FaithLM: Towards Faithful Explanations for Large Language Models

Anonymous ACL submission

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 may not accurately reflect the LLMs' decision-making process due to a lack of fidelity optimization on the derived explanations. Measuring the fidelity of NL explanations is a challenging issue, as it is difficult to manipulate the input context to mask the semantics of these 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.

Numerous studies have attempted to enhance the transparency of decision-making processes in LLMs by providing natural language (NL) explanations. Advanced billion-level LLMs, such as GPT4 (Achiam et al., 2023), mainly leverage their reasoning abilities and internal knowledge for complex downstream problems. However, this complexity poses challenges to faithfully explain the underlying reasons behind their decisions with natural language sentences. In this manner, recent advancements are struggling to generate reliable NL explanations for interpreting LLMs (Ye and Durrett, 2022). Some work attempt to leverage powerful LLMs (Majumder et al., 2021; Chen et al., 2023b) with auxiliary information to generate NL sentences or chain-of-thought (CoT) reasoning (Lanham et al., 2023; Radhakrishnan et al., 2023; Chen et al., 2023a) as the explanations to explain the decision-making process of LLMs. Although existing work emerged that LLMs may possess the ability to self-explain (Madsen et al., 2024; Wang et al., 2022), or follow chain-of-thoughts to explain (Lyu et al., 2023), 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). Thus, the derived NL explanations may not faithfully reflect the decision-making process of LLMs (Zhao et al., 2023; Turpin et al., 2023). Measuring the fidelity of NL explanations is a challenging issue, as the NL explanations may provide crucial information beyond the input context. This makes it hard to mask the semantics of NL explanations by manipulating the input tokens.

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

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. This example indicates that the contrary explanation interrupts the LLM's original prediction process with faithful information, demonstrating that the information in an original explanation is faithful and aligns with LLM's initial answer.

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 approach for measuring the fidelity of NL explanations, we introduce *Faithful LLM Explainers* (`FaithLM`) to generate faithful NL explanations for LLMs. Specifically, `FaithLM` adopts LLMs as explainers 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. To demonstrate the effectiveness of `FaithLM`, we conducted several experiments on four different LLMs under three datasets from different domains. `FaithLM` achieved significantly higher fidelity performance in generating NL explanations and more closely matched the golden explanations compared with state-of-the-art baseline methods. In summary, our contributions can be summarized as follows:

- **Fidelity of NL Explanations:** We propose to measure the fidelity of NL explanation by incorporating its contrary explanation into the query and observing LLM output difference.
- **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 on three datasets show that `FaithLM` can effectively improve the fidelity of NL explanations, revealing a better alignment with the ground-truth explanations than SoTA baseline methods.

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 directly generated $\mathcal{E}_{\text{NL}}$ under single-forward passing may not be faithful and accurate, degrading the user's trust in the prediction made by the targeted LLM. To this end, our work focuses on benefiting the explainer $g(\cdot)$ to generate **more faithful NL explanations regarding the decision of $f(\cdot)$ in a post-hoc manner**, where $f(\cdot)$ can be either closed-source or open-source LLMs.

2.2 Post-hoc Explanations of LLMs

Recent research on LLM explanations has primarily focused on post-hoc approaches due to the inaccessibility of LLM weights and architectures. One group of studies calculates importance scores for specific tokens (Lopardo et al., 2023; Huang et al., 2023), and the other line of work generates natural language sentences (Kumar and Talukdar, 2020; Chen et al., 2021, 2023b; Menon et al., 2023) and CoT reasoning (Lyu et al., 2023; Chen et al., 2023a) as explanations by leveraging LLMs. Despite the advanced capability of powerful LLMs to generate NL explanations, issues with unreliability and non-fidelity persist. While studies like Chen et al. (Chen et al., 2024) utilize internal model weights aiming for reliable explanations generation, accessing these weights is challenging with closed-source LLMs. Considering the non-accessibility of LLMs, such as closed-source LLMs, our goal is to faithfully generate NL explanations instead of exploring the internal mechanisms or neurons of LLMs to generate explanations.

2.3 Limitations of Traditional Fidelity on Natural Language 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 tar-

geted 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 $\boldsymbol{Y} = f(\boldsymbol{X})$. Following the traditional fidelity definition, the fidelity can be 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 $\mathcal{E}_{\text{NL}}$ 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 $\boldsymbol{X}$. For instance, as the example shown in Figure 1, the critical component "similar poles push each other away" in $\mathcal{E}_{\text{NL}}$ does not explicitly appear in the input context. Thus, we cannot simply remove critical components from the question following the traditional definition. In this paper, we propose a solution to systematically address this obstacle by removing the critical components from the semantic level instead of the token level.

3 `FaithLM`: The Explainer LLM Framework

In this section, we systematically introduce the generative explanation framework, `FaithLM`, which derives faithful explanations in natural language. The derived explanations are expected to accurately reflect the predictive decision-making process of targeted LLMs with high fidelity. Specifically, we first introduce the Fidelity Evaluator in Section 3.1 to quantitatively assess the fidelity of the NL explanations. Subsequently, `FaithLM` iteratively optimizes the fidelity of the derived explanations and searches for improved explanation trigger prompts using the proposed Fidelity Evaluator. The optimization frameworks for these processes are detailed in Sections 3.2 and 3.3.

3.1 Fidelity Evaluator for Natural Language Explanations

Due to the limitation of the fidelity metric described in Section 2.3, we introduce the *Fidelity Evaluator* to directly assess the fidelity of NL explanations, as shown in Figure 1. Specifically, we first extend the original fidelity definition to evaluate the fidelity of NL explanations $\mathcal{E}_{\text{NL}}$. Finally, we introduce the fidelity evaluator that follows the proposed fidelity measurement criteria.

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 $\neg\mathcal{E}_{\text{NL}}$ is defined as a statement obtained opposite semantics to the given NL explanation $\mathcal{E}_{\text{NL}}$. 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 $\mathcal{E}_{\text{NL}}$, we use the contrary explanation $\neg\mathcal{E}_{\text{NL}}$ as an extra given condition to the input queries, forming conditional LLM inferences $f(\boldsymbol{X} \mid \neg\mathcal{E}_{\text{NL}})$. 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 $\mathcal{E}_{\text{NL}}$ can be estimated by the prediction difference:

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

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 and Durrett, 2022), which means that the relationship between the reliability of the explanations and the correctness of predictions is significantly high. Motivated by the observation, we propose a framework of 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 $\neg\mathcal{E}_{\text{NL}}$ regarding the original $\mathcal{E}_{\text{NL}}$. The generation process for $\neg\mathcal{E}_{\text{NL}}$ 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 $f(\boldsymbol{X}) - f(\boldsymbol{X} \mid \neg\mathcal{E}_{\text{NL}})$. 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 $\neg\mathcal{E}_{\text{NL}}$ consist of the contrasting key messages against $\mathcal{E}_{\text{NL}}$ that can significantly impact the decision-making process of the targeted LLM. This suggests that the explanation $\mathcal{E}_{\text{NL}}$ contains key components that significantly support the inference of the targeted LLMs.

3.2 `FaithLM` on Fidelity-enhanced Explanation

In this section, we introduce an iterative framework designed to progressively enhance the fidelity of NL explanations. The primary goal of `FaithLM` here is to generate faithful NL explanations with iterative fidelity-enhanced optimization.

Fidelity-enhanced Explanation. The framework of Fidelity-enhanced Explanation is illustrated in Figure 2(a). 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 $\mathcal{E}_{\text{NL}}$ following the goal of fidelity enhancement.

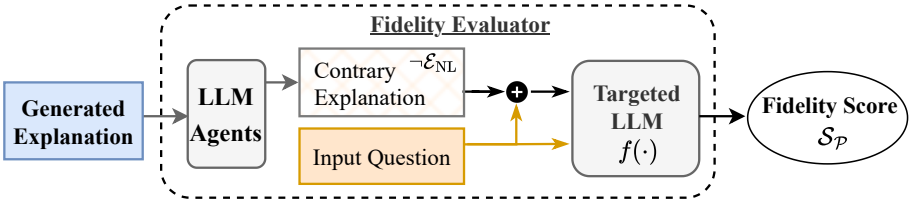


Figure 1: The framework of Fidelity Evaluator. The evaluator calculates the fidelity scores of the derived explanations based on its contrary explanations.

In the first round of enhancement, the LLM explainer generates NL explanations $\mathcal{E}_{\text{NL}}$ following human-crafted explanation trigger prompts $\mathcal{P}_{\mathcal{E}}$ provided in Appendix G. The explanations are then generated by the explainer $g(\mathcal{P}_{\mathcal{E}} | \boldsymbol{X}, \boldsymbol{Y})$. Starting from the second round till converge, `FaithLM` collects a trajectory $\mathcal{T}$ with the NL explanations $\mathcal{E}_{\text{NL}}$ and their corresponding fidelity scores $\mathcal{S}_{\mathcal{E}}$ generated by Fidelity Evaluator. The collection process can be represented as $\mathcal{T} \leftarrow \{\mathcal{T}, [\mathcal{E}_{\text{NL}}, \mathcal{S}_{\mathcal{E}}]\}$, 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 fidelity enhancement process is guided by the system prompts detailed in Figure 13 of Appendix H.

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 $f(\cdot)$.

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**

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 explanations with higher fidelity.

Trigger Prompt Optimization. The framework of Trigger Prompt Optimization is shown in Figure 2(b). 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.

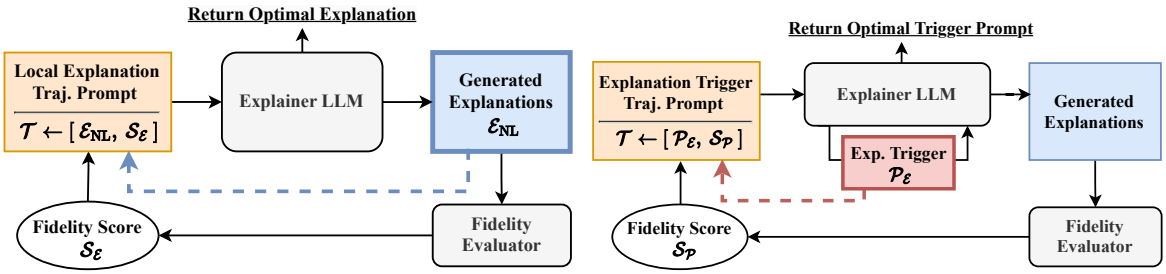
To estimate the fidelity score for a trigger prompt, `FaithLM` first adopts the randomly human-crafted trigger prompt to guide the LLM explainers to generate NL explanations, and then utilize the Fidelity Evaluator to assess the fidelity of the derived explanation. The final estimated score is averaged by the fidelity score $\mathcal{S}_{\mathcal{E}_i}$ of each instance i from 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



(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.

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 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 in our experiments.

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

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:** Does the configurations of LLMs affect the explanation performance of `FaithLM`?

4.1 Dataset and Baseline

Datasets. We evaluate `FaithLM` on three datasets with multiple tasks: 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 of datasets are provided in Appendix A. **Baseline Methods.** We compare `FaithLM` with 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 outputs from the chain-of-thought prompting process 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

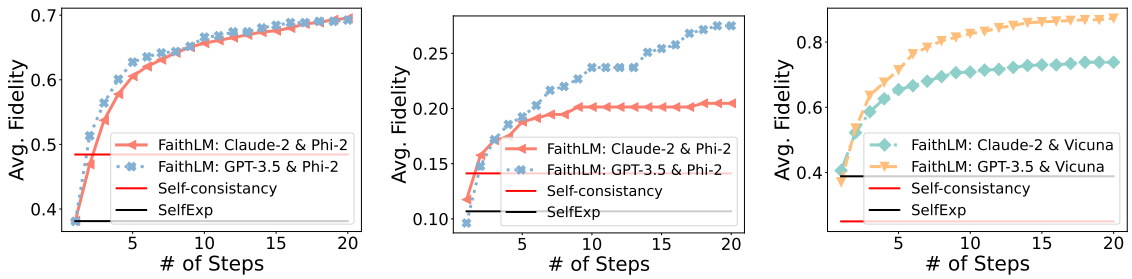


Figure 3: The fidelity evaluation of explanations from FaithLM on ECQA dataset (left), TriviaQA- Long (middle), and COPA dataset (right). The reported scores are the average fidelity on testing instances in each step of fidelity-enhanced optimization.

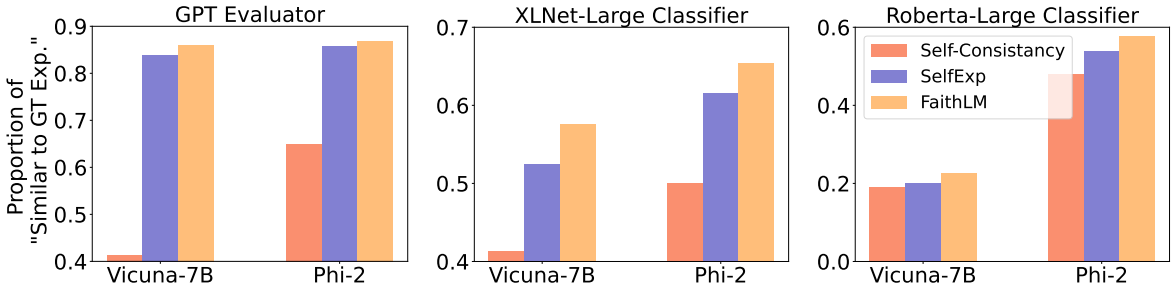


Figure 4: Trustfulness evaluation of the NL explanations. Higher the proportion of "similar to ground-truth explanation," the more consistent the derived explanations are with the ground-truth NL explanations.

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 and 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.

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 of Appendix G.

- **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.

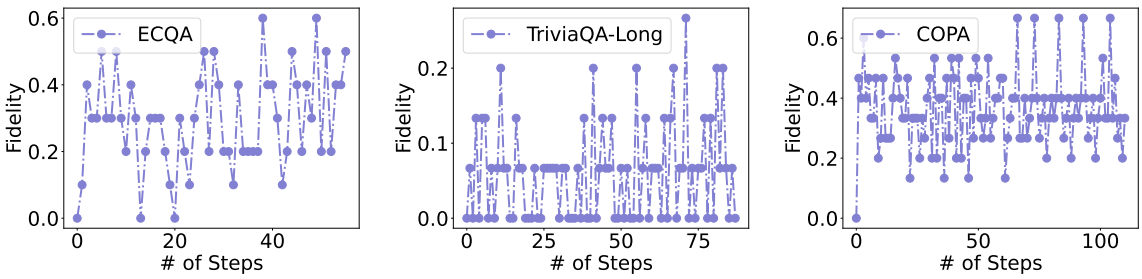
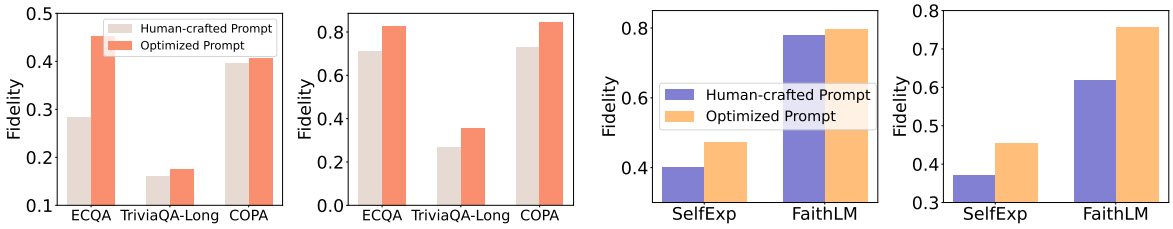


Figure 5: The fidelity in different optimization steps of the trigger prompts (Algorithm 2) on the ECQA, TrivaQA, and COPA datasets. The fidelity grows higher as the number of steps increases.



(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.

Efficacy of Explanation Trigger Prompts. We first show prompt optimization curves of explanation trigger prompts 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 uniformly established at 50 rounds across different explainer and targeted LLMs.

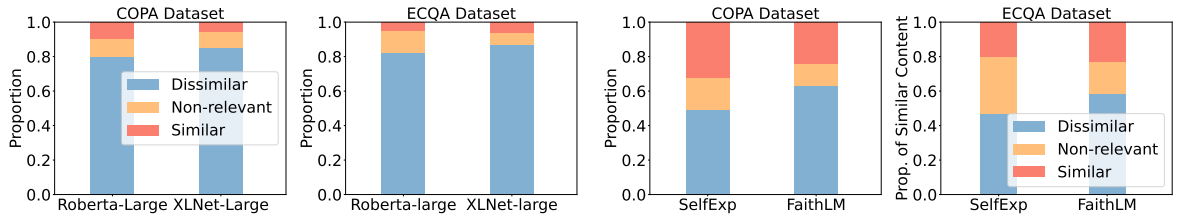
- **Trigger Prompt Optimization Curve.** Figure 5 demonstrates the optimization curves of three datasets. We display the explainer as GPT-3.5-Turbo and Claude-2 and the explainer as Vicuna-7B. We observe that the optimization curve exhibits a generally ascending trend as the step progresses, interspersed with multiple waves throughout the optimization procedure. This indicates that `FaithLM` generates better explanation trigger prompts after the optimization. More results of optimization curves on remaining datasets 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 6(a), including the experiments conducted 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. Additionally, the optimized trigger prompts are effective in improving the fidelity of the derived explanations with or without the optimization of `FaithLM`.

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 LLMs.

4.4 Transferability of Optimized Trigger Prompt (RQ2)

We assess the transferability of ultimately optimized trigger prompts across different unseen datasets within the same domain, as depicted in Figure 6(b). 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



(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.

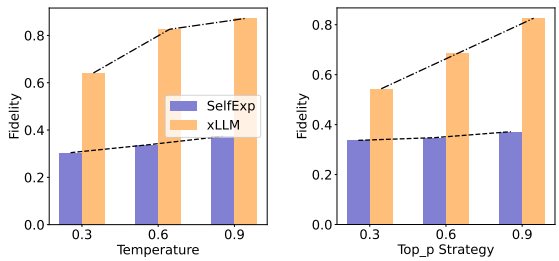


Figure 8: Robustness Analytics of `FaithLM` in different decoding settings, which are Temperature (left) and Top-p strategies (right).

the optimized trigger prompts generated by `FaithLM` possess a great property of data transferability.

4.5 Robustness Analytics of Configuration in `FaithLM` (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 8. 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.

4.6 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 outputs from their original NL explanations. In this section, 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 Table 7 of Appendix F.

The results are shown in Figure 6 under the 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 on the ECQA and COPA datasets, respectively. The results of the GPT-classifier demonstrate that the derived explanations from SelfExp obtain more non-faithful information than `FaithLM`, risking the LLM agent of Fidelity Evaluator in generating non-relevant information as the contrary explanations. Case studies are provided in Appendix I to show the informativeness and readability of contrary explanations.

5 Conclusion

In this paper, we introduce `FaithLM` to explain the decision-making process of LLMs. 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 on three datasets demonstrate the effectiveness of `FaithLM` in terms of the high fidelity of derived explanations, and better alignment with the ground-truth explanations of the datasets. For future work, we plan to extend `FaithLM` to explore high-impact applications, particularly in domains like healthcare, where the need for transparency is critical. This is especially important given the growing reliance on black-box LLMs, which raise significant ethical and regulatory concerns.

6 Limitations

One significant limitation of FaithLM associated with the carbon emissions during the experiments. To generate better faithfulness and truthfulness of the derived explanations, FaithLM requires iterating a few rounds of optimization during the explanation derivation. This leads to extra computational resources to proceed. The extra computational power is thus required for optimizing FaithLM leads to considerable energy consumption, which, in turn, results in a significant carbon footprint. As the demand for more sophisticated LLMs continues to grow, so does their environmental impact. This limitation underscores the urgent need to explore and adopt more sustainable practices and technologies in the development and learning FaithLM with fewer optimization steps to mitigate their ecological footprint.

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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 and 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 and 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.

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.

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

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.)	$\sim$3	$\sim$5	$\sim$3
Execution Cost ($)	$\sim$0.01	$\sim$0.04	$\sim$0.01

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

	bs=32	bs=64	bs=96
Execution Time (Sec.)	$\sim$3	$\sim$5	$\sim$3
Memory Cost (GB)	$\sim$28GB	$\sim$43GB	$\sim$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 9 reveal that FaithLM attains notably higher fidelity scores across all three datasets following 20 steps of optimization. Additionally, Figure 9 illustrates the evolution of the optimization process during the generation of explanations.

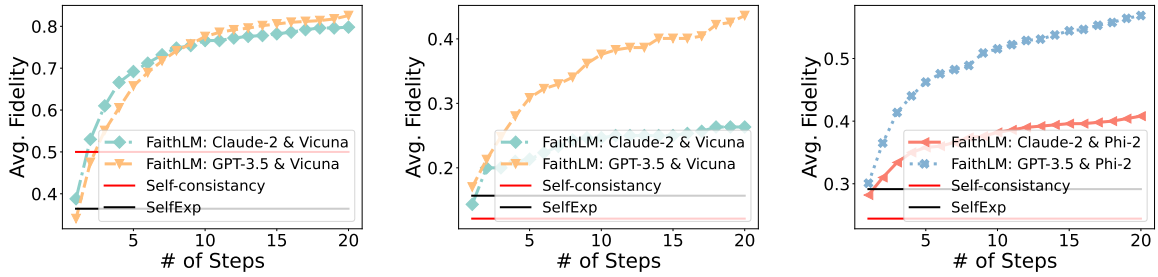

Figure 9: The fidelity evaluation of derived explanations from FaithLM under different settings of predictors and explainers.

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 10 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.

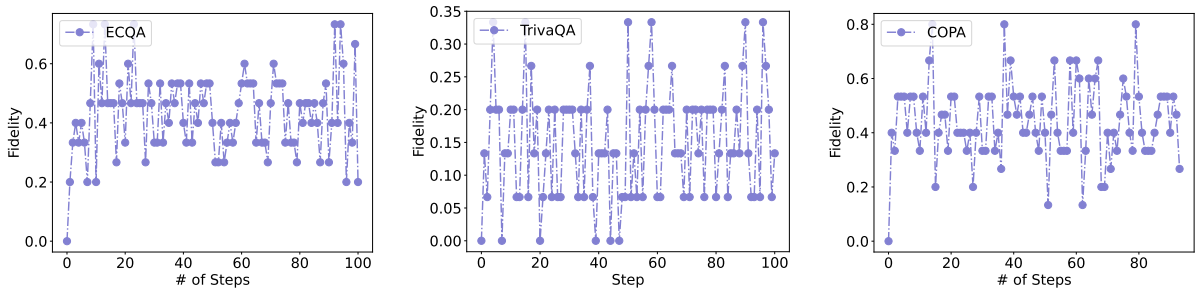

Figure 10: The optimization curve of explanation trigger prompts on ECQA (left), TriviaQA-Long (middle), and COPA dataset (right).

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.

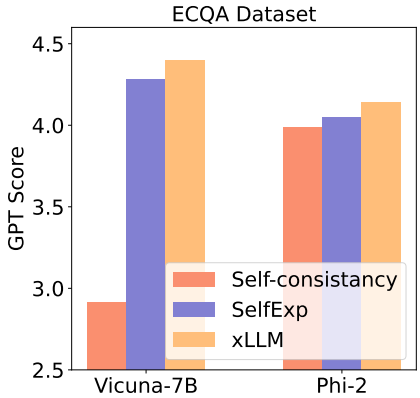

Figure 11: Truthfulness evaluation with ground-truth explanation under GPT-score settings.

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 4.6.

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`.

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

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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.
Ground Truth: The movie received poor reviews.
LLM Answer: 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.
Ground Truth: Dust blew out of the hole.
LLM Answer: 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**)