARC, BIG-Bench Hard (BBH) and BIG-Bench Sub (BB-sub)⁵, respectively.

B.2 Hyperparameters Settings

In our study, we ensure consistency in the hyperparameter settings across all baselines, including our proposed CasCoD approach, to maintain the fairness of our comparative analysis. Here, we detail the hyperparameter configurations employed in our experiments. 893

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Training Steps and Batch Size. The number of training steps is determined based on the size of the training dataset, the batch size, and the number of gradient accumulation steps required. We maintain a consistent batch size across all baselines to eliminate any performance discrepancies that could arise from varying batch sizes.

Learning Rate. Our exploratory experiments initially focus on the standard CoTs distillation method using the LLaMA-2 model, revealing that while the batch size had minimal impact on perfor-

⁵For detailed descriptions of the subtasks in BIG-Bench, please refer to https://github.com/google/BIG-bench/

blob/main/bigbench/benchmark_tasks/README.md.

Models & Tasks	elementary_math_qa	identify_math_theorems	DateUnderstanding	Multi-StepArithmetic	AVG
Std-CoT	11.0	20.7	82.0	8.0	30.4
SCOTT	12.0	34.0	58.0	4.0	27.0
MT-CoT	10.0	9.4	74.0	6.0	24.9
Step-by-step	17.0	32.1	68.0	0.0	29.3
CasCoD	22.0	36.2	86.0	8.0	38.1

Table 5: Accuracy (%) on mathematical reasoning tasks with different distillation methods.



Figure 7: Ablation study on model size in the IND (BBH-test). The dotted line indicates the performance of the teacher LLM under the Zero-shot-CoT setting.

No.	Task	Size	# Choices
1	AQuA-RAT	254	5
2	LogiQA-EN	651	4
3	LSAT-AR	230	5
4	LSAT-LR	510	5
5	LSAT-RC	269	5
6	SAT-Math	220	4
7	SAT-EN	206	4
8	SAT-EN (w/o Psg.)	206	4
	Sum	2546	-

Table 6: Statistics of AGIEval dataset.

mance, the learning rate was a critical factor. We
test learning rates of 1e-4, 2e-4, and 3e-4 and observe optimal performance at 2e-4 across Std-CoT
and other distillation baselines as well as our CasCoD. Therefore, we set the learning rate to 2e-4 for
all methods involved in our study.

917Epochs and Evaluation Strategy. Throughout918our training process, we monitor the training loss919curve and note that it generally plateaued by920the 15th epoch, suggesting that the models have921achieved convergence. Accordingly, we set the922number of epochs to 15 for 7B models. The pro-923cess of determining the number of epochs for other924model sizes follows a similar pattern. To mitigate



Figure 8: Ablation study on training data size in the IND (BBH-test). The dotted line indicates the performance of fine-tuning the student models by standard CoT distillation using the full set (100% of) BBH-train dataset.

Task	Size	# Choices
ARC-E	2376	4-5
ARC-C	1172	4-5

Table 7: Statistics of ARC test dataset.

the potential risk of overfitting and to ensure that our evaluation reflects the most effective model configuration, we systematically select the checkpoints from the epoch that demonstrate the best performance on the IND task. These checkpoints are then used to evaluate performance on OOD tasks. 925

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Finally, the detailed hyperparameters in training and inference can be found in Table 10 and Table 11, respectively.

C Prompts

C.1 Prompts of Generating CoTs for ChatGPT

We use the prompt template shown in Table 12 to call the ChatGPT API to generate the CoTs for the BBH-train datasets.

No.	Task	Size	# Choices
1	Boolean Expressions	250	2
2	Causal Judgement	187	2
3	Date Understanding	250	6
4	Disambiguation QA	250	4
5	Dyck Languages	250	-
6	Formal Fallacies Syllogisms Negation	250	2
7	Geometric Shapes	250	11
8	Hyperbaton (Adjective Ordering)	250	2
9	Logical Deduction (3 objects)	250	3
10	Logical Deduction (5 objects)	250	5
11	Logical Deduction (7 objects)	250	7
12	Movie Recommendation	250	5
13	Multi-Step Arithmetic	250	-
14	Navigate	250	2
15	Object Counting	250	-
16	Penguins in a Table	146	5
17	Reasoning about Colored Objects	250	18
18	Ruin Names	250	11
19	Salient Translation Error Detection	250	6
20	Snarks	178	2
21	Sports Understanding	250	2
22	Temporal Sequences	250	4
23	Tracking Shuffled Objects (3 objects)	250	3
24	Tracking Shuffled Objects (5 objects)	250	5
25	Tracking Shuffled Objects (7 objects)	250	7
26	Web of Lies	250	2
27	Word Sorting	250	-
	Sum	6511	-

Table 8: Statistics of BIG-Bench Hard dataset.

C.2 Prompts of Simulators

We use the prompt templates shown in Table 13 and Table 14 to call the ChatGPT and GPT4 API to predict the answers given a question or with an additional rationale, respectively.

D Case Study

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Here we show 4 cases in Table 15, 16, 17 and 18 to compare the CoT generated by CasCoD with the teacher LLM and the standard CoTs distillation method (Std-CoT). We utilize \checkmark and \times to denote whether the CoT is correct or incorrect, respectively.

Table 15 and 16 show that while Std-CoT correctly predicts the final answer on in-domain tasks, it generates incorrect intermediate reasoning steps, indicating that Std-CoT causes student models to capture spurious correlations between questions and answers, without learning to reason with diversity. This is evidenced by the fact that its generated rationales are almost identical to the teacher's CoTs. In contrast, CasCoD produces more distinct CoTs, differing from the teacher's reasoning format, which indicates an enhancement in the student's reasoning generalizability. Tables 17 and 18 illustrate that on out-of-domain tasks, Std-CoT fails to reason correctly, including logical and factual mistakes, whereas CasCoD can clearly understand the question and provides concise, logically rich

No.	Task	Size	# Choices
1	abstract narrative understanding	100	5
2	anachronisms	100	2
3	analogical_similarity	100	7
4	analytic_entailment	70	2
5	cause_and_effect	100	2
6	checkmate_in_one	100	26
7	cifar10_classification	100	10
8	code_line_description	60	4
9	conceptual_combinations	100	4
10	crass_ai	44	4
11	elementary_math_qa	100	5
12	emoji_movie	100	5
13	empirical_judgments	99	3
14	english_russian_proverbs	80	4
15	entailed_polarity	100	2
16	entailed_polarity_hindi	100	2
17	epistemic_reasoning	100	2
18	evaluating_information_essentiality	68	5
19	fantasy_reasoning	100	2
20	figure_of_speech_detection	59	10
21	goal_step_wikihow	100	4
22	gre_reading_comprehension	31	5
23	human_organs_senses	42	4
24	identify_math_theorems	55	4
25	identify_odd_metaphor	4/	5
20	implicatures	100	25
27	india aguag and affaat	82	25
20	intercent commetry	100	26
29	kanii asoji	100	20
31	kanpada	100	1
32	key value mans	100	
33	logic grid puzzle	100	3
34	logical args	32	5
35	logical fallacy detection	100	2
36	metaphor boolean	100	2
37	metaphor understanding	100	4
38	minute mysteries ga	100	4
39	mnist ascii	100	10
40	moral_permissibility	100	2
41	movie_dialog_same_or_different	100	2
42	nonsense_words_grammar	50	4
43	odd_one_out	86	5
44	parsinlu_qa	100	4
45	physical_intuition	81	4
46	play_dialog_same_or_different	100	2
47	presuppositions_as_nli	100	3
48	riddle_sense	49	5
49	similarities_abstraction	76	4
50	simple_ethical_questions	100	4
51	social_iqa	100	3
52	strange_stories	100	2
53	strategyqa	100	2
54	swahili_english_proverbs	100	4
55	swedish_to_german_proverbs	12	4
56	symbol_interpretation	100	5
5/	umedial	100	3
50	undo_permutation	100	5
39 60	unit_interpretation	100	5
61	vitaminc_fact_verification	100	3
01	willowily	100	2
	Sum	5384	-

Table 9: Statistics of BIG-Bench sub dataset. We filter the original dataset by retrieving tasks with keywords "multiple choice" and randomly sample up to 100 examples per task. Note, the task in BBH will not be involved in BB-sub.

reasoning.

Hyperparameter	TinyLLaMA-1.1B	LLaMA2-7B	LLaMA2-13B
gradient accumulation steps	4	4	8
per device batch size	16	16	8
learning rate	2e-4	2e-4	2e-4
epoches	20	15	10
max length	1024	1024	1024
β of AdamW	(0.9,0.999)	(0.9,0.999)	(0.9,0.999)
ϵ of AdamW	1e-8	1e-8	1e-8
γ of Scheduler	0.95	0.95	0.95
weight decay	0	0	0
warmup ratio	0	0	0
rank of LoRA	64	64	64
α of LoRA	32	32	32
target modules	q_proj, v_proj	q_proj, v_proj	q_proj, v_proj
drop out of LoRA	0.05	0.05	0.05

Table 10: Training hyperparameters.

Arguments	Student	Teacher
do sample	False	True
temperature	-	0.2
top-p	1.0	1.0
top-k	-	-
max new tokens	1024	2048
# return sequences	1	1

Table 11: Generation configs of students and teachers.

{Task Description}. Your response should conclude with the format "Therefore, the answer is". Q: {Task Example Question No.1} A: Let's think step by step. {Human-Curated-CoTs No.1}. Q: {Task Example Question No.2} A: Let's think step by step. {Human-Curated-CoTs No.2}. Q: {Task Example Question No.3} A: Let's think step by step. {Human-Curated-CoTs No.3}. Q: {QUESTION} A: Let's think step by step.

Table 12: Prompt template of gpt-3.5-turbo for generating the CoTs data with 3 shots.

system content	You are a helpful and precise assistant for following the given instruction.
	[Instruction] {Please read the question and then give your answer based on the question without any explanations.}
user content	Task Description: {TASK_DESCRIPTION}
user content	Question: {QUESTION}
	Your Answer:

Table 13: Prompt template of simulators for predicting the answers when given the question.

system content \mid You are a helpful and precise assistant for following the given instruction.		
user content	[Instruction] {Please read the question and the rationale, and then give your answer based on the question and the rationale without any explanations.}	
	Task Description: {TASK_DESCRIPTION}	
	Question: {QUESTION}	
	Rationale: {RATIONALE}	
	Your Answer:	

Table 14: Prompt template of simulators for predicting the answers when given the question and rationale.

Question:	Evaluate the result of a random Boolean expression: not False and False or True or False.
	Rmember that (i) expressions inside brackets are always evaluated first and that (ii) the order of operations from highest priority to lowest priority is "not", "and", "or", respectively.
	We first simplify this expression "Z" as follows: "Z = not False and False or True or False = A and B or C or D" where "A = not False", "B = False", "C = True", and "D = False".
Teacher	Let's evaluate A: A = not False = not (False) = True.
	Plugging in A, B, C, and D, we get: $Z = A$ and B or C or D = True and False or True or False = False or True or False = True.
	Therefore, the answer is True.
	Rmember that (i) expressions inside brackets are always evaluated first and that (ii) the order of operations from highest priority to lowest priority is "not", "and", "or", respectively.
	We first simplify this expression "Z" as follows: "Z = not False and False or True or False = A and B or C or D" where "A = not False", "B = False", "C = True", and "D = False".
Std-CoT	Let's evaluate A: A = not False = not (False) = True.
	Plugging in A, B, C, and D, we get: $Z = A$ and B or C or D = True and False or True or False = False or False or False = False.
	Therefore, the answer is True. 🗡
	Removing the brackets first: (not False and False) or (True or False) or False.
	Let's evaluate these expressions one by one:
	- (not False and False): The boolean expression "not False and False" evaluates to True.
CasCoD	- (True or False): The boolean expression "True or False" evaluates to True.
	- False: The boolean expression False evaluates to False.
	When we evaluate these expressions, we get True.
	Therefore, the answer is True.

Table 15: A boolean-expression case from BIG-Bench Hard.

Question:	Answer extremely simple questions about the colors of objects on a surface. Q:On the table, you see several objects arranged in a row: a burgundy paperclip, a purple cup, a mauve pencil, a yellow keychain, and a silver teddy bear. What is the color of the object furthest from the teddy bear? Options: (A) red (B) orange (C) yellow (D) green (E) blue (F) brown (G) magenta (H) fuchsia (I) mauve (J) teal (K) turquoise (L) burgundy (M) silver (N) gold (O) black (P) grey (Q) purple (R) pink
Teacher	According to this question, the objects are arranged in a row, from left to right, as follows: (1) a burgundy paperclip, (2) a purple cup, (3) a mauve pencil, (4) a yellow keychain, (5) a silver teddy bear.
	The teddy bear is the last item on the list, namely (5). The object furthest from the teddy bear corresponds to (1), which is a burgundy paperclip.
	The color of the paperclip is burgundy. Therefore, the answer is (L) \checkmark
Std-CoT	According to this question, the objects are arranged in a row, from left to right, as follows: (1) a burgundy paperclip, (2) a purple cup, (3) a mauve pencil, (4) a yellow keychain, (5) a silver teddy bear. The object furthest from the teddy bear is the mauve pencil, which is the third item on the list.
	The color of the mauve pencil is mauve. Therefore, the answer is (L).
CasCoD	Rationale: According to this question, the objects are arranged in a row, from left to right, as follows: (1) a burgundy paperclip, (2) a purple cup, (3) a mauve pencil, (4) a yellow keychain, (5) a silver teddy bear.
	The object furthest from the teddy bear corresponds to (1), which is a burgundy paperclip.
	The color of the paperclip is burgundy.
	Therefore, the answer is (L).

Table 16: A reasoning about colored objects case from BIG-Bench Hard.

Question:	h = 3a + 28.6 A pediatrician uses the model above to estimate the height h of a boy, in inches, in terms of the boy's age a , in years, between the ages of 2 and 5. Based on the model, what is the estimated increase, in inches, of a boy's height each year? Options: (A)3 (B)5.7 (C)9.5 (D)14.3
Teacher	Step 1: We are given the model $h = 3a + 28.6$ which represents the estimated height h of a boy in terms of his age a . Step 2: We need to find the estimated increase in height each year. This means we need to find the change in height for a change in age of 1 year. Step 3: To find the change in height, we can subtract the height at age $a + 1$ from the height at age a . So, the change in height is $(3(a + 1) + 28.6) - (3a + 28.6)$. Step 4: Simplifying the expression, we get $3a + 3 + 28.6 - 3a - 28.6$. Step 5: The terms $3a$ and $-3a$ cancel out, leaving us with $3 + 3$. Step 6: The change in height is 6 inches.
	Therefore, the answer is (A) 3.
Std-CoT	This question focuses on the increase in height each year. According to the model, the height of a boy between the ages of 2 and 5 is approximately 36 inches. Therefore, the estimated increase in height each year is 3 inches. Therefore, the answer is (A).
CasCoD	Rationale: This question asks about the estimated increase, in inches, of a boy's height each year. According to the model, the height of a boy increases by 3 inches each year between the ages of 2 and 5. Therefore, the answer is (A) 3 inches.

Table 17: A sat-math case from AGIEval.

Question:	Which gas is the most abundant in Earth's atmosphere? Options: (A) oxygen (B) nitrogen (C) water vapor (D) carbon dioxide
Teacher	First, we know that Earth's atmosphere is primarily composed of gases.
	Second, we need to determine which gas is the most abundant.
	Third, we can eliminate options (A) oxygen and (C) water vapor because they are present in smaller quantities compared to the other gases.
	Finally, we are left with options (B) nitrogen and (D) carbon dioxide.
	Considering that nitrogen makes up about 78% of Earth's atmosphere, while carbon dioxide only makes up about 0.04%, it is clear that nitrogen is the most abundant gas in Earth's atmosphere.
	Therefore, the answer is (B) nitrogen.
Std-CoT	The percentage of each gas in the atmosphere is given by the following table:
	Gas Percentage
	oxygen 20.95
	nitrogen 78.09
	water vapor 0.4
	carbon dioxide 0.04
	According to this table, oxygen is the most abundant gas in Earth's atmosphere. Therefore, the answer is (A). 🗡
CasCoD	Rationale: According to the World Bank, the composition of Earth's atmosphere is approximately 78% nitrogen, 21% oxygen, 0.93% argon, and small amounts of other gases. Nitrogen is the most abundant gas in Earth's atmosphere.
	Therefore, the answer is (B).

Table 18: A case from AI2 Reasoning Challenge.