Toward Explanations for Large Language Models in Natural Language

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Abstract

Large Language Models (LLMs) have become proficient in addressing complex tasks by leveraging their extensive internal knowledge and reasoning capabilities. However, the black-box nature of these models complicates the task of explaining their decision-making processes. While recent advancements demonstrate the potential of leveraging LLMs to self-explain their predictions through natural language (NL) explanations, their explanations or chain-of-thoughts may not accurately reflect the LLMs' decision-making process due to a lack of true decision-making pivots involved. Measuring the fidelity of NL explanations is a challenging but important issue, as it is difficult to manipulate the input context to mask the semantics of these explanations, but it can effectively assess the quality of explanations. To this end, we introduce FaithLM for explaining the decision of LLMs with NL explanations. Specifically, FaithLM designs a method for evaluating the fidelity of NL explanations by incorporating the contrary explanations to the query process. Moreover, FaithLM conducts an iterative process to improve the fidelity of derived explanations. Experiment results on three datasets from multiple domains demonstrate that FaithLM can significantly improve the fidelity of derived explanations, which also provides a better alignment with the ground-truth explanations. Our source code is available at `https://anonymous.4open.science/r/xLLM-305B/`.

1 Introduction

Large language models (LLMs) exhibit remarkable performance in various natural language processing tasks, such as the GPT4 (Achiam et al., 2023), LLaMA (Touvron et al., 2023), and Claude (AnthropicAI, 2023). However, these language models are commonly regarded as intricate black-box systems. The opacity of their internal mechanisms poses a significant challenge when trying to explain their decision-making process. The lack of transparency in LLMs, especially in API-accessed LLM services, inferences contradict the practical requirements of stakeholders and are in opposition to regulatory standards in various domains, such as GDPR (Goodman et al., 2017; Floridi, 2019). The imperative arises to develop explainability mechanisms for LLMs, particularly for their use in high-stakes applications such as healthcare. In this work, we focus on "LLM explanation", rather than "LLM reasoning" or "LLM self-refinement", to interpret the model prediction behaviors after providing the final responses. (More illustrations of their discrepancy are in Section 2.2).

Numerous studies have attempted to enhance the transparency of decision-making processes in LLMs by providing natural language (NL) explanations. However, recent advancements are struggling to generate reliable NL explanations for interpreting LLMs (Ye & Durrett, 2022), which fail to provide the underlying true explanation behind their decisions-making. Some work attempt to leverage powerful LLMs (Majumder et al., 2021; Chen et al., 2023b;a) with auxiliary information to generate NL sentences or heatmap of input tokens as model explanations. Although existing work emerged that LLMs may possess the ability to self-explain (Madsen et al., 2024), their explanation-generating process usually overlooks the fidelity, a fundamental metric for evaluating the quality of explanations (Chuang et al., 2023; Wang et al., 2023), which means that the explanations from the existing work may not accurately reflect "why model generate this answers" (Zhao et al., 2023; Turpin et al., 2023) (i.e., low fidelity for the NL explanations). Some work attempts to leverage chain-of-thought (CoT) reasoning steps as the post-hoc model explanation (Lyu et al., 2023; Radhakrishnan et al., 2023). However, these reasoning steps are not considered as model

Question and LLM Answer	Faithful NL Explanation	Question conditioned with Contrary NL Explanation
Question: Can the positive pole from two magnets pull each other closer? **Original Answer: No**	Each magnet has a positive pole and a negative pole, and **similar poles push each other away.**	**Question:** Each magnet has a positive pole and a negative pole, and **similar poles pull each other closer.** Can the positive pole from two magnets pull each other closer? **New Answer: Yes**

Table 1: An example of measuring fidelity of NL explanations. The LLM first answers the question in **No**. Given a faithful explanation *"similar poles pull each other away,"* with its contrary NL explanation, the LLM changes the answer from **No** to **Yes** when introduced contrary NL explanation as an extra condition to LLM.

explanations (Tanneru et al., 2024), as they are only the intermediate outputs in resulting answers without fidelity guarantee. Generally, prior work define this manner as failing to provide faithful explanations (or low fidelity) for a given generated answer. These CoT steps are produced without a thorough fidelity check (i.e., one that involves masking out the key factors) to ensure they genuinely influence the final answer. These steps are only the intermediate results during the LLM prediction and their fidelity remains unknown. A proper fidelity measurement requires masking the critical features or key messages in the explanation and observing the model's performance afterward (Du et al., 2019), but neither of them are monitored or adopted before claiming CoT reasoning as model explanations. Measuring the fidelity of NL explanations now become a important but challenging issue, as we can monitor and optimization the explanation generation process based on fidelity improvement. The ones may provide crucial information beyond the input context, but the faithful information may appear in semantic levels, making it hard to measure by manipulating the tokens for fidelity measurement.

To overcome this challenge, we propose a method to measure the fidelity of NL explanations. We give an example to convey the motivation in Table 1. Specifically, the fidelity of an explanation can be measured by leveraging its contrary explanation as extra conditions of the input context, and observing the LLM's output difference compared with its initial output. Here, a contrary explanation refers to a statement with opposite semantics to the original explanation. By incorporating the contrary explanation to the input context, we can identify an explanation as high fidelity if there is a significant change in the LLM's output, such as from **No** to **Yes**. This change indicates that the crucial information present in the original explanation is substituted with the opposite meaning context in the contrary explanation, where the crucial information is essential to the LLM's decision-making process. Based on this observation, we propose to extend the applicability of fidelity to the evaluation on NL explanations. This extension follows the integration of contrary explanations to represent the concepts of masking important features in traditional fidelity measurement.

Building upon this new fidelity measurement, we introduce *Faithful LLM Explainers* (FaithLM) to generate faithful NL explanations for LLMs. Specifically, FaithLM adopts LLMs as explainer to generate the NL explanations and explanation trigger prompts, and iteratively optimizes the derived NL explanations and trigger prompts with the goal of fidelity enhancement. During the iterative process, FaithLM computes the fidelity of each derived explanation and optimized prompt based on our proposed fidelity measurement method, and progressively improves their fidelity through in-context learning. We conducted the experiments on four different LLMs under three datasets. FaithLM achieves significantly higher fidelity in generating NL explanations and more closely matched the golden explanations compared with state-of-the-art baseline methods. Our contributions can be summarized as follows:

- **Fidelity of NL Explanations:** We propose the way to measure the fidelity of NL explanations by introducing a contradictory explanation and observing how the LLM's output changes.

- **Faithful LLM Explainers:** FaithLM improves the fidelity of NL explanations, aiming at faithfully explaining the decision-making process of LLMs.

- **Fidelity and Truthfulness:** Experimental results show that FaithLM can improve the fidelity of NL explanations, revealing a better alignment with the ground-truth explanations.

2 Preliminaries

2.1 Notations and Objectives

We aim to explain the decisions of arbitrary targeted LLMs $f(\cdot)$ with NL explanations in a post-hoc manner. Given an input $\boldsymbol{X}$, the targeted LLMs generate an output $\boldsymbol{Y} = f(\boldsymbol{X})$. Our objective is to produce an NL explanation $\mathcal{E}_{\text{NL}}$ that faithfully explains the reasons behind the prediction of $\boldsymbol{Y} = f(\boldsymbol{X})$. In this work, we employ an LLM as the explainer $g(\cdot)$ to generate the NL explanation $\mathcal{E}_{\text{NL}} = g(\cdot \mid \boldsymbol{X}, \boldsymbol{Y})$. However, the $\mathcal{E}_{\text{NL}}$ under single-forward passing generated directly from LLMs may not be faithful and accurate. The consistency between $f(\cdot)$ and $g(\cdot)$ is ensured through an iterative optimization process monitored by fidelity scores. To this end, the explainer $g(\cdot)$ to generate **more faithful NL explanations regarding the decision of** $f(\cdot)$ **in post-hoc**, where $f(\cdot)$ can be either closed-source or open-source LLMs.

2.2 Difference between LLM Explanation and Chain-of-thoughts

Due to the limited accessibility of LLM APIs, recent research on LLM explanations has largely relied on post-hoc explanation approaches (Chen et al., 2023b). However, some studies conflate 'LLM reasoning' and "LLM self-refinement' with 'LLM explanations' when discussing these post hoc LLM explanations, even though these three terms are not identical and with different goals. We illustrate the difference as follows.

LLM reasoning and Chain-of-thoughts refers to the internal process the model undergoes when it encounters a query or instruction, such as weighting probabilities and generating words step by step plus verification, with the goal of improving performance on reasoning tasks. Some advantages rely on providing chain-of-thought (CoT) reasoning (Lanham et al., 2023; Radhakrishnan et al., 2023; Chen et al., 2023a; Wang et al., 2022) to present the hidden inference steps that the model goes through. These studies show that CoT Manuvinakurike et al. (2025) can improve reasoning performance, but does not necessarily provide an explanation or even count as explanations of how or why an LLM arrives at its answers (Tanneru et al., 2024), where "good fidelity" in the series of work is typically defined by the alignment between the content of CoT and the final answer (Lyu et al., 2023; Radhakrishnan et al., 2023). Another line of work leverages self-refinement techniques (Lightman et al., 2023; Madaan et al., 2024; Tian et al., 2024), which employ self-reasoning or knowledge supervision as feedback, to iteratively enhance reasoning performance. Although these advancements introduce robust self-feedback loops that effectively boost reasoning accuracy, the "feedback" during optimization is neither necessarily faithful nor equivalent to LLM explanations (Tanneru et al., 2024). Notably, this feedback may be wrong yet still guide LLMs toward a correct reasoning direction. Due to its non-stationary nature, it yields non-faithful outputs when treated as an LLM explanation, which is also very distinct from the goal of "LLM explanation" tasks.

LLM Explanations. Unlike LLM reasoning and self-refinement, *LLM explanation* focuses on clarifying why the model provides a particular answer after generating its final decision (Siegel et al., 2024). The concept of fidelity in an LLM explanation (Du et al., 2019; Zhao et al., 2023), which differs from LLM reasoning and self-refinement, refers to whether the model's prediction would change if the key knowledge provided explanation were removed. If removing the knowledge causes a drastic change in the model's prediction, we can conclude that the derived explanation is faithful to the LLMs prediction (i.e., the actual reasons that results the predictions). In this work, we focus on LLM explanation, rather than LLM reasoning or self-refinement.

2.3 Limitations of Traditional Fidelity Measurement on NL Explanations

The fidelity metric measures the fidelity of the given explanation, which is broadly applicable when ground-truth explanations are unavailable. In the NLP scenario, fidelity has been used to evaluate the heatmap-formatted explanations (Lopardo et al., 2023; Huang et al., 2023), where the heatmap one highlights the important tokens of the input. Specifically, fidelity evaluates the explanation by removing the important tokens from the input $\boldsymbol{X}$ and checking the prediction difference of the targeted LLM. Following the definition of fidelity (Miró-Nicolau et al., 2024). Given a sequence of tokens $\boldsymbol{I} = \{t_1, \cdots, t_M\} \subseteq \mathcal{E}_{\text{NL}}$, which is identified as an important component of explanation to the prediction of a targeted LLM $\boldsymbol{Y} = f(\boldsymbol{X})$. The traditional fidelity can be

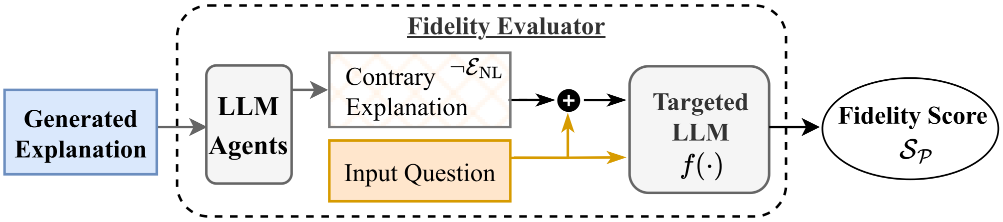


Figure 1: The framework of Fidelity Evaluator. The evaluator calculates the fidelity scores of the derived explanations based on its contrary explanations.

estimated as:

$$\text{Fidelity} = f(\boldsymbol{X}) - f(\boldsymbol{X} \setminus \boldsymbol{I}),$$

where "$\boldsymbol{X} \setminus \boldsymbol{I}$" denotes token removal from $\boldsymbol{X}$ in $\boldsymbol{I}$.

If important component $\boldsymbol{T}$ achieves higher fidelity, this demonstrates that $\mathcal{E}_{\mathrm{NL}}$ comprises the crucial tokens that significantly influence the predictions of the targeted LLMs. However, it is challenging to evaluate the fidelity of NL explanations throughout the fidelity defined above, as the critical components in NL explanations may not contain in the input context $\boldsymbol{X}$.Some work (Lanham et al., 2023) attempts to measure fidelity by modifying the output chain-of-thought (CoT) reasoning to overcome this challenge. However, altering only the output does not guarantee changes in the model's pre-filling probability and may therefore meet self-consistency, but rather than the definition of fidelity. Thus, we cannot simply remove or modify critical components from the question following the traditional definition. Unlike the previous approaches, we propose a solution to address this obstacle by removing the critical components from the semantic meaning instead of the tokens.

3 FaithLM: The Explainer LLM Framework

In this section, we introduce a generative explanation framework, FaithLM, which derives faithful explanations in NL format. The derived explanations are expected to accurately reflect the predictive decision-making process of targeted LLMs with high fidelity after optimizing under FaithLM.

3.1 Fidelity Evaluator for Natural Language Explanations

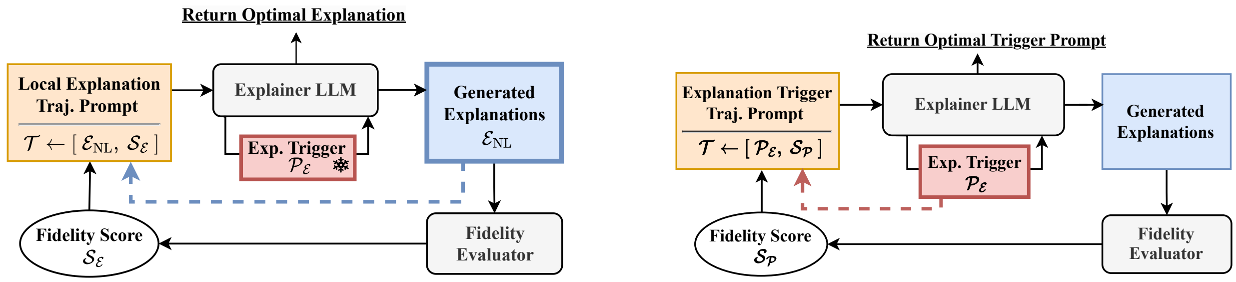
We introduce the *Fidelity Evaluator* to assess the fidelity of NL explanations shown in Figure 1.

Fidelity of NL Explanations. To assess the fidelity of NL explanations, we extend the traditional fidelity definition to equip it with special constraints regarding NL explanations. To address this challenge, we propose formulating the fidelity of NL explanation as the prediction difference caused by the “contrary explanation". Specifically, the contrary explanation $\neg\mathcal{E}_{\mathrm{NL}}$ is defined as a statement obtained opposite semantics to the given NL explanation $\mathcal{E}_{\mathrm{NL}}$. For instance, if the explanation is *"similar poles* ***push each other away,"*** then the contrary explanation would be *"similar poles* ***pull each other closer."*** To estimate the fidelity of $\mathcal{E}_{\mathrm{NL}}$, we use the contrary explanation $\neg\mathcal{E}_{\mathrm{NL}}$ as an extra given condition to the input queries, forming conditional LLM inferences $f(\boldsymbol{X} \mid \neg\mathcal{E}_{\mathrm{NL}})$. This operation results in different prediction results for targeted LLMs compared to the original predictions, which compels the targeted LLMs to follow contrary information from the explanations of the input queries. In this manner, the fidelity $\mathcal{S}_{\mathcal{E}}$ of $\mathcal{E}_{\mathrm{NL}}$ can be estimated by the prediction difference:

$$\mathcal{S}_{\mathcal{E}} := f(\boldsymbol{X}) - f(\boldsymbol{X} \mid \neg\mathcal{E}_{\mathrm{NL}}). \tag{1}$$

This formulation aligns with the traditional definition of fidelity by observing the prediction difference of the LLM when considering input with and without the component supplied by the explanations.

Fidelity Evaluator. Unreliable explanations derived from LLMs often present incorrect predictions (Ye & Durrett, 2022), which means that the relationship between the reliability of the explanations and the correctness of the predictions is significantly high. Motivated by the observation, we propose a framework



(a) Fidelity-enhanced Explanation (b) Trigger Prompt Optimization

Figure 2: An overview of FaithLM framework for two different optimization objectives. The blue dotted line reveals the trajectory to optimize the NL explanation (Section 3.2), and the red dotted line indicates the trajectory of the explanation trigger prompt optimization (Section 3.3). "Traj. Prompt" denotes the trajectory system prompt shown in Section H.

for the Fidelity Evaluator as illustrated in Figure 1. Specifically, we utilize a powerful LLM agent, such as GPT-3.5, to generate the contrary explanation $\neg\mathcal{E}_{\mathrm{NL}}$ regarding the original $\mathcal{E}_{\mathrm{NL}}$. The generation process for $\neg\mathcal{E}_{\mathrm{NL}}$ is guided by the prompt provided in Appendix G. Given the contrary explanation as a condition for the input context, the Fidelity Evaluator computes the fidelity scores according to the difference of output logits $f(\boldsymbol{X}) - f(\boldsymbol{X} \mid \neg\mathcal{E}_{\mathrm{NL}})$. Intuitively, if the targeted LLMs' output probability changes significantly enough to flip the result (i.e., judgements or choices), it implies that the contrary explanations $\neg\mathcal{E}_{\mathrm{NL}}$ consist of the contrasting key messages against $\mathcal{E}_{\mathrm{NL}}$ that can significantly impact the decision-making process of the targeted LLM. This suggests that the explanation $\mathcal{E}_{\mathrm{NL}}$ contains key components that significantly support the inference of the targeted LLMs. Unlike previous approaches, we did not utilize counterfactual explanations to measure fidelity, as the ones may contain contexts different from the target-to-assessed explanation $\mathcal{E}_{\mathrm{NL}}$ (Parcalabescu & Frank, 2024), leading to inaccurate assessment. In this work, we introduce a "contrary explanation" (i.e., not the counterfactual explanations) that preserves the opposite meaning of existing information in $\mathcal{E}_{\mathrm{NL}}$, enabling LLM explanation to have better chance to reflect the true decision-making pivots that lead to the given prediction.

3.2 FaithLM on Fidelity-enhanced Explanation

In this section, we introduce an iterative framework designed to progressively enhance the fidelity of NL explanations with iterative fidelity-enhanced optimization.

Fidelity-enhanced Explanation. The framework of fidelity-enhanced explanation is illustrated in Figure 2a. Since the initial explanation may be unreliable and unfaithful, we propose a fidelity-enhanced optimization approach designed to progressively generate explanations with higher fidelity. We aim to explain the response $\boldsymbol{Y}$ produced by the targeted LLM $f(\cdot)$ in response to the given input queries $\boldsymbol{X}$ with NL explanations $\mathcal{E}_{\mathrm{NL}}$ following the goal of fidelity enhancement. In the first round of enhancement, the LLM explainer generates NL explanations $\mathcal{E}_{\mathrm{NL}}$ following a given human-crafted explanation trigger prompt $\mathcal{P}_{\mathcal{E}}$ provided in Appendix G. The explanations are then generated by the explainer $g(\mathcal{P}_{\mathcal{E}} \mid \boldsymbol{X}, \boldsymbol{Y})$. Starting from the second round till converge, FaithLM collects a trajectory $\mathcal{T}$ with the NL explanations $\mathcal{E}_{\mathrm{NL}}$ and their corresponding fidelity scores $\mathcal{S}_{\mathcal{E}}$ generated by Fidelity Evaluator. The collection process can be represented as $\mathcal{T} \leftarrow \{\mathcal{T},\ [\mathcal{E}_{\mathrm{NL}},\ \mathcal{S}_{\mathcal{E}}]\}$, where $\mathcal{T}$ initially starts as an empty trajectory. Following this trajectory, the LLM explainer generates new explanations with the goal of achieving higher fidelity scores in subsequent iterations. This process is guided by the system prompts detailed in Figure 13.

The trajectory $\mathcal{T}$ is continuously updated by incorporating each newly derived explanation with its assessed fidelity score until the convergence. Regardless of any given explanation trigger prompts $\mathcal{P}_{\mathcal{E}}$, FaithLM can all systematically guide the generation of NL explanations, progressively improving fidelity scores by following the reference path established in the trajectory.

Algorithm of Fidelity-enhanced Explanation. The outline of FaithLM for Fidelity-enhanced Explanation is detailed in Algorithm 1. Specifically, in the first iteration, FaithLM generates the NL explanations using the human-craft prompts (line 1). starting from the second iteration till the convergence or optimization ends, FaithLM estimates the fidelity of the derived NL explanations (line 4). Then, we incorporate the explanation and its corresponding fidelity score to the trajectory (line 5), and update the explanations with the goal of achieving higher fidelity scores in subsequent iterations (line 6). The iteration terminates at a predetermined step or ceases earlier as soon as FaithLM observes a flipping performance from the targeted LLM $f(\cdot)$.

3.3 FaithLM on Trigger Prompt Optimization

Despite the success of enhancing fidelity in Section 3.2, the low quality of the explanation trigger prompts $\mathcal{P}_{\mathcal{E}}$ may still hinder the optimization process of receiving a high-fidelity explanation. Given that the unknown preference for prompts from LLMs, human-crafted trigger prompts used in Fidelity-enhanced Explanation Optimization might lead to sub-optimal fidelity enhancement in the derived explanations. In this section, we hereby propose a new optimization pipeline under FaithLM, aiming to optimize the trigger prompt $\mathcal{P}_{\mathcal{E}}$ for generating NL explanations with higher fidelity scores as the LLM explanations of input each input query.

Algorithm 1 Fidelity-enhanced explanation

Input: Input $\boldsymbol{X}$, output $\boldsymbol{Y}$, targeted LLMs $f(\cdot)$, human-crafted prompt $\mathcal{P}_{\mathcal{E}}$, and LLM explainer $g(\cdot)$.
Output: NL explanation $\mathcal{E}_{\text{NL}}$.
1: $\mathcal{E}_{\text{NL}} \sim g(\mathcal{P}_{\mathcal{E}} \mid \boldsymbol{X}, \boldsymbol{Y})$
2: $\mathcal{T} = \varnothing$
3: **while** *steps not end* **and** *decision not flips* **do**
4: Estimate the fidelity score $\mathcal{S}_{\mathcal{E}}$ of $\mathcal{E}_{\text{NL}}$
5: Append $\mathcal{T} \leftarrow \mathcal{T} \cap [\mathcal{E}_{\text{NL}},\ \mathcal{S}_{\mathcal{E}}]$
6: Update $\mathcal{E}_{\text{NL}} \sim g(\mathcal{T} \mid \boldsymbol{X}, \boldsymbol{Y})$
7: **end while**

Trigger Prompt Optimization. The framework of Trigger Prompt Optimization is shown in Figure 2b. The framework aims to optimize the trigger prompt to generate NL explanations with higher fidelity. Different from the optimization goal in Section 3.2, the trajectory in this task collects the trigger prompts $\mathcal{P}_{\mathcal{E}}$ and their fidelity scores $\mathcal{S}_{\mathcal{P}}$. The trajectory is constructed by the system optimization prompts detailed in Figure 12.

To estimate the fidelity score for a trigger prompt, FaithLM first adopts the randomly human-crafted trigger prompt to guide the LLM explainers to generate NL explanations, and then utilize the Fidelity Evaluator to assess the fidelity of the derived explanation. The final estimated score is averaged by the fidelity score $\mathcal{S}_{\mathcal{E}_i}$ of the hold-out dataset $(\boldsymbol{X}_i, \boldsymbol{Y}_i) \in \mathcal{D}$. Formally, the fidelity score for a trigger prompt $\mathcal{P}_{\mathcal{E}}$ is as follows:

$$\mathcal{S}_{\mathcal{P}} = \mathbb{E}_{\mathcal{E}_i \sim g(\mathcal{P}_{\mathcal{E}} | \boldsymbol{X}_i, \boldsymbol{Y}_i)} \left[\mathcal{S}_{\mathcal{E}_i} \right], \tag{2}$$

where $\mathcal{S}_{\mathcal{E}i}$ represents the fidelity score of the explanation $\mathcal{E}_i$, which is generated by $g(\mathcal{P}_{\mathcal{E}} | \boldsymbol{X}_i, \boldsymbol{Y}_i)$, as assessed by the Fidelity Evaluator in Section 3.1.

During the optimization, the trajectory begins from an empty set and starts to incorporate newly derived trigger prompts with the fidelity scores in each optimization iteration. Following this trajectory, the LLM explainer generates a new trigger prompt with the goal of achieving higher fidelity scores of explanations in subsequent iterations. After several rounds of iterations, FaithLM ultimately yields an optimal explanation trigger prompt with the highest fidelity score for the LLM explainer to generate a more faithful NL explanation.

Algorithm of Trigger Prompt Optimization. The outline of FaithLM for Trigger Prompt Optimization is detailed in Algorithm 2, which focuses on optimizing the trigger prompt for generating NL explanations. Specifically, in each iteration, LLM explainer $g(\cdot)$ leverages the trigger prompt to generate the NL explanations and estimates its fidelity (lines 4-7). The fidelity scores of the trigger prompts average the fidelity scores of the entire hold-out dataset (lines 8). Afterward, the trajectory appends the trigger prompt with its corresponding fidelity score (line 9), and updates the trigger prompt as a new sequence of words to achieve higher fidelity scores (line 10). Through multiple iterations, FaithLM progressively

Algorithm 2 Trigger Prompt Optimization.

Input: Hold-out dataset $\mathcal{D}$, Targeted LLMs $f(\cdot)$, and LLM explainers $g(\cdot)$.
Output: Optimal explanation trigger prompt $\mathcal{P}_{\mathcal{E}}$.
1: Initialize human-crafted $\mathcal{P}_{\mathcal{E}}$
2: Initialize $\mathcal{T} = \{\varnothing\}$
3: **while** (Steps Not End) **do**
4: **for** $(\boldsymbol{X}_i, \boldsymbol{Y}_i) \sim \mathcal{D}$ **do**
5: $\mathcal{E}_i \leftarrow g(\mathcal{P}_{\mathcal{E}} \mid \boldsymbol{X}_i, \boldsymbol{Y}_i)$
6: Estimate the fidelity score $\mathcal{S}_i$ of $\mathcal{E}_i$
7: **end for**
8: $\mathcal{S}_{\mathcal{P}} = \mathbb{E}_{\mathcal{E}_i \sim g(\mathcal{P}_{\mathcal{E}} | \boldsymbol{X}_i, \boldsymbol{Y}_i)} \left[\mathcal{S}_{\mathcal{E}_i} \right]$
9: Append $\mathcal{T} \leftarrow \mathcal{T} \cap (\mathcal{P}_{\mathcal{E}}, \mathcal{S}_{\mathcal{P}})$
10: Update $\mathcal{P}_{\mathcal{E}} \leftarrow g(\mathcal{P}_{\mathcal{E}} \mid \mathcal{D})$
11: **end while**

guides the trigger prompt to generate explanations with higher fidelity scores, following the reference path established in the trajectory. The iteration process terminates at a predetermined 20 step.

4 Experiment

In this section, we conduct experiments to evaluate the performance of FaithLM, aiming to answer the following three research questions: **RQ1:** How does FaithLM perform in generating explanations in terms of efficacy? **RQ2:** Can optimized explanation trigger prompts transfer between different datasets? **RQ3:** How does the contrary explanations affect the explanation performance?

4.1 Datasets and Baselines

Datasets. Three datasets with multiple tasks are included: ECQA (Aggarwal et al., 2021) dataset on commonsense question-answer task, TrivaQA-Long (Bai et al., 2023; Joshi et al., 2017) dataset on reading comprehension task, and COPA (Kavumba et al., 2019; Roemmele et al., 2011) dataset on commonsense causal reasoning task. More details are provided in Appendix A. **Baseline Methods.** Two state-of-the-art baseline methods: `SelfExp` (Madsen et al., 2024) and `Self-consistency` (Wang et al., 2022). The former ones instruct LLMs to generate explanations using prompt engineering under single-forward inference, and the later ones leverage the chain-of-thought outputs as the model explanations.

4.2 Experiment Settings

We introduce the experimental settings for evaluating FaithLM. Two distinct types of explanation tasks and evaluation settings are as follows.

Fidelity-enhanced Explanation In this task, our goal is to produce NL explanations that exhibit a higher fidelity. The fidelity is exploited as a metric to evaluate fidelity. FaithLM is evaluated across all testing instances, where an NL explanation is generated for each instance, and the averaged fidelity score is calculated, serving as the reported metric to evaluate fidelity.

Explanation Trigger Prompt Optimization. In this task, we aim to optimize the explanation trigger prompt that benefits FaithLM in generating better explanations. The optimization process is conducted on the same dataset, where 30 instances are sampled as a hold-off dataset in each optimization step from the training set. During the optimization process, the fidelity score of a trigger prompt is calculated as the average of the fidelity scores from the selected instances.

Evaluation Metrics. The quality of the derived NL explanation is evaluated under the fidelity and truthfulness metrics. The fidelity follows Section 3.1, which observes the flipping rate of the targeted LLMs by incorporating contrary explanations to the input. The evaluation of truthfulness assesses the correlation between the derived NL explanations to the ground-truth explanations Specifically, we leverage GPT-3.5 and two well-trained natural language inference (NLI) models, Roberta-Large and XLNet-Large (Nie et al., 2020) from the huggingface hub (Wolf et al., 2019), as the evaluators. With the same evaluators setup, the truthfulness evaluation follows the settings from (Liu et al., 2023), and uses the evaluation prompt provided in Appendix F. Specifically, the evaluators assess the derived explanations and ground-truth explanations, determining whether the two sentences belong to “similar content", “dissimilar content," or “non-relevant content". Higher the proportion of “similar content", the more consistent results with ground-truth NL explanations.

Implementation Details. In the experiments, we explore two variants of LLMs as the targeted LLMs $f(\cdot)$: Vicuna-7B (Chiang et al., 2023) and Phi-2 (Javaheripi & Bubeck, 2023), two types of LLMs as the explainers $g(\cdot)$ in FaithLM: GPT-3.5-Turbo and Claude-2 (Anthropic, 2023). The LLM agent for generating the contrary explanations takes the same LLMs as those used by the explainers. All reported results are calculated from the average scores of 3 times repetitions with the grid search on the performance. The settings for predictors are uniform, with Phi-2 (2.7B) and Viucua-7B receiving identical hyperparameter configurations during the experiments conducted in this study. The hyper-parameter settings and device configuration, including temperature and total optimization steps, of FaithLM are given in Appendix C and D, respectively.

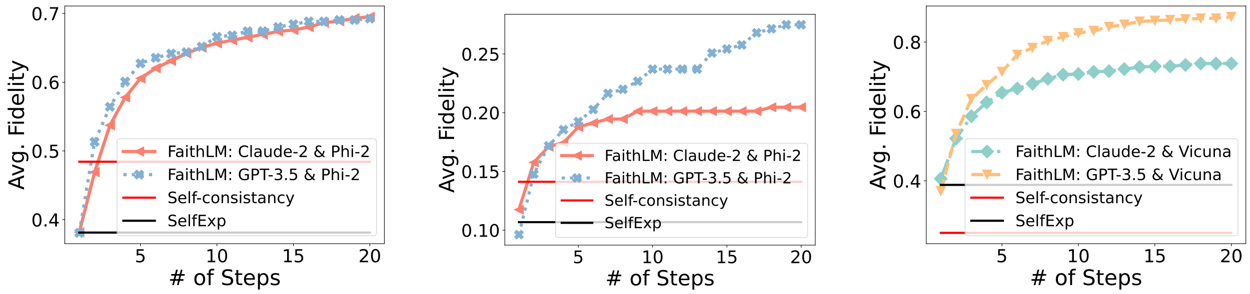


Figure 3: Fidelity evaluation of explanations on ECQA (left), TriviaQA-Long (middle), and COPA (right). Scores are average fidelity on test instances at each step of fidelity-enhanced optimization.

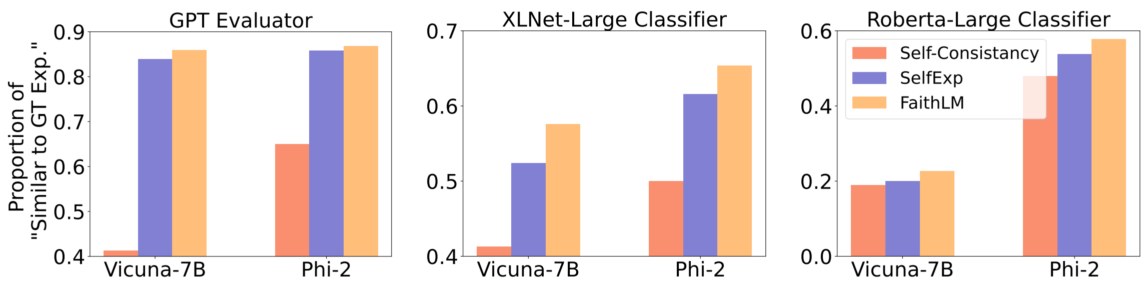


Figure 4: Trustfulness evaluation of the NL explanations. A higher proportion of “similar to ground-truth explanation," indicates more consistent generated explanations with the ground-truth.

4.3 Explanation Efficacy of FaithLM (RQ1)

Efficacy of Derived Explanations. We assess the efficacy of derived explanations under the fidelity metric. FaithLM adopts the trajectory system prompts in Figure 13 of Appendix H. The generation of contrary explanations is guided by the prompt in Table 8.

- **Fidelity Evaluation.** The results in Figure 3 demonstrate that FaithLM achieves significantly higher fidelity scores across all three datasets compared with two baselines after 20 steps of optimization. Moreover, the optimization curve of fidelity demonstrates that 20 rounds of optimization are sufficient to converge. A similar phenomenon occurs across different settings of explainers and targeted LLMs. Additional results are provided in Appendix E.

- **Truthfulness Evaluation.** To evaluate the truthfulness of explanations, we show the proportions of “similar to ground-truth explanations" in the ECQA dataset, as depicted in Figure 4. We leverage GPT evaluators and well-trained NLI evaluators to assess whether the given explanations are within similar content to ground-truth explanations. The results show that FaithLM’s explanations are more consistent with the ground-truth NL explanations, indicated by a larger proportion of “similar to ground-truth explanations" generated by FaithLM than baseline methods.

Efficacy of Explanation Trigger Prompts. We first show prompt optimization curves on three different datasets, and then leverage the optimal explanation trigger prompts to generate explanations via FaithLM. In the experiments, we randomly select 15 instances from the training dataset in each optimization round, and compute the average fidelity scores of the newly derived trigger prompts. After the progress is terminated, we evaluate the optimized trigger prompts on the testing set. The optimization step is established at 50 rounds across different explainer and targeted LLMs.

- **Trigger Prompt Optimization Curve.** Figure 5 demonstrates the optimization curves of three datasets. We display the explainer as GPT-3.5-Turbo and Claude-2 and the explainer as Vicuna-7B. We observe that the optimization curve exhibits a generally ascending trend as the step progresses, interspersed with

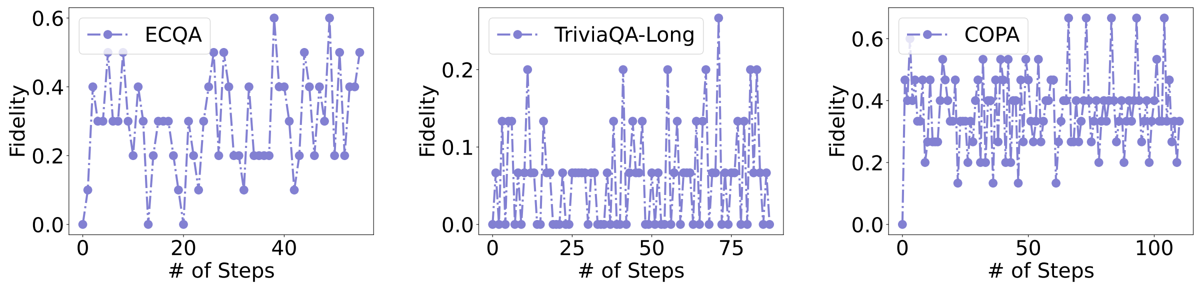
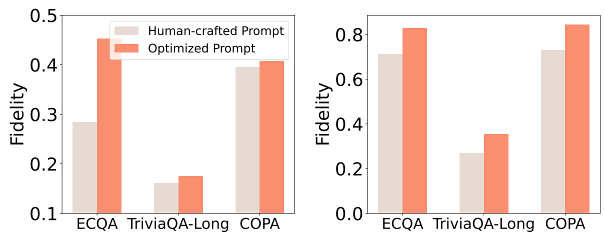
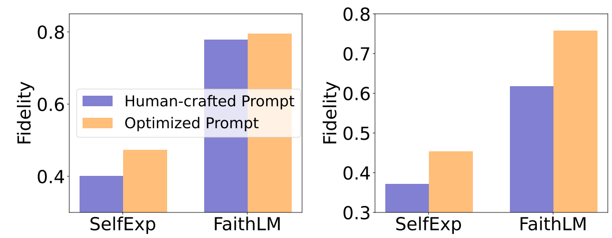


Figure 5: The fidelity in different optimization steps of the trigger prompts (Algorithm 2) on the ECQA, TrivaQA, and COPA datasets. The fidelity grows higher as the number of steps increases.



(a) Robustness analytics of trigger prompts



(b) Transferability results of trigger prompts

Figure 6: Assessment on the adaptation of the optimized explanation trigger prompts. Figure (a) reveals the robustness evaluation, and figure (b) illustrates the results on transferability.

multiple waves throughout the optimization procedure. This indicates that FaithLM generates better explanation trigger prompts after the optimization. More results are provided in Appendix E.

- **Explanation Generation by Optimized Trigger Prompts.** We utilize the optimized explanation trigger prompts to generate explanations following Algorithm 1. The results are displayed in Figure 6a, including the ones using all three datasets with Claude-2 as the explainer and Vicuna-7B as the targeted LLM. We observe that optimized explanation trigger prompts obtain higher fidelity scores than the initial human-crafted trigger prompt in generating explanations. This trend is consistent across all datasets, regardless of whether the explanations are refined by Algorithm 1.

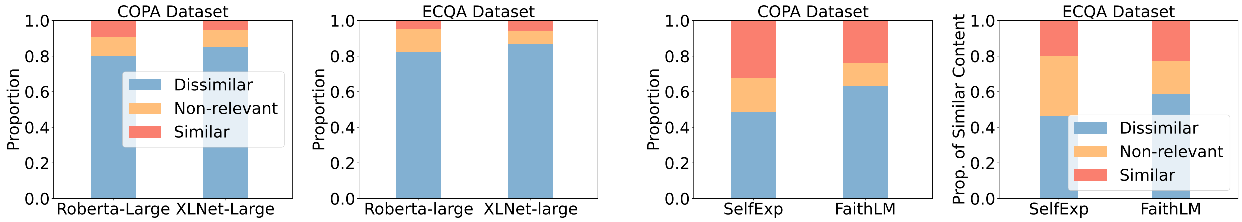
A Case Study of FaithLM. The case studies illustrate the evolving trend via FaithLM, including derived NL explanations, explanation trigger prompts, and contrary explanations in Appendix I. These studies demonstrate that the explanations generated by FaithLM are informative and readable, which enables humans to understand the reasons behind the decision-making process of target LLMs.

4.4 Transferability of Trigger Prompt (RQ2)

We assess the transferability of ultimately optimized trigger prompts across different unseen datasets within the same domain, as depicted in Figure 6b. Specifically, we transfer the optimized trigger prompts from the ECQA to the Social-IQA dataset, and from the COPA to the XCOPA datasets, without any additional optimization. Specifically, the Social-IQA dataset is dedicated to commonsense question-answering (similar to the ECQA dataset), while the XCOPA dataset specializes in causal reasoning (similar to the COPA dataset). We adopt the Vicuna-7B as the targeted LLM, and Claude-2 as the explainer on these transfer tasks. The fidelity of the derived NL explanation on the target dataset is shown in Figure 6(b). The optimized trigger prompts show better explanation efficacy than human-crafted prompts when it is transferred in similar domain. This shows that the optimized trigger prompts generated by FaithLM possess a great property of data transferability.

4.5 Ablation Studies on Contrary Explanation in FaithLM (RQ3)

The quality of contrary explanations $\neg\mathcal{E}_{\text{NL}}$ determines the efficacy of FaithLM. We leverage the powerful LLMs as the LLM agent to generate contrary explanations, requesting the delivery of high-quality opposite-meaning



(a) Evaluated by pre-trained NLI classifiers (b) Evaluated by GPT-3.5 Evaluator

Figure 7: Ablation studies on evaluating contrary explanation. The results show that contrary explanations obtain opposite meanings to the derived explanations.

outputs from their original NL explanations. We evaluate the quality of contrary explanations, aiming to observe the semantic differences between the original NL explanations and their contrary explanations. To examine the quality, we employ the GPT classifier and two well-trained NLI classifiers, Roberta-Large and XLNet-Large (Nie et al., 2020). We leverage each classifier to distinguish whether the relationship between the "original NL explanations" and "contrary explanations" belong to the category of "similar meaning (entailment)," "dissimilar meaning (contradiction)," or "non-relevant (neutral)." We follow the evaluation settings from (Liu et al., 2023) on GPT-classifier with evaluation prompt provided in Appendix F. The results show in Figure 7 with randomly sampled 100 instances from the ECQA and COPA datasets. We observe that the two NLI classifiers achieve up to 86% and 82% in the "dissimilar meanings"" category. The results show that SelfExp obtains more non-faithful information than FaithLM, risking to generate non-relevant explanations. Case studies are provided in Appendix I, showing informativeness and readability of contrary explanations.

5 Conclusion

In this paper, we introduce FaithLM to explain the decision-making process of LLMs, instead of providing reasoning or self-refinement feedback as model explanation. Specifically, FaithLM employs a fidelity enhancement strategy to progressively refine the fidelity of derived explanations and explanation trigger prompts. FaithLM conducts an iterative process to improve the fidelity of derived explanations. Experimental results demonstrate the effectiveness of FaithLM, and better alignment with the ground-truth explanations. This suggest that the decision-making process are truly reflected. For future work, we plan to extend FaithLM in healthcare, where the needs for transparency is critical given the growing reliance on black-box LLMs.

References

Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. Gpt-4 technical report. *arXiv preprint arXiv:2303.08774*, 2023.

Shourya Aggarwal, Divyanshu Mandowara, Vishwajeet Agrawal, Dinesh Khandelwal, Parag Singla, and Dinesh Garg. Explanations for CommonsenseQA: New Dataset and Models. In *Proceedings of the 59th Annual Meeting of the Association for Computational Linguistics and the 11th International Joint Conference on Natural Language Processing*, pp. 3050–3065. Association for Computational Linguistics, 2021.

Anthropic. Claude 2, July 2023. URL `https://www.anthropic.com/index/claude-2`.

AnthropicAI. Introducing claude. *See https://www.anthropic.com/index/introducing-claude*, 2023.

Yushi Bai, Xin Lv, Jiajie Zhang, Hongchang Lyu, Jiankai Tang, Zhidian Huang, Zhengxiao Du, Xiao Liu, Aohan Zeng, Lei Hou, Yuxiao Dong, Jie Tang, and Juanzi Li. Longbench: A bilingual, multitask benchmark for long context understanding, 2023.

Qianglong Chen, Feng Ji, Xiangji Zeng, Feng-Lin Li, Ji Zhang, Haiqing Chen, and Yin Zhang. Kace: Generating knowledge aware contrastive explanations for natural language inference. In *Proceedings of the*

59th Annual Meeting of the Association for Computational Linguistics and the 11th International Joint Conference on Natural Language Processing (Volume 1: Long Papers), pp. 2516–2527, 2021.

Yanda Chen, Ruiqi Zhong, Narutatsu Ri, Chen Zhao, He He, Jacob Steinhardt, Zhou Yu, and Kathleen McKeown. Do models explain themselves? counterfactual simulatability of natural language explanations. *arXiv preprint arXiv:2307.08678*, 2023a.

Zichen Chen, Ambuj K Singh, and Misha Sra. Lmexplainer: a knowledge-enhanced explainer for language models. *arXiv preprint arXiv:2303.16537*, 2023b.

Jiale Cheng, Xiao Liu, Kehan Zheng, Pei Ke, Hongning Wang, Yuxiao Dong, Jie Tang, and Minlie Huang. Black-box prompt optimization: Aligning large language models without model training. *arXiv preprint arXiv:2311.04155*, 2023.

Wei-Lin Chiang, Zhuohan Li, Zi Lin, Ying Sheng, Zhanghao Wu, Hao Zhang, Lianmin Zheng, Siyuan Zhuang, Yonghao Zhuang, Joseph E. Gonzalez, Ion Stoica, and Eric P. Xing. Vicuna: An open-source chatbot impressing gpt-4 with 90%* chatgpt quality, March 2023. URL `https://lmsys.org/blog/2023-03-30-vicuna/`.

Yu-Neng Chuang, Guanchu Wang, Fan Yang, Zirui Liu, Xuanting Cai, Mengnan Du, and Xia Hu. Efficient xai techniques: A taxonomic survey. *arXiv preprint arXiv:2302.03225*, 2023.

Mengnan Du, Ninghao Liu, and Xia Hu. Techniques for interpretable machine learning. *Communications of the ACM*, 63(1):68–77, 2019.

Luciano Floridi. Establishing the rules for building trustworthy ai. *Nature Machine Intelligence*, 1(6):261–262, 2019.

Bryce Goodman, Seth Flaxman, and Y X. European union regulations on algorithmic decision-making and a "right to explanation". *AI magazine*, 38(3):50–57, 2017.

Qingyan Guo, Rui Wang, Junliang Guo, Bei Li, Kaitao Song, Xu Tan, Guoqing Liu, Jiang Bian, and Yujiu Yang. Connecting large language models with evolutionary algorithms yields powerful prompt optimizers. *arXiv preprint arXiv:2309.08532*, 2023.

Shiyuan Huang, Siddarth Mamidanna, Shreedhar Jangam, Yilun Zhou, and Leilani H Gilpin. Can large language models explain themselves? a study of llm-generated self-explanations. *arXiv preprint arXiv:2310.11207*, 2023.

Mojan Javaheripi and Sébastien Bubeck. Phi-2: The surprising power of small language models, December 2023.

Mandar Joshi, Eunsol Choi, Daniel Weld, and Luke Zettlemoyer. triviaqa: A Large Scale Distantly Supervised Challenge Dataset for Reading Comprehension. *arXiv e-prints*, art. arXiv:1705.03551, 2017.

Pride Kavumba, Naoya Inoue, Benjamin Heinzerling, Keshav Singh, Paul Reisert, and Kentaro Inui. When choosing plausible alternatives, clever hans can be clever. In *Proceedings of the First Workshop on Commonsense Inference in Natural Language Processing*, pp. 33–42, Hong Kong, China, November 2019. Association for Computational Linguistics. doi: 10.18653/v1/D19-6004. URL `https://aclanthology.org/D19-6004`.

Sawan Kumar and Partha Talukdar. Nile: Natural language inference with faithful natural language explanations. *arXiv preprint arXiv:2005.12116*, 2020.

Tamera Lanham, Anna Chen, Ansh Radhakrishnan, Benoit Steiner, Carson Denison, Danny Hernandez, Dustin Li, Esin Durmus, Evan Hubinger, Jackson Kernion, et al. Measuring faithfulness in chain-of-thought reasoning. *arXiv preprint arXiv:2307.13702*, 2023.

Hunter Lightman, Vineet Kosaraju, Yura Burda, Harri Edwards, Bowen Baker, Teddy Lee, Jan Leike, John Schulman, Ilya Sutskever, and Karl Cobbe. Let's verify step by step. *arXiv preprint arXiv:2305.20050*, 2023.

Yang Liu, Dan Iter, Yichong Xu, Shuohang Wang, Ruochen Xu, and Chenguang Zhu. Gpteval: Nlg evaluation using gpt-4 with better human alignment. *arXiv preprint arXiv:2303.16634*, 2023.

Gianluigi Lopardo, Frederic Precioso, and Damien Garreau. Faithful and robust local interpretability for textual predictions. *arXiv preprint arXiv:2311.01605*, 2023.

Qing Lyu, Shreya Havaldar, Adam Stein, Li Zhang, Delip Rao, Eric Wong, Marianna Apidianaki, and Chris Callison-Burch. Faithful chain-of-thought reasoning. *arXiv preprint arXiv:2301.13379*, 2023.

Aman Madaan, Niket Tandon, Prakhar Gupta, Skyler Hallinan, Luyu Gao, Sarah Wiegreffe, Uri Alon, Nouha Dziri, Shrimai Prabhumoye, Yiming Yang, et al. Self-refine: Iterative refinement with self-feedback. *Advances in Neural Information Processing Systems*, 36, 2024.

Andreas Madsen, Sarath Chandar, and Siva Reddy. Are self-explanations from large language models faithful? In Lun-Wei Ku, Andre Martins, and Vivek Srikumar (eds.), *Findings of the Association for Computational Linguistics: ACL 2024*, pp. 295–337, Bangkok, Thailand, August 2024. Association for Computational Linguistics. doi: 10.18653/v1/2024.findings-acl.19. URL `https://aclanthology.org/2024.findings-acl.19/`.

Bodhisattwa Prasad Majumder, Oana-Maria Camburu, Thomas Lukasiewicz, and Julian McAuley. Knowledge-grounded self-rationalization via extractive and natural language explanations. *arXiv preprint arXiv:2106.13876*, 2021.

Ramesh Manuvinakurike, Emanuel Moss, Elizabeth Anne Watkins, Saurav Sahay, Giuseppe Raffa, and Lama Nachman. Thoughts without thinking: Reconsidering the explanatory value of chain-of-thought reasoning in llms through agentic pipelines. *arXiv preprint arXiv:2505.00875*, 2025.

Rakesh R Menon, Kerem Zaman, and Shashank Srivastava. Mantle: Model-agnostic natural language explainer. *arXiv preprint arXiv:2305.12995*, 2023.

Miquel Miró-Nicolau, Antoni Jaume-i Capó, and Gabriel Moyà-Alcover. A comprehensive study on fidelity metrics for xai. *arXiv preprint arXiv:2401.10640*, 2024.

Christoph Molnar. Interpretable machine learning: A guide for making black box models explainable. 2022.

Yixin Nie, Adina Williams, Emily Dinan, Mohit Bansal, Jason Weston, and Douwe Kiela. Adversarial NLI: A new benchmark for natural language understanding. In *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics*. Association for Computational Linguistics, 2020.

Ankit Pal, Logesh Kumar Umapathi, and Malaikannan Sankarasubbu. Medmcqa: A large-scale multi-subject multi-choice dataset for medical domain question answering. In Gerardo Flores, George H Chen, Tom Pollard, Joyce C Ho, and Tristan Naumann (eds.), *Proceedings of the Conference on Health, Inference, and Learning*, volume 174 of *Proceedings of Machine Learning Research*, pp. 248–260. PMLR, 07–08 Apr 2022. URL `https://proceedings.mlr.press/v174/pal22a.html`.

Letitia Parcalabescu and Anette Frank. On measuring faithfulness or self-consistency of natural language explanations. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pp. 6048–6089, 2024.

Ansh Radhakrishnan, Karina Nguyen, Anna Chen, Carol Chen, Carson Denison, Danny Hernandez, Esin Durmus, Evan Hubinger, Jackson Kernion, Kamilė Lukošiūtė, et al. Question decomposition improves the faithfulness of model-generated reasoning. *arXiv preprint arXiv:2307.11768*, 2023.

Melissa Roemmele, Cosmin Adrian Bejan, and Andrew S Gordon. Choice of plausible alternatives: An evaluation of commonsense causal reasoning. In *2011 AAAI Spring Symposium Series*, 2011. URL `https://people.ict.usc.edu/~gordon/publications/AAAI-SPRING11A.PDF`.

Noah Shinn, Federico Cassano, Ashwin Gopinath, Karthik R Narasimhan, and Shunyu Yao. Reflexion: Language agents with verbal reinforcement learning. In *Thirty-seventh Conference on Neural Information Processing Systems*, 2023.

Noah Y Siegel, Oana-Maria Camburu, Nicolas Heess, and Maria Perez-Ortiz. The probabilities also matter: A more faithful metric for faithfulness of free-text explanations in large language models. *arXiv preprint arXiv:2404.03189*, 2024.

Alon Talmor, Jonathan Herzig, Nicholas Lourie, and Jonathan Berant. CommonsenseQA: A question answering challenge targeting commonsense knowledge. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers)*, pp. 4149–4158, Minneapolis, Minnesota, June 2019. Association for Computational Linguistics. doi: 10.18653/v1/N19-1421. URL `https://aclanthology.org/N19-1421`.

Sree Harsha Tanneru, Dan Ley, Chirag Agarwal, and Himabindu Lakkaraju. On the hardness of faithful chain-of-thought reasoning in large language models. *arXiv preprint arXiv:2406.10625*, 2024.

Paul Thomas, Seth Spielman, Nick Craswell, and Bhaskar Mitra. Large language models can accurately predict searcher preferences. *arXiv preprint arXiv:2309.10621*, 2023.

Ye Tian, Baolin Peng, Linfeng Song, Lifeng Jin, Dian Yu, Haitao Mi, and Dong Yu. Toward self-improvement of llms via imagination, searching, and criticizing. *arXiv preprint arXiv:2404.12253*, 2024.

Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, et al. Llama: Open and efficient foundation language models. *arXiv preprint arXiv:2302.13971*, 2023.

Miles Turpin, Julian Michael, Ethan Perez, and Samuel R Bowman. Language models don't always say what they think: Unfaithful explanations in chain-of-thought prompting. *arXiv preprint arXiv:2305.04388*, 2023.

Guanchu Wang, Yu-Neng Chuang, Fan Yang, Mengnan Du, Chia-Yuan Chang, Shaochen Zhong, Zirui Liu, Zhaozhuo Xu, Kaixiong Zhou, Xuanting Cai, et al. Leta: Learning transferable attribution for generic vision explainer. *arXiv preprint arXiv:2312.15359*, 2023.

Xuezhi Wang, Jason Wei, Dale Schuurmans, Quoc Le, Ed Chi, Sharan Narang, Aakanksha Chowdhery, and Denny Zhou. Self-consistency improves chain of thought reasoning in language models. *arXiv preprint arXiv:2203.11171*, 2022.

Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, et al. Huggingface's transformers: State-of-the-art natural language processing. *arXiv preprint arXiv:1910.03771*, 2019.

Chengrun Yang, Xuezhi Wang, Yifeng Lu, Hanxiao Liu, Quoc V Le, Denny Zhou, and Xinyun Chen. Large language models as optimizers. *arXiv preprint arXiv:2309.03409*, 2023.

Xi Ye and Greg Durrett. The unreliability of explanations in few-shot prompting for textual reasoning. *Advances in neural information processing systems*, 35:30378–30392, 2022.

Haiyan Zhao, Hanjie Chen, Fan Yang, Ninghao Liu, Huiqi Deng, Hengyi Cai, Shuaiqiang Wang, Dawei Yin, and Mengnan Du. Explainability for large language models: A survey. *arXiv preprint arXiv:2309.01029*, 2023.

Appendix

A Details about Datasets

The experiments are conducted on the three NLU datasets. The details of the datasets are provided as follows:

- **ECQA (Aggarwal et al., 2021).** ECQA is an extension of the CQA dataset (Talmor et al., 2019). Specifically, based on the CQA dataset, it annotates the positive or negative properties and golden explanations for the QA pairs. Due to API cost budgets, we evaluate our framework on the first 500 instances in the ECQA dataset.
- **TriviaQA LongBench (Joshi et al., 2017).** TriviaQA LongBench (TriviaQA-Long) is a reading comprehension dataset. It includes 300 question-answer-evidence triples sourced from the Longbench (Bai et al., 2023) dataset[1]. This dataset features question-answer pairs crafted by trivia enthusiasts, accompanied by independently sourced evidence documents, providing supervision for answering these questions.
- **Balanced COPA (Roemmele et al., 2011; Kavumba et al., 2019).** The Balanced COPA (COPA) dataset is a collection of 500 questions for commonsense causal reasoning. Each question consists of a premise and two alternatives, where the task is to select the alternative that more plausibly has a causal relation with the premise.

B Related Work

B.1 Post-hoc Explanation

Post-hoc explanation techniques have undergone significant development and discussion, driven by the widespread adoption of black-box ML models across various data modalities. A multitude of post-hoc algorithms has been introduced from two aspects: local and global explanations (Molnar, 2022; Du et al., 2019). Explanations aim to explain the reasoning behind an individual model for each input instance, while global explanations aim to uncover the overall functioning of a complex model (Chuang et al., 2023). Considering various purposes of explanation, the explanation techniques mainly showcase the explanation from two perspectives, including feature attributions and counterfactual examples. Feature attribution aims to provide users with important scores for each feature's impact on model predictions, while counterfactual examples aim to offer alternative instances that explicitly assist users in grasping the model's decision-making process. In recent years, with the growing proficiency and wide usage of black-box LLMs, especially closed-source LLMs service, post-hoc explanations have become increasingly prominent and have garnered significant attention in NLP research due to the inaccessibility of LLMs' model weights and structure (Zhao et al., 2023).

B.2 Explainability of LLMs

The majority of explanation efforts in LLM research have centered on delivering explanations. One group of studies calculates importance scores for specific tokens (Lopardo et al., 2023; Huang et al., 2023), another line of progress generates NL explanations by leveraging the pre-trained LLMs with internal model knowledge sources (Kumar & Talukdar, 2020; Chen et al., 2023b; Menon et al., 2023), the other group of work leverages LLMs themselves to generate chain-of-thought (CoT) reasoning (Lanham et al., 2023; Radhakrishnan et al., 2023; Chen et al., 2023a;a) as the self-explanations through the one feed-forward inference process. Furthermore, some studies aim to yield counterfactual explanations by pre-trained LLMs to assist users in better understanding the decision-making process from LLMs (Chen et al., 2021; 2023a). Although NL explanations offer fantastic human-understandable insights than token-wise explanations, the explanations can lose their fidelity via one feed-forward inference process of pre-trained LLMs. Unreliability and non-fidelity of NL explanations are still a concern (Ye & Durrett, 2022; Turpin et al., 2023). Given our primary aim of producing faithful explanations, our efforts are to generate NL explanations to improve the likelihood of accurately representing the decision-making process of LLMs.

[1] https://huggingface.co/datasets/THUDM/LongBench/

B.3 LLMs as Optimizers

LLMs as optimizers is a novel paradigm, describing optimization problems in natural language and utilizing the reasoning capabilities of LLMs for optimizing (Yang et al., 2023). Depicting optimization problems in natural language enables the optimization of diverse tasks without defining formal specifications, such as prompt optimization (Yang et al., 2023; Cheng et al., 2023; Guo et al., 2023), agent learning (Shinn et al., 2023), and model labeling (Thomas et al., 2023). Based on this optimization paradigm, our work introduces a generative explanation framework with a novel estimation method of sentence-level fidelity.

C Hyper-parameter Settings of FaithLM

The hyper-parameters of FaithLM are given in Table 2. The configuration for explainers is consistent across Claude-2 and GPT-3.5-Turbo, provided that the parameters are adjustable. Likewise, the settings for predictors are uniform, with Phi-2 and Viucua-7B receiving identical hyperparameter configurations during the experiments conducted in this study.

	Dataset	ECQA	TriviaQA-Long	COPA
Fidelity-enhanced Optimization	Optimization Steps	20	20	20
	Temperature of Predictor LLMs	0.7	0.5	0.7
	Temperature of Explainer LLMs	0.9	0.9	0.9
	Top-P of Explainer LLMs	0.9	0.9	0.9
Trigger-oriented Optimization	Optimization Steps	50	100	100
	Sampled Instances	30	30	30
	Temperature of Predictor LLMs	0.7	0.5	0.7
	Temperature of Explainer LLMs	0.9	0.9	0.9
	Top-P of Explainer LLMs	0.9	0.9	0.9

Table 2: Hyper-parameters and optimization settings in FaithLM.

D Computation Infrastructure and Costs

D.1 Computation Infrastructure

For a fair comparison of testing algorithmic throughput, the experiments are conducted based on the following physical computing infrastructure in Table 3.

Device Attribute	Value
Computing infrastructure	GPU
GPU model	Nvidia-A40
GPU number	1
GPU Memory	46068 MB

Table 3: Computing infrastructure for the experiments.

D.2 Computation Costs

The computational costs associated with FaithLM primarily differ from the inference costs of local LLMs and the expenses related to API-accessed LLMs. The computational costs depend on the parameter scale and variants of LLMs used in the FaithLM framework, shown in Table 4 and 5.

	ECQA	TrivaQA	COPA
Execution Time (Sec.)	∼3	∼5	∼3
Execution Cost ($)	∼0.01	∼0.04	∼0.01

Table 4: Computing costs of FaithLM with GPT-3.5 on each dataset.

	bs=32	bs=64	bs=96
Execution Time (Sec.)	∼3	∼5	∼3
Memory Cost (GB)	∼28GB	∼43GB	∼59GB

Table 5: Computing costs of FaithLM with Vicuna-7B under different batch size (bs).

E Additional Experimental results of FaithLM

E.1 Optimization Procedure of derived explanations

We demonstrate more evaluation results on derived explanations from FaithLM. The outcomes depicted in Figure 8 reveal that FaithLM attains notably higher fidelity scores across all three datasets following 20 steps of optimization. Additionally, Figure 8 illustrates the evolution of the optimization process during the generation of explanations.

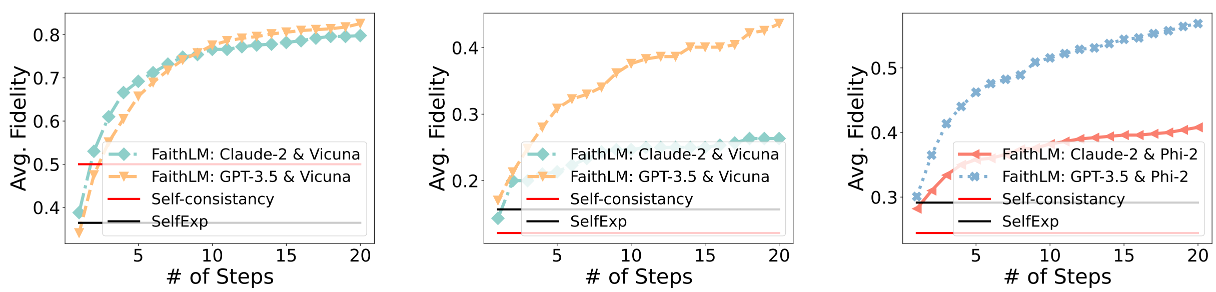


Figure 8: The fidelity evaluation of derived explanations from FaithLM under different settings of predictors and explainers.

E.2 Additional Optimization Curve of Explanation Trigger Prompt

We demonstrate more evaluation results on the optimization curve of explanation trigger prompts of FaithLM. The optimization curve shown in Figure 9 generally displays an upward trend with the progression of steps, interspersed with several fluctuations throughout the optimization process. This suggests that FaithLM can successfully generate improved explanation trigger prompts after optimization.

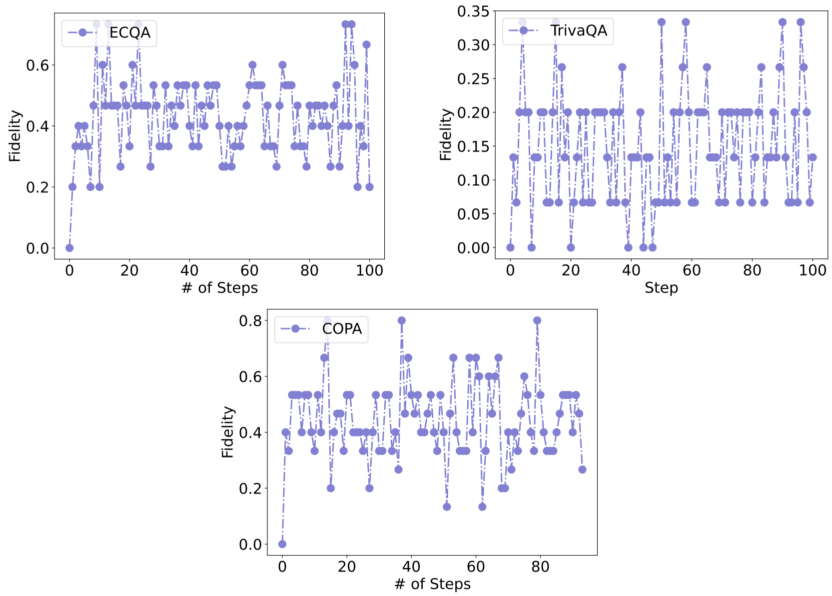


Figure 9: The optimization curve of explanation trigger prompts on ECQA (left), TriviaQA-Long (middle), and COPA dataset (right).

E.3 Additional Experiments on Diverse Domains of Dataset

We further have conducted additional experiments on one new MedMCQA dataset (Pal et al., 2022) in the healthcare domain. We evaluate the FaithLM using a fidelity assessment under Natural Language Explanation Generation settings. All experimental configurations follow the settings in Section 4.2. The experimental results are shown in the table below. We observe that FaithLM outperforms the baseline method, which is consistent with the experimental results across other domain datasets that were evaluated in our work.

	SelfExp	Self-consistency	FaithLM
Fidelity	0.6956	0.4715	**0.9565**

Table 6: Additional experimental results on MedMCQA dataset.

E.4 Additional Experiments on Truthfulness Evaluation

We further lunch additional experiments on all evaluators with different evaluation settings to measure the relevance between derived explanations and ground-truth explanations. The evaluators assesses their relevance using a GPT-Score in GPT evaluator on a scale of one to five. If the two provided explanations are classified under the “similar content" category or receive a GPT-Score close to five, this indicates that the derived explanations are highly similar to ground-truth explanations.

F Details of Evaluation Prompt Usage

We provide a listing of the evaluation prompts in Table 7 utilized in assessing the performance of FaithLM. The first row reveals the evaluation prompt on comparing the derived explanation with the ground-truth (GT) explanation in the ECQA dataset in Section 4.3; and the second row demonstrates the evaluation prompt on activating the GPT classifier and the GPT scorer for assessing contrary explanations in Section 4.5.

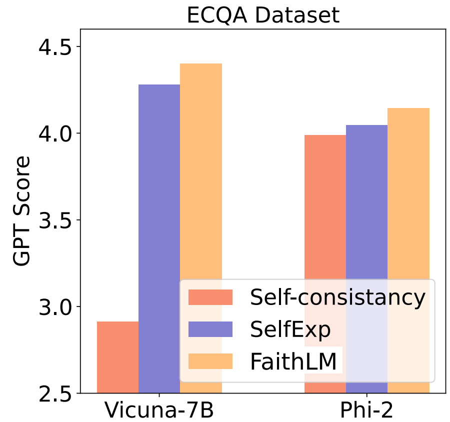


Figure 10: Truthfulness evaluation with ground-truth explanation under GPT-score settings.

Evaluation Task	Evaluation Prompts
Ground-truth Explanation	Given a user instruction and two AI assistant responses, your job is to classify whether the relation of two responses in S1 and S2 belongs to G-1, G-2, or G-3. The meaning of class is as follows: (G-1) relevant contents, (G-2) irrelevant contents, or (G-3) irrelevant contents. Judge responses holistically, paying special attention to whether two responses have similar contents. Judge responses with only ONE class label as your final answer. **S1:{*derived explanation*}. S2:{*GT-Explanation*}.** Please ONLY response your in either G-1, G-2, or G-3; THERE SHOULD BE NO OTHER CONTENT INCLUDED IN YOUR RESPONSE.
GPT classifier for Contrary Explanations	Given a user instruction and two AI assistant responses, your job is to classify whether two responses in S1 and S2 belong to G-1, G-2, or G-3. The meaning of class is as follows: (G-1) same semantic meaning, (G-2) opposite semantic meaning, and (G-3) no relation. Judge responses holistically, paying special attention to whether two responses have the same semantic meaning. Judge responses with only ONE class label as your final answer. **S1:{*derived explanation*}. S2:{*Contrary Explanations*}.** Please ONLY respond in either G-1, G-2, or G-3; THERE SHOULD BE NO OTHER CONTENT INCLUDED IN YOUR RESPONSE.
GPT scorer of Contrary Explanations	Given a user instruction and two AI assistant responses, your job is to rate from ONE to FIVE to judge whether two responses in S1 and S2 have the same semantic meaning or not. A FIVE score refers to being totally the same, and ONE score refers to being totally the opposite. Judge responses holistically, paying special attention to whether two responses have the same semantic meaning. The judge responds with the rates between ONE and FIVE. **S1:{*derived explanation*}. S2:{*Contrary Explanations*}.** Please ONLY respond to the rate value; THERE SHOULD BE NO OTHER CONTENT INCLUDED IN YOUR RESPONSE.

Table 7: Evaluation Prompts given to GPT-3.5-Turbo used in assessing the efficacy of FaithLM.

F.1 Robustness Analytics of Configuration (RQ3)

In this section, the robustness test of the explainer LLMs is conducted under the analytics of hyper-parameters that are highly dependent on the outputs of LLMs. We focus on two different hyper-parameters: Temperature and Top-p. The experiments are conducted under the explainer GPT-3.5-Turbo and the predictor Vicuna-7B. We evaluate the following temperatures and top-p of the explainer LLM in the range of {0.3, 0.6, 0.9}. The results are shown in Figure 11. We observe that the explainer LLMs perform inferior when the temperature and Top-p are low, reflecting that the lower exploration of explainer LLM may degrade the optimization ability in explanation generation. The explainer LLMs are encouraged to obtain the temperatures and top-p around 0.9. The small values of the temperatures and top-p may lead to low flexibility in updating new explanations. In contrast, large temperatures and top-p may impact explainer LLMs disobeying the given optimization trajectory. Thus, in the main experiments, all reported performances are under the settings of temperature 0.9 and top-p 0.9, achieving the best performance for generating explanations.

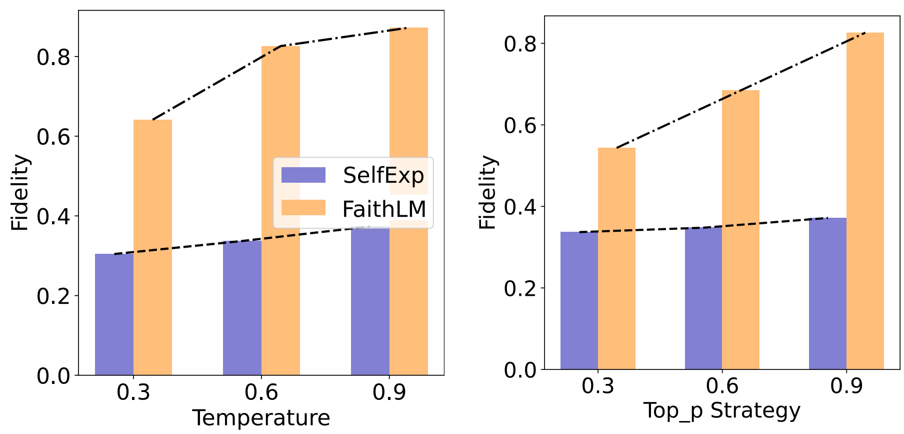


Figure 11: Robustness Analytics of FaithLM: Temperature (left) and Top-p strategies (right).

G Details of Prompts Usage in FaithLM

We provide a listing of the prompts in Table 7 utilized in FaithLM in different tasks. The first row demonstrates the initial explanation trigger prompt leveraging in both fidelity-enhanced optimization and trigger-oriented optimization. The second row shows the prompt for the LLM agent to generate the contrary explanations.

Conducted Task	Evaluation Prompts
Explanation Generation	Please provide objective explanations of why the model generates the answers to the given questions based on your thoughts. Explain the reason why the model provides the answer, no matter if it is wrong or correct. Make sure not to answer the questions or provide any suggestions to better answer the questions by yourself. **Q:{*Question*}. A:{*Targeted LLM-generated Answer*}.**
Contrary Explanations Generation	Please generate one example of obtaining the opposite meaning from a given sentence. Make sure you output sentences only. **Sentences:{*derived explanation*}.**

Table 8: The example of prompts that are given to two explainer LLMs and LLM agent for contrary explanation.

H Trajectory System Prompts Usage in FaithLM

We present a detailed listing of the trigger-oriented trajectory prompt in Figure 12 and the explanation-oriented prompt in Figure 13, as utilized within the FaithLM framework.

H.1 Trigger-oriented Trajectory Prompt

System instruction: Your task is to generate the general prompts <INS> for language model generating model explanations of each question. Below are some previous prompts with their scores in the Inputs. The score is calculated as the flipping answer rates and ranges from 0 to 1.

Inputs: The following exemplars show how to apply your text:
Text: Please provide objective explanations of why model generates the answers.
Score: 0.21

Text: Provide a concise, objective explanation of only the key reasoning or assumptions that likely led the model to generate this specific response.
Score: 0.53

......

Trajectory Instruction: Generate a prompt <INS> that is different from all prompt <INS> in Inputs above and has a higher score than all the prompts <INS> from Inputs. The prompts should begin with <INS> and end with <INS> and follow the format of the examples in Inputs. The prompts should be concise, effective, and generally applicable to all problems above.

Response: <A Newly Generated Trigger Prompt>

Figure 12: A examples of **trigger-oriented trajectory prompt**. This prompt populates in both LLM explainers, which are Cluade2 and GPT-3.5-Turbo. The output of FaithLM optimized under trigger-oriented trajectory prompt is append after the **Response** label.

H.2 NL Explanation-oriented Trajectory Prompt

System instruction: You have some texts along with their corresponding scores. The texts are the possible explanation of the following given question and answer. The texts are arranged in random order based on their scores, where higher scores indicate better quality. The scores are calculated as how relative the texts are toward the given question and answer as the explanation. The scores range from 0 to 1 based on your output text.

Inputs: The following exemplars show how to apply your text:
Text: The model generates the answer "farmland" because an apple tree is likely found in abundance in farmland.
Score: 0.0

Text: The model generates the answer "farmland" because **apple trees require open spaces and fertile soil**, both of which are commonly found in farmland.'
Score: 1.0

. . . . . .

Trajectory Instruction: You replace <EXP> with your text. We say your output is bad if your output obtains lower scores than the previous text, and we say your output is good if your output obtains higher scores than the previous text. Please provide new objective text to describe why the answers are given to the questions based on your thoughts. Explain the reason, no matter if the answer is wrong or correct. Make sure not to answer the questions or provide any suggestions to better answer the questions by yourself. Every explanation should begin with <EXP>. Make sure not to repeat the input queries and answers. Please only output the explanation sentences.

Response: <A Newly Generated Trigger Prompt>

Figure 13: A examples of **explanation-oriented trajectory prompt**. This prompt populates in both LLM explainers, which are Cluade2 and GPT-3.5-Turbo. The output of FaithLM optimized under trigger-oriented trajectory prompt is append after the **Response** label.

I Case Studies of FaithLM

I.1 Explanations Generation

We demonstrate the case studies of explanation results generated by FaithLM after fidelity-enhanced optimization in the following two Figure 14 and Figure 15. The results show that FaithLM can generate faithful explanations that truly express the decision-making process of targeted LLMs.

Case Study 1

Question: What is the cause of the Promise? Premise: The movie tickets sold out. Choices: [choice] It was opening day for the movie. [choice] The movie received poor reviews.

<u>Ground Truth:</u> The movie received poor reviews.

<u>**LLM Answer:**</u> It was opening day for the movie. **(wrong)**

derived explanation: The model likely selected that answer because opening day tends to have very high demand for movies, often resulting in sold out showings. While there could be other reasons for the sell out, high opening day demand is a reasonable explanation given the limited context provided.

Case Study 2

Question: What is the effect of the Promise? Premise: I drilled a hole in the wall. Choices: [choice] A mouse crawled out of the hole. [choice] Dust blew out of the hole.

<u>Ground Truth:</u> Dust blew out of the hole.

<u>**LLM Answer:**</u> Dust blew out of the hole. **(correct)**

derived explanation: Dust exiting the hole in the wall is a reasonable effect to expect when drilling into a wall. Without further context, there is no reason to assume a mouse coming out of the hole is likely based solely on the premise that a hole was drilled. The model selected the choice directly supported by the information provided in the premise.

Figure 14: Case Study: **derived explanations** (Dataset: **COPA**; Targeted Model $f(\cdot)$: **Claude-2**; Explainer $g(\cdot)$: **Vicuna**)

Case Study 1

Question: Where would you get a dog if you do not have one?
Choices: [choice] pet store [choice] outside [choice] neighbor's house [choice] park [choice] rug
Ground Truth: store
LLM Answer: store **(correct)**
Derived explanation: The model suggested "pet store" as the place to get a dog if you don't already have one because pet stores are a common retail business where people can purchase dogs as pets.

Case Study 2

Question: Where would you put coins if you want to bring them with you?
Choices: [choice] medium [choice] water fountain [choice] wishing well [choice] desk [choice] purse
Ground Truth: purse
LLM Answer: desk **(wrong)**
Derived explanation: The model may have predicted "desk" because desks often have drawers or containers where coins could be stored temporarily. However, a purse is the most practical option for carrying coins when leaving.

Figure 15: Case Study: **Derived explanations** (Dataset: **ECQA**; Targeted Model $f(\cdot)$: **Claude-2**; Explainer $g(\cdot)$: **Phi**)

I.2 Explanation Trigger Prompts

The demonstrations in the explanation trigger prompts generated by FaithLM in Figure 16. The results show that FaithLM can generate explanation trigger prompts that lead explainer LLMs to generate explanations and obtain higher fidelity.

Initial Explanation Trigger Prompt:

Please provide objective explanations of why model generates the answers to the given questions based on your thoughts. Explain the reason why the model provides the answer, no matter if it is wrong or correct. Make sure not to answer the questions or provide any suggestions to better answer the questions by yourself.

Optimized Trigger Prompt (Dataset: **ECQA**; Targeted Model $f(\cdot)$: **Phi-2**; Explainer $g(\cdot)$: **Claude-2**):

Explain your reasoning clearly and impartially based solely on the factual inputs, without assumptions. Succinctly identify factual connections and provide clarification if helpful. I tried distilling this down to: clear, impartial reasoning solely from the facts; succinctly identifying factual connections without assumptions; and providing clarification if helpful. The aim is simplified yet effective guidance that remains focused and broadly applicable to explain reasoning across diverse queries.

Optimized Trigger Prompt (Dataset: **COPA**; Targeted Model $f(\cdot)$: **Vicuna-7B**; Explainer $g(\cdot)$: **Claude-2**):

Provide a concise, objective explanation of only the key reasoning or assumptions that likely led the model to generate this specific response, without repeating the original input or assessing quality. Use the <EXP> tag and avoid adding any personal perspectives. I have focused on providing clear, minimal guidelines to elicit explanations that specifically convey the core logic behind each individual response from the model's perspective, rather than overall performance evaluation or subjective opinions. The key aspects aim to produce focused explanations to better understand the model's reasoning, while maintaining brevity and objectivity.

Optimized Trigger Prompt (Dataset: **TriviaQA**; Targeted Model $f(\cdot)$: **GPT-3.5**; Explainer $g(\cdot)$: **GPT-3.5**):

Create concise and insightful explanations for the model's answers by thoroughly analyzing the relevant information in the passages and their connection to the given questions. Begin each explanation with <EXP> and avoid introducing new information or personal opinions. Use precise and concise language to focus on the key points and enhance the clarity and comprehensibility of the explanations. Strive for brevity without sacrificing coherence to ensure the explanations are easily understandable by a wide range of readers. Avoid repetition of the questions or answers and provide valuable insights into the model's reasoning process to improve the effectiveness and impact of the explanations.

Figure 16: Case Study: Generation of **Explanation Trigger Prompts**

I.3 Contrary Explanation

We demonstrate results on contrary explanations leveraged in Fidelity Evaluator. The results in Figure 17 show that the contrary explanation obtains the opposite meaning of the given explanation.

Case Study 1

Question: The child wanted to test electricity, so what did he feel as a result?
Choices: [choice] cause fire [choice] shock [choice] short fuse [choice] kill if used improperly [choice] produce heat
Ground Truth: shock
LLM Answer: cause fire **(wrong)**
Given Explanation: The model likely incorrectly associated testing electricity with igniting a fire, rather than understanding that direct contact can cause an electric shock. It failed to comprehend the potential outcomes of unsafe electrical contact.
Contrary Explanation: The model correctly predicted that testing electricity would not cause a fire. It likely fully understood that direct contact with electricity can cause a shock rather than ignite a fire.

Case Study 2

Question: Where would you put coins if you want to bring them with you?
Choices: [choice] medium [choice] water fountain [choice] wishing well [choice] desk [choice] purse
Ground Truth: purse
LLM Answer: purse **(correct)**
Given Explanation: A purse is a personal item that people often carry with them when going places. It has compartments to store small items like coins, so putting coins in your purse allows you to easily bring them along wherever you go.
Contrary Explanation: The purse is not a good place to put coins if you don't want to bring them with you, because purses are designed for other items, not coins.

Figure 17: Case Study: **Contrary Explanation** (Dataset: **ECQA**; Targeted Model $f(\cdot)$: **Claude-2**; Explainer $g(\cdot)$: **Vicuna**)