

# Making Reasoning Matter: Measuring and Improving Faithfulness of Chain-of-Thought Reasoning

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## Abstract

Large language models (LLMs) have been shown to perform better when asked to reason step-by-step before answering a question. However, it is unclear to what degree the model’s final answer is faithful to the stated reasoning steps. In this paper, we perform a causal mediation analysis on twelve LLMs to examine how intermediate reasoning steps generated by the LLM influence the final outcome and find that LLMs do not reliably use their intermediate reasoning steps when generating an answer. To address this issue, we introduce FRODO, a framework to tailor small-sized LMs to generate correct reasoning steps and robustly reason over these steps. FRODO consists of an *inference module* that learns to generate correct reasoning steps using an implicit causal reward function and a *reasoning module* that learns to faithfully reason over these intermediate inferences using a counterfactual and causal preference objective. Our experiments show that FRODO significantly outperforms four competitive baselines. Furthermore, FRODO improves the robustness and generalization ability of the reasoning LM, yielding higher performance on out-of-distribution test sets. Finally, we find that FRODO’s rationales are more faithful to its final answer predictions than standard supervised fine-tuning.

## 1 Introduction

Chain-of-thought (CoT) reasoning techniques have been shown to improve the performance of large language models (LLMs) by generating step-by-step reasoning traces before generating a final answer (Wei et al., 2022). Many works suggest that the reasoning process described in CoT explanations may be a possible description of how models make predictions (Kojima et al., 2022; Yao et al., 2023; Sun et al., 2023). However, despite the remarkable success of CoT in many reasoning tasks, recent works show that LLMs-generated reasoning

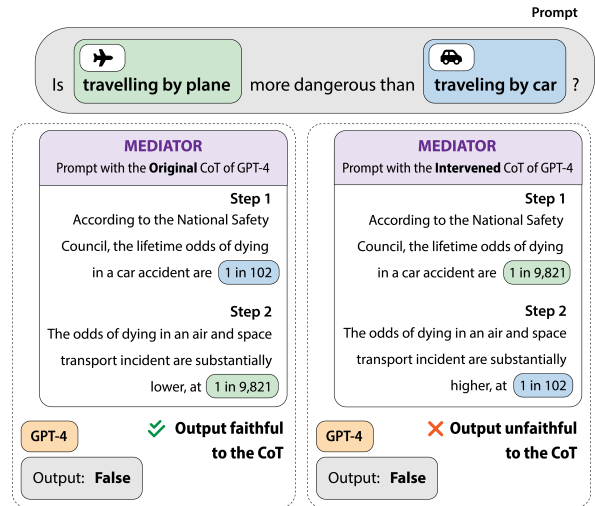


Figure 1: An example of our proposed causal analysis to measure the faithfulness of the final output to the CoT generated by the model. We perturbed CoT rationales and studied the causal impact on the model’s behaviour.

traces can be incorrect (Zhang et al., 2023) and unfaithful (Turpin et al., 2023).

Reasoning implicitly involves two steps: identifying the rules and facts (inference chains) necessary to reach a conclusion and then robustly using them to reach said conclusion (Levesque, 1986). Our paper studies whether LLMs reliably use inference chains to arrive at a conclusion.<sup>1</sup> In standard CoT, LLMs can generate plausible explanations with the final answer not necessarily guaranteed to follow the reasoning chain or imply a causal relation between the reasoning chain and the model’s outcome (Lyu et al., 2023). Most recent efforts have either focused on the performance of LLMs on various reasoning tasks or their faithfulness in CoT generation, ignoring the sequential relationship between CoT and the final answer (Huang and Chang, 2023; Lanham et al., 2023).

<sup>1</sup>In our paper, reasoning faithfulness refers to how reliably the model uses its reasoning steps to arrive at a correct answer.

In this work, we address this gap by introducing a methodology for interpreting the relationship between the CoT trace and the final answer based on causal mediation analysis (Pearl, 2001). Causal mediation analysis is a method of causal inference that studies the change in a response variable following an intervention or treatment. More concretely, we use this method to measure and interpret the contribution of a reasoning chain (mediator) to the final answer (observed output), as shown in Fig. 1. We propose multiple interventions on the model inputs and mediators (reasoning chain) to unveil the causal effect of specific reasoning steps in a model’s output.

We apply this framework and study the causal impact of CoT rationales on the behaviour of twelve different state-of-the-art LLMs on three different complex reasoning tasks (*mathematical*, *commonsense*, and *causal understanding*). We observe a large variation across tasks and models in how strongly reasoning traces causally affect the model’s prediction. In particular, we find that instruction-tuned models (GPT-3.5-Instruct, Brown et al., 2020b; Mistral-Instruct-7B, Jiang et al., 2023b) have a stronger causal effect on the final answer when conditioned on the reasoning trace than models trained with RLHF (e.g., ChatGPT; Llama-2-7B-Chat, Touvron et al., 2023). Similar to Turpin et al. (2023), when we intervene in the reasoning problem, we observe that ChatGPT and GPT-3.5-Instruct are inconsistent at generating plausible reasoning chains. Finally, we find GPT-4 (Achiam et al., 2023) only changes its answer 30% of the time when conditioned on perturbed counterfactual reasoning chains. In Figure 1, we see one example where GPT-4 does not faithfully change its final answer when provided with intervened counterfactual CoT. These results indicate two issues: (i) LLMs can generate unfaithful and implausible reasoning chains, and (ii) LLMs are inconsistent when reasoning over their own generated reasoning traces.

To address these issues, we introduce a novel method, FRODO, comprising two modules. The first module tailors small-sized LMs to generate correct reasoning chains (inference module), while the second module takes the reasoning chains as input and faithfully reasons over them to arrive at the correct answer (reasoning module). To learn to generate correct reasoning chains, we use the DPO algorithm (Rafailov et al., 2023), which enables the model to prefer correct reasoning chains

over counterfactual ones with implicit feedback. Instead of relying on human labeling, we obtain preference data by prompting LLMs to generate correct and counterfactual reasoning chains. Second, we train another small-sized LM to improve the causal effect between the reasoning chain and the final answer using a counterfactual and causal preference ranking objective.

We evaluate FRODO on four reasoning tasks (Quarel, StrategyQA, OpenBookQA, QASC) using multiple model backbones of different scales, and demonstrate that FRODO achieves an absolute accuracy improvement of 2% ~ 3% over standard supervised fine-tuning or CoT distillation methods. We assess robustness by examining how models alter their answers when intervened with counterfactual reasoning chains. FRODO exhibits significant (+4.5%) improvement in robustness. Finally, FRODO generalizes better to out-of-distribution test sets, showing a +2.6% performance improvement over supervised fine-tuning.<sup>2</sup>

## 2 Reasoning Chain as a Mediator

**Problem Formulation.** Reasoning is often a process that involves composing multiple inference steps to reach a conclusion or make a decision. We informally conceptualize each reasoning task as requiring a model  $f: X \rightarrow Y$  to map an input  $x \in X$  to an output  $y \in Y$  by making correct or plausible inference steps  $R$ .

**Causal Interpretation.** The causal graph is a probabilistic graphical model used to describe how variables interact, expressed by a directed acyclic graph consisting of the sets of nodes ( $N$ ) denoting the variables and a set of directed edges ( $E$ ) indicating the causal relationships between these variables denoting the causality.

**Causal Mediation Analysis.** It is a method to measure how an independent variable (or treatment) affects a dependent variable (or outcome) mediated by intermediate variables (Pearl, 2001; Robins, 2003). Causal mediation analysis aims to decompose the total effect of the independent variable ( $X$ ) on the dependent variable ( $Y$ ) into two components: the direct effect and the indirect effect (Pearl, 2001). In this work, we view the reasoning process as a causal graph, framing the input (reasoning problem)  $X$  and the output  $Y$  as random variables and the reasoning steps as mediator variable  $R$ . We use mediation analysis to interpret the

<sup>2</sup>Code and data will be released upon publication.

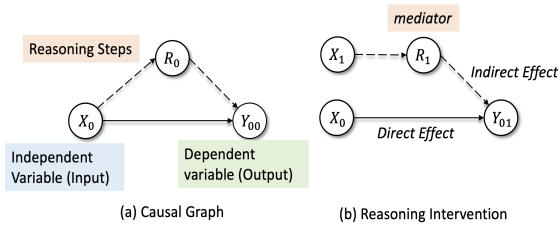


Figure 2: Causal graph for natural language reasoning, modeling  $P(Y|do(x))$ .  $X_0$ : original reasoning problem,  $X_1$ : intervened reasoning problem.  $R_0$ : Reasoning steps for  $X_0$ ,  $R_1$ : Reasoning steps for  $X_1$ . Outputs  $Y_{00}$  or  $Y_{01}$  are model outputs given  $X_0$  and  $R_0$  or  $X_0$  and  $R_1$ .

role of reasoning steps as mediators between model inputs and model outputs. Let  $X_0$  denote the initial reasoning problem,  $R_0$  the reasoning chain given  $X_0$ . Let  $Y_{00}$  denote the potential outcome when the treatment and mediator variables are  $X_0$  and  $R_0$ , respectively. Meanwhile,  $Y_{01}$  denotes the potential outcome when treatment is set to  $X_0$ , and  $R_1$  is the reasoning chain for the reasoning problem  $X_1$ .

*Direct Effect (DE) measures how much an intervention  $X$  changes an outcome variable  $Y$  directly, without passing through a hypothesized mediator  $R$ .* The direct effect of  $X = X_0$  on  $Y$  can be defined as  $\mathbb{E}[Y_{00} - Y_{10}]$ , which can be seen as the correctness comparison between the two potential outcomes given two different treatments, i.e.,  $X = X_0$  and  $X = X_1$ . It is computed by applying the intervention  $X$  but holding  $R$  fixed to its original value ( $R_0$ ).

*Indirect Effect (IE) measures how much an intervention  $X$  changes  $Y$  indirectly through  $R$ .* The indirect effect can be defined as  $\mathbb{E}[Y_{00} - Y_{01}]$ . It is computed by setting  $R$  to its value under the intervention  $X$  while keeping everything else to its original value.

More concretely, according to Pearl (2001), in our scenario, a high direct effect means the model emphasizes the reasoning problem more than the reasoning steps. In contrast, a high indirect effect means the model emphasizes the reasoning steps more than the problem input.

**Reasoning Intervention.** Following Pearl (2001), we conduct counterfactual reasoning to measure the causal effect of a treatment variable on a response variable. We first perform targeted interventions on the input text  $X$  and measure their effect on the reasoning outcome  $Y$  by keeping  $R$  fixed (direct effect). Further, we also perform interventions on the mediator  $R$  and measure their effect on  $Y$  (indirect effect). We perform the following steps to automatically generate an

Variables	Example
$X_0$	<i>Is Poseidon similar to the god <u>Vulcan</u>?</i>
$R_0$	<i>Poseidon is a god from Greek mythology, known as the <u>god of the sea</u>, earthquakes, and horses. <u>Vulcan</u> is a god from Roman mythology, known as the <u>god of fire</u>, metalworking, and the forge. Although both are gods, they represent different elements and aspects, and come from different mythologies.</i>
$X_1$	<i>Is Poseidon similar to the god <u>Neptune</u>?</i>
$R_1$	<i>Poseidon is a god from Greek mythology, known as the <u>god of the sea</u>, storms, and earthquakes. <u>Neptune</u> is a god from Roman mythology, who is also known as the <u>god of the sea</u>. Both Poseidon and Neptune share similar roles and attributes in their respective mythologies.</i>

Table 1: An example from StrategyQA dataset, where  $X_1 =$  intervened reasoning problem;  $R_0$  and  $R_1 =$  reasoning steps (generated by GPT-4).

intervention on  $X$  and  $R$ .

**Step 1: Intervention Data Generation.** We use a large language model (GPT-4) to automatically generate an alternative value  $X_1$  for the treatment variable.<sup>3</sup> The input to LLM includes instruction and few-shot examples, taking the format shown in Table 20. LLMs can be sensitive to instructions and few-shot examples; hence, we randomize the prompt by manually creating a set of semantically similar instructions. Then, we randomly sample from the instruction set each time.

**Step 2: Manual Data Curation.** To retain high-quality data for our analysis, we manually filter out generated samples from Step 1 that are invalid or low-quality. Table 1 shows an example where given the original input reasoning question  $X_0$ , the model generated  $X_1$ , where it replaces “*Vulcan*” with “*Neptune*”.

**Step 3: Generate Reasoning Chain.** Finally, to get the indirect effect, we generate the reasoning chain ( $R_0, R_1$ ) for each reasoning problem  $X_0$  or  $X_1$  by providing LLMs with some high-level descriptions about each reasoning task and reasoning prompt – “*Let’s think step by step*”(see App. Table. 19).

Our experiments show a large variation in the causal effects of COT in the final answer depends on the tasks (see Table 2, 3). We also observe that vanilla LMs (<10 billion parameters) exhibit a less significant causal effect of COT on the final answer.

### 3 FRODO

In this section, we introduce FRODO, a framework that tailors small-sized LMs (<10B parameters) to

<sup>3</sup>See Table. 23 for details on task-specific interventions.

be strong rationalizers and perform reasoning faithfully over the rationales. FRODO aims to improve the synergy between the reasoning chain and the final answer. We first describe how we obtain silver reasoning chains from LLMs (§3.1). Then, we introduce our inference module that trains a model to generate rationales (§3.1) followed by the reasoner module and its training objectives (§3.2).

### 3.1 Inference Module

In this work, we assume no gold rationales to train our model. Hence, similar to recent works (Liu et al., 2022, 2023; Wang et al., 2023; Ramnath et al., 2024), we automatically obtain the silver rationale from LLM (GPT-3) using in-context learning. A common approach is fine-tuning a smaller text-to-text model on the silver rationales generated by LLMs with a standard language modeling loss. Recent studies have shown that fine-tuning models (<5B) on reasoning chains may struggle to *align* the reasoning chains with the provided reasoning question during inference (Yang et al., 2023; Fu et al., 2023). Additionally, learning to generate a reasoning chain means learning to decompose complex reasoning into smaller reasoning steps implicitly. However, Shridhar et al. (2023) showed that fine-tuning could lead to learning shortcuts and degrade performance. Recent studies have demonstrated that feedback-based methods can help the model align better with the human goal. Hence, we use Direct Preference Optimization (DPO) (Rafailov et al., 2023) for aligning LMs to learn to generate correct reasoning chains.

**Preference Data.** We prompt the LLM to generate correct reasoning chains ( $R_w$ ) and incorrect reasoning chains ( $R_l$ ) for each reasoning problem. In our experiments, we consider two kinds of reasoning chains as incorrect: *counterfactual chains* (alternative chains that can lead to different outcomes) and *irrelevant chains*. We assume that models that can understand and learn to prefer correct reasoning chains over counterfactual chains will become more robust and enhance generalization. Hence, we manually construct correct and incorrect intermediate reasoning steps and demonstrate the model with these annotated examples before a new instance is provided. In this way, we obtain a preference data  $D \in \{X, R_w, R_l\}$  that contains reasoning problems ( $X$ ) and pairs of reasoning steps that lead to correct ( $Y_w$ ) or incorrect outcomes ( $Y_l$ ).

**Training.** Given a reasoning problem  $\{x \in X\}$  and instruction prompt  $p \in \{\text{correct or counterfac-$

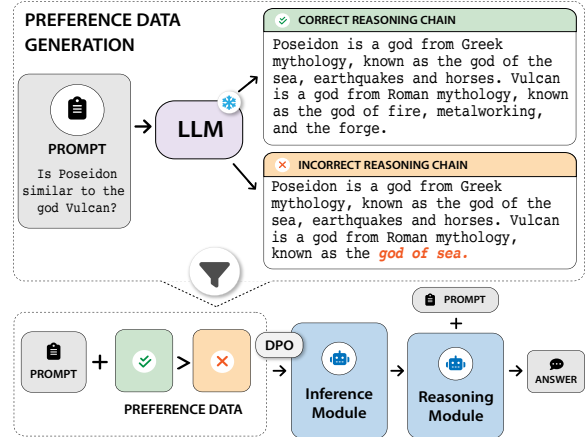


Figure 3: An overview of FRODO.

tual}, our goal is to train models that could generate reasoning steps ( $r_w$  or  $r_l$ ). We propose to adopt Direct Preference Optimization (DPO) (Rafailov et al., 2023), an effective algorithm for aligning language models with implicit rewards. DPO assumes that we only have access to some pairwise preference data  $x \rightarrow \{r_w > r_l\}$  for each problem  $x \in X$ . Hence, while training a model ( $\pi_\theta$ ) to generate correct reasoning steps, we consider counterfactual and irrelevant reasoning steps as less preferred. Training a DPO model includes two phases: (i) supervised fine-tuning (SFT) and (ii) Preference Learning (PL) phase.

**SFT.** We begin by fine-tuning a pre-trained LM with a maximum log-likelihood objective to obtain  $\pi_{sft}$ .

**PL Phase.** Contrary to traditional RL approaches, which initially train a reward model and subsequently derive a policy from it, DPO enables extracting policy through implicit reward learning. DPO adopts a binary classification loss:

$$\mathcal{L}_{DPO} = -\mathbb{E}_{\{x, r_w > r_l\}} \log \sigma(f_\theta(r_w, x) - f_\theta(r_l, x)) \quad (1)$$

where  $f_\theta$  is the implicit reward model. Intuitively, the gradient of the loss function  $\mathcal{L}_{DPO}$  increases the likelihood of the preferred completions  $r_w$  and decreases the likelihood of counterfactual reasoning chains  $r_l$ . See Appendix A.1 for more details. During inference, the reasoning module uses the generated reasoning steps by  $\pi_\theta$  model for a given reasoning problem.

### 3.2 Reasoning Module

Given a reasoning question  $x \in X$  and reasoning steps  $r_w$  (correct) and  $r_l$  (counterfactual)<sup>4</sup>, our goal

<sup>4</sup>Please note that in the reasoner module, we only consider counterfactual reasoning steps as negative samples.

is to train a model ( $\pi_\gamma$ ) that can generate a correct answer  $y_w$ . To encourage our reasoner module to reason faithfully over the reasoning steps, we train the model with a linear combination of two losses: an indirect effect loss and a supervised margin rank loss,  $\mathcal{L} = \lambda_{\text{LM}} * \mathcal{L}_{\text{LM}} + \lambda_{\text{counter}} * \mathcal{L}_{\text{counter}} + \lambda_{\text{PREF}} * \mathcal{L}_{\text{PREF}}$ , which we describe below.

**Language Model Loss.** We use the standard training objective to maximize the likelihood of the correct answer using cross-entropy loss, computed as:

$$\mathcal{L}_{\text{LM}} = -\log P(y_w|x, r_w) \quad (2)$$

**Counterfactual Loss.** To encourage the model to reason robustly and faithfully towards the reasoning steps, we propose training the model to learn how different reasoning chains (correct or counterfactual) can lead to different outcomes. Hence, inspired by the causal mediation theory (Pearl, 2001), we use the following loss:

$$\mathcal{L}_{\text{counter}} = -\log P(y_l|x, r_l) \quad (3)$$

Similar to (Wang et al., 2023; Roese, 1997), we posit that adding a counterfactual objective can help the model to avoid learning reasoning shortcut between a question and the gold answer since now the model is tasked to answer differently for the same question.

**Margin-Ranking Loss.** It has been shown (Khosla et al., 2020) that contrastive loss and ranking loss help to improve model robustness and generalization against input variation. Hence, we propose to use the margin ranking loss that aims to maximize the margin between positive examples (i.e., statements containing questions, correct reasoning steps and correct answers) and negative examples (i.e., statements containing questions, counterfactual reasoning steps and correct answers).

$$\mathcal{L}_{\text{PREF}} = \max(0, t * \text{IE} + m) \quad (4)$$

where  $t$  is the label (indicating which sample in the pair is better)=1,  $m$  is the margin=1.0, and the indirect effect  $\text{IE} = h(x, r_w, y_w) - h(x, r_l, y_w)$  where  $h$  is the logits.

## 4 Experiments

**Datasets.** We conduct the causal mediation analysis on three datasets: STRATEGYQA (Geva et al., 2021), GSM8K (Cobbe et al., 2021), and Causal Understanding (Suzgun et al., 2023). We evaluate FRODO on four datasets: STRATEGYQA,

QUAREL (Tafjord et al., 2018), OPENBOOKQA (Mihaylov et al., 2018), and QASC (Khot et al., 2020). We report more details about each dataset in App. A.4. For all the datasets, we do not use human-written rationales. We used rationales generated by prior work (Ramnath et al., 2024) using GPT-3 (TEXT-DAVINCI-003) as silver rationales for supervision. For counterfactual rationales, we use chain-of-thought prompts on these datasets (Table. 19) and sample 2 rationales for each training instance with a temperature of 0.5.

**Evaluation Metrics.** To evaluate the causal effects, we report the average indirect and direct effects of the LLMs. We use the following formula to calculate the scores:  $\text{IE} = \text{Avg}[\text{Acc}(Y_{00}) - \text{Acc}(Y_{01})]$ , and  $\text{DE} = \text{Avg}[\text{Acc}(Y_{00}) - \text{Acc}(Y_{10})]$  where  $X_0$  and  $R_0$  original reasoning problem and reasoning chains. We measure two kinds of causal effects: **natural** and **controlled** for different types of LLMs. *Natural Indirect Effect (NIE)*: for models that have emergent capabilities (>100B parameters) of generating plausible reasoning chains, we measure the causal effect of  $X$  on  $Y$  that uses  $R$  generated by the same model. *Controlled Indirect Effect (CIE)*: for models with <20B parameters, we evaluate the causal effect by providing reasoning chains generated by GPT-4. Further, to measure the *robustness* of models, we use controlled indirect effect. To evaluate the *faithfulness* of the rationales generated by the small-sized models, we use LAS (Hase et al., 2020) to measure how well the rationales help a simulator to predict a student’s predictions  $a'$ , namely  $\text{Acc}(\text{qr} \rightarrow a') - \text{Acc}(\text{q} \rightarrow a')$ . Similar to Wang et al. (2023), we implement each simulator with a fine-tuned T5-large model respectively.

**Implementation Details.** We use GPT-4 to generate intervened reasoning problems  $X_1$  and reasoning chains ( $R_0$  or  $R_1$ ) to perform the causal mediation analysis. We report the prompts used in Table.19, 20 and hyperparameters in App. A.4.

**Baselines.** We perform the causal analysis on a series of language models that are diverse in terms of scale, training, and data: LLaMa-2 (Touvron et al., 2023), Mistral (Jiang et al., 2023b), ChatGPT (Brown et al., 2020a), GPT-4 (OpenAI, 2023), Flan-T5 (Chung et al., 2022), Flan-Alpaca (Chung et al., 2022), Stable-Vicuna (Chiang et al., 2023). We compare FRODO with four strong baselines: (1) SFT + CoT: Finetuning a T5-large or T5-3B or LLaMa-2-7B with LoRA or Mistral-7B with LoRA on silver rationales, then train another model with LM objective to perform the reasoning, Rainier

Models	StrategyQA			GSM8k			Causal Understanding		
	CoT (%)	NIE	NDE	CoT (%)	NIE	NDE	CoT (%)	NIE	NDE
ChatGPT	69.2	15.3	9.1	70.1	56.3	1.01	58.8	21.1	27.4
GPT-4	93.5	40.0	22.2	81.1	21.01	30.01	72.5	29.1	48

Table 2: **Causal Effects** of generated CoT and reasoning problems on the outputs, with both Natural Indirect Effect (NIE) and Natural Direct Effect (NDE). CoT (%) represents the accuracy of the models.

(Liu et al., 2022), (3) Crystal (Liu et al., 2023), (4) Mario (Ramnath et al., 2024) and (5) SCOTT (Wang et al., 2023). More details about all the baselines are reported in App. A.5.

## 5 Results

In Table. 2, 3, we report the results of the causal mediation analysis for twelve models. In section §4, we provide the details about the implementation, evaluation metrics and datasets.

**Natural Direct and Indirect effects.** We first evaluate the indirect and direct effects of the reasoning chain and reasoning problems on the final outputs. For models (>100B) with the emergent ability to generate plausible reasoning chains, we report *natural* indirect effects and direct effects (see §2). Table 2 shows the zero-shot performance of the ChatGPT and GPT-4 models. We observe that for StrategyQA and Causal Understanding tasks, GPT-4 has a higher natural indirect effect than ChatGPT, suggesting that it is able to better reason over the reasoning steps for these tasks. However, for mathematical reasoning (GSM8K), ChatGPT has a better indirect effect. Qualitatively, we find that for mathematical reasoning, when we provide intervened reasoning steps, GPT-4 considers them incorrect and continues to generate correct reasoning steps. This results in a lower indirect effect score. Moreover, GPT-4 exhibits a more pronounced direct effect than ChatGPT, suggesting that its outputs are more causally sensitive to reasoning problems. In general, our experiments show a large variation in the causal effects of CoT in the final answer depending on the tasks.

**Controlled Direct and Indirect effects.** Table 3 shows the results of causal mediation analysis for 12 different LMs. In these experiments, we examined the causal behaviour using reasoning chains generated by GPT-4 (controlled setting). Our study suggests that vanilla LMs (<20B) (in a zero-shot setting) are systematically unfaithful and consistently fail to reason over the mediator. Increasing the model size (7B to 70B) improves the indirect effect (makes them more faithful), indicating the importance of model size. We find that in-context

learning and instruction-tuning improve the indirect effect over models trained only with language modelling objectives (e.g., LLaMA and Mistral), indicating that these methods help the model align better with the reasoning chains. We observe that models trained with RLHF objective (ChatGPT, Llama-2-7B-Chat) have a more direct effect than an indirect effect, suggesting that training on human feedback might have disincentive faithful reasoning (Sharma, 2023). Models that are instruction-tuned or trained on the chain of thought (e.g., Flan-T5) during the pre-training phase have a better indirect effect across different reasoning tasks, suggesting that fine-tuning on CoT can make the model more faithful. Similar to Turpin et al. (2023), we observe inverse scaling for certain tasks. In our case, the indirect effect worsens with increasingly capable models, indicating that sheer scale might not guarantee faithful reasoning. Interestingly, we also observe that none of the models has high indirect or direct effects on the causal understanding task. One intuitive reason is that the causal understanding task is challenging, and the model’s (<10B) performance is nearly random; hence, the effects are not strong. Overall, we observe that LLMs are inconsistent in faithfully performing reasoning over the CoT.

**Comparing FRODO with Baselines.** We now empirically compare FRODO with three strong baseline models (see Table 4). We consider T5-large (770M) as the inference and reasoning modules. We have the following three observations. First, we present the performance of GPT-3.5 on these tasks. We observe the performance on StrategyQA is much lower than on other tasks, indicating the rationales generated for this task can be unfaithful. Hence, similar to (Ramnath et al., 2024), for training FRODO, we use only the instances where the answer predicted by GPT-3.5 is correct. Second, for all four datasets, we observe that FRODO outperforms the strong self-rationalization baselines. FRODO, on average, improves the performance by +4.1 and +3 accuracy points compared to the SFT + CoT and MARIO (the strongest baseline), respectively, across all four tasks. Since SFT + CoT

	Models	StrategyQA			GSM8k			Causal		
		CIE	CDE	p-value	CIE	CDE	p-value	CIE	CDE	p-value
AR	<b>LLaMA-2-7B</b>	24.5	25	<0.001	27.5	8.5	<0.001	2.3	1.1	<0.005
	<b>Mistral-7B</b>	21.2	17.9	<0.001	25.1	3.8	<0.001	2.3	0.6	<0.009
	<b>LLaMA-3-70B</b>	26.6	30.6	<0.001	57.2	5.2	<0.005	8.0	5.1	<0.002
In-context	<b>LLaMA-2-7B</b>	24.9	10	<0.005	45.6	0.9	<0.005	5.6	5.6	<0.009
MoE	<b>Mistral-8-7B</b>	21	11	<0.001	47.4	2.9	<0.003	5.1	4.6	<0.001
RLHF	<b>LLaMA-2-7B-Chat</b>	8.4	30.5	<0.010	1.4	36.7	<0.010	-2.3	8.6	<0.016
	<b>Stable Vicuna-13B</b>	3.5	2.5	<0.001	45.1	2.4	<0.010	0.6	0.1	<0.010
	<b>ChatGPT</b>	2.6	13.6	<0.016	57.8	16.6	<0.010	4.6	10.8	<0.001
Instruct Tuned	<b>Mistral-Instruct-7B</b>	31.6	31.9	<0.001	35.5	4.7	<0.001	7.4	8	<0.005
RLHF + Instruct Tuned	<b>GPT-3.5-Instruct</b>	26.1	27.3	<0.005	<b>62.6</b>	14.7	<0.005	<b>8.5</b>	10.7	<0.005
Instruct-Tuned + CoT Tuned	<b>Flan-T5-11B</b>	<b>36.9</b>	35.7	<0.001	31.23	12.2	<0.001	7.4	13.1	<0.001
	<b>Flan-Alpaca-11B</b>	31.2	47.9	<0.001	25	7.9	<0.001	3.4	9.2	<0.001

Table 3: **Causal Effects** of CoT. The reported results are zero-shot performance. CIE: Controlled Indirect Effect, CDE: Controlled Direct Effect. The p-value represents the significance of the results

Models	StrategyQA	QuaRel	OBQA	QASC
<b>GPT-3.5<sup>o</sup></b>	69.7	83.4	84.5	80.3
<b>SFT</b>	57.6	74.6	65.0	58.6
<b>SFT + CoT</b>	63.6	77.7	65.5	59.4
<b>Rainier</b>	–	–	69.7	54.9
<b>Crystal</b>	–	–	64.2	56.8
<b>MARIO</b>	65.1	79.9	66.1	60.1
<b>FRODO</b>	<b>68.4*</b>	<b>83.4*</b>	70.2 <sup>+</sup>	<b>64.2*</b>
<b>-DPO</b>	66.2	82.2	68.1	62.4
<b>-CL</b>	65.2	82.1	66.4	60.1
<b>-MRL</b>	65.5	81.3	66.2	62.1
<b>SFT</b>	63.1	81.29	72.0	67.8
<b>SFT + CoT</b>	65.1	84.2	73.3	72.0
<b>SCOTT</b>	61.5	–	–	65.0
<b>Crystal</b>	–	–	78.3	74.3
<b>FRODO</b>	<b>82.1*</b>	<b>93.5*</b>	<b>80.1*</b>	<b>75.9*</b>
<b>LlaMa-2-7B</b>	67.2	56.8	47.5	49.6
<b>SFT + CoT</b>	79.4	68.4	62.8	54.6
<b>FRODO</b>	81.5 <sup>+</sup>	73.5 <sup>+</sup>	71.4 <sup>+</sup>	63.4 <sup>+</sup>
<b>Mistral-7B</b>	58.2	56.8	82.1	65.2
<b>SFT + CoT</b>	78.2	70.8	83.5	70.1
<b>FRODO</b>	81.9 <sup>+</sup>	78.2 <sup>+</sup>	84.9 <sup>+</sup>	72.3 <sup>+</sup>

Table 4: Performance of small-sized LMs (770M-7B) on four different reasoning tasks. The base models are T5-large (770M), T5-3B (3B), LLaMa-2-7B and Mistral-7B. We report accuracy (%).<sup>o</sup>: few-shot performance, \*: p-value<0.01, +: p-value<0.05

and MARIO use the same knowledge from GPT-3.5, our results suggest that both our inference and reasoning modules bring substantial performance gains to the model. Third, it is worth noting that increasing (770M to 3B) the model size does not hamper the performance of FRODO. Fourth, we also report the performance of the LLaMa-2-7B and Mistral-7B models. We show that FRODO further improves the performance of model size 7B.

**Ablation.** To obtain a better insight into the contribution of each component of FRODO, we perform an ablation study (see Table. 4). First, when we do not use the DPO to train our inference module, we see a consistent drop (-1.9%) in performance across the four tasks, indicating the importance of incorporating implicit feedback provided by the

DPO in the model’s training. Further, we observe a considerable drop in performance when we do not use counterfactual (-3.1%) and margin ranking loss (-2.8%). This result highlights the model’s ability to benefit from including counterfactual examples.

Models	StrategyQA	QuaRel
<b>SFT</b>	19.4	19.4
<b>SFT + CoT</b>	32.2	29.2
<b>FRODO</b>	<b>39.9</b>	<b>31.2</b>
<b>-CL</b>	34.6	28.7
<b>-MRL</b>	36.2	30.6

Table 5: **Robustness Performance** of LLMs on Reasoning over a Chain. We report CIE scores.

## 6 Analysis

### 6.1 Quantitative Analysis

**Robustness.** In Table 5, we report the controlled indirect effect that indicates how robustly models are able to change their answers when provided with controlled (generated by GPT-4) counterfactual reasoning chains. For STRATEGYQA, we observe that FRODO significantly improves the robustness performance for T5-3B (+7.7 pp.). Further, for the QuaRel task, we observe +2 pp. improvement over the SFT + CoT method. Qualitatively, we find that for the MCQA tasks, the gold rationales often contain the answer; hence, the SFT + CoT learns to copy those as answers. Further, we perform an ablation to understand which component contributes most to the model’s robustness. We find that counterfactual loss brings the most gain in robustness.

**Generalization.** The idea is to test our model’s capability to determine if it can improve out-of-distribution (OOD) generalization. Table 7 shows the OOD performance, where we compare our method with SFT+CoT. We trained the models on the OBQA and QASC datasets and evaluated

551 them on the StrategyQA task. We conclude  
 552 that FRODO significantly helps improve the  
 553 model’s generalizability to a dataset unseen during  
 554 fine-tuning.

## 555 6.2 Qualitative Analysis

557 **Causal Analysis.** To understand the reason for the  
 558 inconsistency in the causal effect, we analyze its re-  
 559 lationship with problem complexity. In Table 6, we  
 560 report the indirect effect of CoT with respect to the  
 561 number of reasoning steps for GSM8K problems.  
 562 We observe that with the increase in the number of  
 563 reasoning steps, the indirect effect drops for both  
 564 LLaMa-3 and ChatGPT. It indicates that the length  
 565 of the reasoning steps has an inverse effect on the  
 566 faithfulness of these models. Table 16 shows a few  
 567 examples of different models’ unfaithful reasoning  
 over the chain of thought.

No. RS	LLaMa-3-70B	ChatGPT
2	<b>66.92</b>	65.6
3	50.31	<b>53.9</b>
4	43.2	<b>61.2</b>
5	41.8	<b>55</b>
6	<b>37.5</b>	21
7	0	25
overall	<b>57.2</b>	56.3

Table 6: **Indirect Effect.** No. RS = Number of Reasoning Steps. IE:  $Avg[Acc(Y_{00}) - Acc(Y_{01})]$

568 **FRODO Analysis.** To further understand the  
 569 findings in §5, we manually analyze the relevance  
 570 of the 100 CoT generated by SFT and DPO. We  
 571 observed that SFT generates 74% and 54% rele-  
 572 vant CoT, whereas DPO generated CoT 77% and  
 573 59% relevant for QuaRel and OBQA tasks, respec-  
 574 tively. Further, we observe two types of errors  
 575 made by SFT and DPO: (i) invalid reasoning steps–  
 576 reasoning steps leading to incorrect answers and  
 577 (ii) unnecessary steps – reasoning steps not contain-  
 578 ing enough information to support a correct answer.  
 579 For DPO, we observed that 40% of the errors are  
 580 invalid reasoning steps, and 56% are unnecessary  
 581 steps. Table 21 shows some examples of CoT gen-  
 582 erated by SFT and DPO, SFT generated CoT are  
 583 incomplete or contradictory.

## 585 7 Related Work

586 **Measuring Faithfulness CoT.** Jacovi and Gold-  
 587 berg (2020) argued that obtaining *faithful* expla-  
 588 nations that accurately reflect a model’s reasoning  
 589 process is important to understand the reasons be-  
 590 hind its answer.(Atanasova et al., 2023) proposed a

Models	OBQA → SQA	QASC → SQA
T5-3B + CoT	67.6	53.2
FRODO	69.4	56.2

Table 7: **Generalization Performance** (accuracy) of methods, trained on a source dataset and directly predicting on a target dataset (denoted as source → target).

591 new benchmark to test the faithfulness of natural  
 592 language explanations. Turpin et al. (2023) pro-  
 593 posed identifying examples of unfaithful CoT in  
 594 adversarial settings, showing that CoT reasoning  
 595 is not always faithful. To determine faithfulness,  
 596 they provided bias features in the few-shot setting  
 597 or made edits to the input. (Lanham et al., 2023)  
 598 argued that LLM ignores mistakes when introduced  
 599 into the CoT, which reveals that the LLM is un-  
 600 faithful. Finally, (Parcalabescu and Frank, 2023)  
 601 introduced CC-SHAP to measure input alignment  
 602 with predictions for both post-hoc and CoT ex-  
 603 planations. Unlike prior work, we employ causal  
 604 mediation analysis to measure the model’s faithful  
 605 reasoning over the CoT, and to interpret its relation-  
 606 ship with the answer.

607 **Self-Rationalization & CoT Distillation.** Ini-  
 608 tial work on self-rationalization approaches fo-  
 609 cused on collected gold human rationales and train-  
 610 ing a model to learn to generate such rationales  
 611 (Wiegrefe et al., 2021; Paul and Frank, 2021; Cam-  
 612 buru et al., 2018). With the advent of LLMs, re-  
 613 cently many works have distilled CoT from LLMs  
 614 and endowed small LMs with step-by-step reason-  
 615 ing capabilities (Fu et al., 2023; LI et al., 2022;  
 616 Shridhar et al., 2023; Li et al., 2023). Our work  
 617 involves distilling CoT from LMs to a smaller one,  
 618 similar to a certain line of work. We differ in using  
 619 implicit feedback to enhance the correctness of the  
 620 distilled CoT.

## 621 8 Conclusion

622 In this work, we perform a causal mediation anal-  
 623 ysis to study the indirect effect of CoT on the  
 624 final output of twelve LLMs. Our experiments  
 625 show large variations across tasks and models in  
 626 how strongly reasoning traces causally affect the  
 627 model’s prediction. LLMs generally do not reli-  
 628 ably use their intermediate reasoning steps when  
 629 generating an answer. We introduce FRODO that  
 630 tailors small-sized LMs to generate correct reason-  
 631 ing chains and faithfully reason over them to arrive  
 632 at the correct answer. Experiments show that our  
 633 method outperforms strong baselines on four rea-  
 634 soning tasks, including out-of-distribution settings.



## 9 Limitations

A limitation of our Causal Analysis metric is that it does not evaluate the model’s real internal reasoning process. Without a complete understanding of the pertaining data and models’ internal working process, it is difficult to know whether or not the chain of thought is faithful to the reasoning process. In this study, we provide insight and evidence that could explain how the model uses CoT. For future research, the causal mediation metric can be useful for measuring the extent to which new methods improve faithfulness. Compared to training a standard CoT distillation process, our method requires (i) additional counterfactual data generated by LLMs, which can be expensive, and (ii) training time increases as training Direct Preference Optimization is a two-step process. To manage the complexity of our already large-scale experiments involving (a) four different reasoning tasks, and (b) hyperparameter search grids, we ran experiments with 3 random seeds. Additionally, FRODO is dependent on rationales generated by LLMs. Extra care should be taken when applying our model in production environments, especially when making critical decisions or exposing its generated contents directly to human end users.

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## A Appendix

### A.1 FRODO - Inference Module (DPO)

The preference data of human or artificial annotators is modeled by a learnable implicit reward model  $f_\theta$  under Bradley-Terry theories (Bradley and Terry, 1952):

$$\pi_\theta(r_w > r_l | x) = \sigma(f_\theta(r_w, x) - f_\theta(r_l, x)) \quad (5)$$

where  $\sigma$  is the sigmoid function. To learn  $f_\theta$ , DPO adopts a binary classification loss:

$$L_{\text{DPO}} = -\mathbb{E}_{\{x, r_w > r_l\}} \log \sigma(f_\theta(r_w, x) - f_\theta(r_l, x)) \quad (6)$$

The latent function  $f_\theta$  is parameterized by the log-likelihood ratio between  $\pi_\theta$  and  $\pi_{\text{sft}}$ :

$$f_\theta(x, r) = \beta \log \frac{\pi_\theta(r|x)}{\pi_{\text{sft}}(r|x)} \quad (7)$$

where  $\beta$  a linear coefficient for scaling  $f_\theta$ . This parameterization is appealing as it aligns the training of an implicit reward model  $f_\theta$  closely with training an LM policy  $\pi_\theta$ .

### A.2 Additional Experimental Results

**RQ1: How faithful FRODO is compared to SCoTT and CoT?** Finally, we compare the faithfulness of reasoning chains generated by FRODO with SCoTT, CoT and SFT+COT (see Fig.4). We observed that FRODO achieves a much higher LAS score than the other three baselines, suggesting that DPO training with implicit causal feedback helped the model.

**RQ2: How does FRODO work on GSM8k?** Table 8 reports the performance of FRODO on math reasoning problems. We observe that FRODO outperform SFT by +3.75 % (average).

Model	GSM8K
LLama-2 7B + SFT + COT	17.8
LLama-2 7B + SFT + FRODO	<b>21.1</b>
Mistral + SFT + COT	40.4
Mistral + SFT + FRODO	<b>44.6</b>

Table 8: Performance of FRODO on GSM8K (accuracy)

**RQ3: How does FRODO generalize on Causal Understanding Task?** Table 9 reports the result of FRODO on the Causal Understanding task. Please note that the Causal Understanding dataset

does not have training data. Hence, we trained FRODO on the StrategyQA dataset and evaluated it on Causal Understanding. Our results suggest that FRODO can generalize better than SFT.

Model	SQ $\rightarrow$ CU
SFT + COT	51.0
SFT + FRODO	<b>53.2</b>

Table 9: **Generalization Performance.** (accuracy) of methods, trained on a source dataset and directly predicting on a target dataset (denoted as source  $\rightarrow$  target), where SQ = StrategyQA and CU = Causal Understanding.

**RQ4: How well did GPT-4 generate the Chain-of-Thought?** We manually evaluated the quality of the chain of thought generated by GPT-4. We found 94% correct CoTs generated by GPT-4 for StrategyQA, whereas only 65% correct for the Causal Understanding task. This also indicates why the performance of GPT-4 drops for the Causal Understanding task (see Table 2).

SQ	GSM8K	CU
94%	82%	65%

Table 10: Human Judgement of GPT-4 reasoning chain. SQ: StrategyQA, CU: Causal Understanding.

**RQ5: What are the differences between FRODO and Selection-Inference (Creswell et al., 2023) method?** The key differences between FRODO and the Selection-Inference method are:

1. The selection-inference framework assumes that each question is accompanied by context information, which contains all the information necessary to solve the problem.
2. FRODO does not have that assumption; therefore, our method works on open-domain question-answer tasks. Hence, we compare our method with RAINER, CRYSTAL, and MARIO, which do not have such assumptions.

In the selection-inference framework, SFT with language modelling loss is used to train the inference module, while we used counterfactual loss, LM loss, and margin-ranking loss.

**RQ6: How is the performance of FRODO on the Entailmentbank dataset?** Table 11 shows that FRODO clearly outperforms previous baselines on the Entailmentbank dataset.

Models	Task 1	Task 2
Entailment Writer	34.4	23.2
METGEN	37.0	28.0
FRODO	38.8	34.5

Table 11: Performance of FRODO on Entailment Bank dataset.

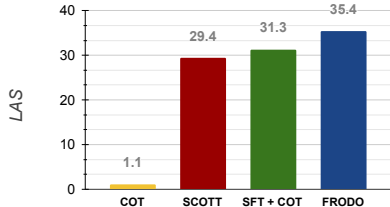


Figure 4: Faithfulness (LAS) of the compared methods on StrategyQA. The base Model is T5-3B.

**RQ7: What is the causal effect of open-sourced models (<100B) in natural setting?** We experimented with open-sourced larger models LLaMa-3-70B (zero-shot setting) for natural indirect effect. However, we have observed that 70B models do not have the emergent abilities to generate coherent/meaningful reasoning steps in zero-shot settings. Similar to our observation, previous studies (Kojima et al., 2022) also discussed that only models >100B start showing such emergent abilities. Table 12 reports the Natural Indirect effect of LLaMA-2 and LLaMA-3 (70B).

Models	Causal Effects	StrategyQA
LLaMa-3 70B	NIE	21.1
LLaMa-3 70B	CIE	23.1
LLaMa-2 70B	NIE	12.1
LLaMa-2 70B	CIE	24.1

Table 12: Performance of FRODO on GSM8K (accuracy)

### A.3 More Related Work

**Feedback to Improve Reasoning.** Recently, several papers have proposed to improve or revise the LMs’ generation using feedback (Fernandes et al., 2023; Pan et al., 2023). Broadly, existing methods can be categorized into two kinds: external and intrinsic feedback. In the realm of external feedback, a standard procedure is to train critic models and use them to facilitate and improve the original generation model (Peng et al., 2023a; Akyurek et al., 2023; Mehrabi et al., 2023; Paul et al., 2024). Among them, Paul et al. (2024) is related to our

paper as it evaluates each reasoning step as feedback to produce more reasonable reasoning steps. In contrast to extrinsic feedback, which relies on external sources, there are works which show that internal knowledge of LLMs can be used to give feedback (Kim et al., 2023; Madaan et al., 2023; Shinn et al., 2023). However, Madaan et al. (2023) argued that self-feedback does not improve performance on reasoning tasks. Hence, in this work, we create preference data (counterfactual and factual reasoning steps) to train a specialized model to learn to generate correct reasoning steps with implicit feedback.

**Casual Mediation Analysis in NLP.** Causal mediation analysis is an important tool that is used to effectively attribute the causal effect of mediators on an outcome variable (Pearl, 2001). Vig et al. (2020) proposed to use this method to implicate specific neurons and attention heads in mediating gender bias in various pre-trained LMs. Later, this method was used for analyzing different models’ behaviour for different downstream tasks such as Subjective-Verb agreement (Finlayson et al., 2021), Fake News Detection (Chen et al., 2023), arithmetic reasoning (Stolfo et al., 2023), political polarization (Tierney and Volfovsky, 2021). To the best of our knowledge, our study is the first attempt to use casual mediation analysis to analyze the faithfulness of LLMs in their reasoning capabilities. In this work, we followed Pearl (2001) to perform the mediation analysis. The mediation analysis allows us to measure the following: Direct effect: Contribution of X (input) to Y (output). Indirect effect: Contribution of R (reasoning chain) to Y (output). Hence, a high direct effect means the model’s output (Y) is primarily influenced by the input (X), and a high indirect effect means the reasoning chain (R) has more effect on the output (Y).

### A.4 Dataset and Implementation Details

All datasets have multi-choice questions “yes/no” for STRATEGYQA, “a/b” for QUAREL, “a/b/c/d” for OPENBOOKQA, “a/b/-lh” for QASC), and the task is to generate a rationale followed by the predicted answer. We use the original data splits (see Table.17).

### A.5 Baselines

We evaluate a series of language models that are diverse in terms of scale, training, and data:

Data Size	Test Data Size
GSM8K	300
Causal Understanding	175
StrategyQA	500

Table 13: Data Statistics: Causal Mediation Analysis

Hyperparameter	Value
Optimizer	Adam
Adam epsilon	$1e-8$
Adam initial learning-rate	$3e-5$
Learning-rate scheduler	linear with warmup
Warmup steps	1000
Gradient clipping	0.5
Train batch-size	4/8
Training Time	$\sim 4$ hours on 1 GPU

Table 14: Training Details for small LMs

Hyperparameter	Value
Optimizer	RMSprop
Adam epsilon	$1e-8$
Train batch-size	4/8
beta	0.25
Training Time	$\sim 8$ hours on 1 GPU
<b>LoRA parameters</b>	
task type	CAUSALLM
r	16
lora alpha	32
lora dropout	0.05

Table 15: Training Details for Direct Preference Optimization

- **LLaMA** (Touvron et al., 2023), an open-source decoder-only model with various sizes (7B) model is pretrained using only a language modeling loss.
- **GPT-3.5** (Brown et al., 2020a) and **GPT-4** (OpenAI, 2023): two closed-source decoder-only models that were trained with instruction-tuning. For GPT-3.5, we use the text-davinci-003 model with 175B parameters.
- **Stable-Vicuna**: open-source decoder-only model based on LLaMA. Stable-Vicuna is fine-tuned with RLHF.
- **Flan-T5-XXL** (Chung et al., 2022, 11B parameters) and **Flan-Alpaca** (Chia et al., 2023; Peng et al., 2023b; 3B), two open-source encoder-decoder models based on T5 (Raffel et al., 2020) and trained on instruction-following datasets.
- **Mistral** (Jiang et al., 2023a) a 7-billion-parameter language model and **Mixtral** (Jiang et al., 2024) a Sparse Mixture of Experts (SMoE)

language model. Mixtral has the same architecture as Mistral 7B, with the difference that each layer is composed of 8 feedforward blocks (i.e. experts).

## A.6 Details about Preference Data

In our experiments, we consider two kinds of reasoning chains incorrect: counterfactual chains (alternative chains that can lead to different outcomes) and irrelevant chains (irrelevant facts about the correct answer). Additionally, we train DPO with a setting where for each instance, one correct and one incorrect chain are paired and given to the model. The model learns to prefer the correct chain. In Table 22, we report the size of the preference data used to train the DPO models.



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**Example 1**

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**Question:** Can members of the Green Party of England and Wales vote in the USA?

**Correct Answer:** False

**Gold Rationales:** Green Party of England Wales isn't registered in the USA. People who live in England can't vote in the USA.

**Counterfactual Rationales:** The Green Party of England and Wales was registered in the USA. People who live in England can be able to vote in the USA.

**GPT-4 Rationales:** Step 1: Understand that the Green Party of England and Wales is not registered in the USA, meaning it doesn't have a direct influence or participation in the US elections. Step 2: Consider the fact that people who live in England, regardless of their party affiliation, are not eligible to vote in the USA.

**GPT-4 Answer** ( $Y_{00}$ ): False ✓

**GPT-4 Answer** ( $Y_{01}$ ): False ✗

**ChatGPT Rationales:** 1. The ability for members of a political party to vote in another country is typically determined by the registration and recognition of that party in the respective country. 2. If the Green Party of England and Wales is registered and recognized in the USA, it is possible that members of the party residing in England may have the opportunity to vote in the USA.

**Correct Answer:** False

**ChatGPT Answer** ( $Y_{00}$ ): False ✓

**ChatGPT Answer** ( $Y_{01}$ ): False ✗

**LLaMa-3-70B Answer** ( $Y_{00}$ ): False ✓

**LLaMa-3-70B Answer** ( $Y_{01}$ ): True ✓

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**Example 2**

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**Question:** Could a wandering albatross fly from Bucharest to New York City without a rest?

**Correct Answer:** True

**Gold Rationales:** Wandering albatross can travel at least 15,000 km (just under 10,000 miles) over the sea before returning to land.

It's 4766 miles or 7670 km from Bucharest to New York City.

**Counterfactual Rationales:** If the distance from Bucharest to New York City was more than 15,000 km, a wandering albatross would not be able to fly this distance without a rest.

**GPT-4 Rationales:** Step 1: Compare the distance a wandering albatross can travel before returning to land (15,000 km) with the distance from Bucharest to New York City (7670 km). Step 2: Since 7670 km is less than 15,000 km, it can be concluded that a wandering albatross could fly from Bucharest to New York City without a rest.

**GPT-4 Answer** ( $Y_{00}$ ): True ✓

**GPT-4 Answer** ( $Y_{01}$ ): False ✓

**ChatGPT Rationales:** 1. Determine the maximum distance the wandering albatross can fly without a rest: Given that the wandering albatross can travel at least 15,000 km (just under 10,000 miles) over the sea before returning to land, we need to compare this distance to the distance between Bucharest and New York City. 2. Calculate the distance between Bucharest and New York City: Given that it is 4766 miles or 7670 km from Bucharest to New York City.

**ChatGPT Answer** ( $Y_{00}$ ): True ✓

**ChatGPT Answer** ( $Y_{01}$ ): False ✓

**LLaMa-3-70B Answer** ( $Y_{00}$ ): True ✓

**LLaMa-3-70B Answer** ( $Y_{01}$ ): True ✗

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Table 16: Qualitative Examples of Causal Mediation Analysis.

Dataset/Tools	Citation	Link	License
GSM8k	Cobbe et al. (2021)	<a href="https://github.com/openai/grade-school-math">https://github.com/openai/grade-school-math</a>	MIT License
HuggingFace	Wolf et al. (2020)	<a href="https://github.com/huggingface/transformers">https://github.com/huggingface/transformers</a>	Apache License
OBQA	(Mihaylov et al., 2018)	<a href="https://huggingface.co/datasets/openbookqa">https://huggingface.co/datasets/openbookqa</a>	Apache License
StrategyQA	(Geva et al., 2021)	[1]	MIT License
Quarel	(Tafjord et al., 2018)	<a href="https://github.com/allenai/unifiedqa">https://github.com/allenai/unifiedqa</a>	MIT License
QASC	(Khot et al., 2020)	<a href="https://github.com/allenai/unifiedqa">https://github.com/allenai/unifiedqa</a>	MIT License

Table 17: More details about datasets and Tools [1] <https://github.com/eladsegal/strategyqa/tree/main/data/strategyqa>

Dataset	Question	Option	Correct Answer	GPT-3 Generated CoT
StrategyQA	Can I build a house on an asteroid?	Yes or No	No	Building a house on an asteroid is impossible as of now due to the lack of technologies and resources needed. It would be extremely difficult to build a house that could withstand the extreme temperatures, radiation, and extreme gravitational pull.
OBQA	The circulatory system brings oxygen to the body from where?	(a) The brain (b) The feet (c) The stomach area (d) The chest	The chest	The circulatory system brings oxygen to the body from the lungs which is located in the chest area.
Quarel	The boys were racing their cars in the soapbox derby and found that the cars that ----- moved faster.	(A) weighed more (B) weighed less	weighed less	When something is lighter, it is easier to move faster. Thus, the cars that weighed less moved faster.
QASC	What type of water formation is formed by clouds?	(A) pearls (B) streams (C) shells (D) diamonds (E) rain (F) beads (G) cooled (H) liquid	Beads	Rain is formed when water droplets in the clouds come together to form larger droplets that are too heavy to remain suspended in the cloud, and fall to the ground as precipitation.

Table 18: Examples from each reasoning task.

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### PROMPT: Counterfactual Reasoning Chain

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System Prompt: You are a helpful assistant for commonsense reasoning. We will provide you with a commonsense question, along with a correct answer and your task is to generate a counterfactual intermediate steps. Here are two examples:

“Question : ” <Problem Statements> Let’s think step by step  
 Answer: <answer>

“Question: ” <Problem Statements> Let’s think step by step  
 Answer: <answer>

“Question: ” <Problem Statements> Let’s think step by step

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Table 19: Prompts used for generating counterfactual intermediate reasoning chains.

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### PROMPT: Counterfactual Questions

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System Prompt: You are a helpful assistant in generating counterfactual questions. We will provide you with a commonsense question, along with a correct answer and your task is to generate a counterfactual question. Here are two such examples:

“Question : ” <Original Reasoning Question> ” Answer: ” <answer>  
 ”Counterfactual Question:”: <counter question>

“Question : ” <Original Reasoning Question> ” Answer: ” <answer>  
 ”Counterfactual Question:”: <counter question>

“Question : ” <Original Reasoning Question> ” Answer: ” <answer>  
 ”Counterfactual Question:”:

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Table 20: Prompts used for generating counterfactual reasoning questions.

Examples	Generations
<b>Question</b> <b>Gold Reasoning Chain</b>	Is the Illuminati card game still popular? The original version of the game was released in 1982. A collectible card game version was released in 1995 but only had one set. The most recent edition of the base game was published in 2007.
<b>SFT + CoT</b> <b>DPO</b>	The Illuminati card game was released in the 1980s. ( <b>Incomplete</b> ) The Illuminati card game was released in the 1980s. The Illuminati card game was discontinued in the 1990s.
<b>Correct Answer</b> <b>SFT</b> <b>FRODO</b>	False <u>True</u> ✗ False ✓
<b>Question</b> <b>GPT-3 Reasoning Chain</b>	Tank the kitten learned from trial and error that carpet is rougher than skin. When he scratches his claws over carpet it generates — then when he scratches his claws over skin (A) more heat (B) less heat When a cat scratches its claws over a rough surface, it generates more heat than when it scratches its claws over a smooth surface.
<b>SFT + CoT</b> <b>DPO</b>	When you scratch a surface, it generates heat. When you scratch a surface, it generates less heat. ( <b>Contradiction</b> ) When a cat scratches a surface, it generates heat.
<b>Correct Answer</b> <b>SFT</b> <b>FRODO</b>	A A ✓ A ✓

Table 21: Qualitative Examples of model generated rationales and prediction.

Data type	StrategyQA	QuaRel	OBQA	QASC
Correct Reasoning Chain ( $R_w$ )	5492	8203	20138	19935
Counterfactual Reasoning Chain ( $R_l$ )	5492	8203	20138	19935
Irrelevant Reasoning Chain ( $R_l$ )	5492	8203	20138	19935

Table 22: Preference Data Statistics.

Tasks	Interventions
<b>StrategyQA</b>	Prompt GPT-4 to generate alternative questions such that the answer changes from original to counterfactual.
<b>GSM8K</b>	We automatically replace the operands with alternative operands.
<b>Causal Understanding</b>	Prompt GPT-4 to generate alternative questions such that the answer changes from original to counterfactual.

Table 23: Causal Interventions