

# Unleashing the Potential of Large Language Models as Prompt Optimizers: An Analogical Analysis with Gradient-based Model Optimizers

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## Abstract

Automatic prompt optimization is an important approach to improving the performance of large language models (LLMs). Recent research demonstrates the potential of using LLMs as prompt optimizers, which can generate improved task prompts via iterative refinement. In this paper, we propose a novel perspective to investigate the design of LLM-based prompt optimizers, by drawing an analogy with gradient-based model optimizers. To connect these two approaches, we identify two pivotal factors in model parameter learning: *update direction* and *update method*. Focused on the two aspects, we borrow the theoretical framework and learning methods from gradient-based optimization to design improved strategies for LLM-based prompt optimizers. By systematically analyzing a rich set of improvement strategies, we further develop a capable Gradient-inspired LLM-based Prompt Optimizer called **GPO**. At each step, it first retrieves relevant prompts from the optimization trajectory as the update direction. Then, it utilizes the generation-based refinement strategy to perform the update, while controlling the edit distance through a cosine-based decay strategy. Extensive experiments demonstrate the effectiveness and efficiency of GPO. In particular, GPO brings an additional improvement of up to 56.8% on Big-Bench Hard and 55.3% on MMLU compared to baseline methods. The code is available at <https://github.com/RUCAIBox/GPO>.

## 1 Introduction

Nowadays, prompting has become the pivotal approach to unleashing the power of large language models (LLMs) (Zhao et al., 2023; Touvron et al., 2023; OpenAI, 2023). However, prompt engineering is not easy and requires extensive trial-and-error efforts since LLMs are sensitive to prompts (Zhao

et al., 2021; Lu et al., 2022; Wei et al., 2023). Although general guidelines for high-quality prompts exist (Kojima et al., 2022; Amatriain, 2024), they cannot always lead to optimal task performance.

To improve the task performance of LLMs, *automatic prompt optimization* has been proposed (Zhou et al., 2023). Early work either directly performs discrete optimization through methods like reinforcement learning (Deng et al., 2022; Zhang et al., 2023) or performs continuous optimization in the embedding space of LLMs (Shin et al., 2020; Lin et al., 2023; Chen et al., 2023). However, these methods often require access to the logits or internal states of LLMs, which is infeasible for those only accessible through APIs. In addition, they need to be specially trained for each task. Considering these issues, recent work proposes to model the optimization problem in natural language and using LLMs as *prompt optimizers* (Zhou et al., 2023; Yang et al., 2023; Ma et al., 2024). In this approach, LLMs can perform optimization with only outputs from the task model and quickly adapt to various tasks without training. However, such a method raises a new challenge for the design of *meta-prompt*, which is the prompt for LLMs to perform prompt optimization.

To tackle this issue, we aim to investigate the design of meta-prompts. In existing approaches, meta-prompts are often hand-crafted (Yang et al., 2023) or optimized with heuristic algorithms (Fernando et al., 2023). Despite the flexibility, these studies still lack principled guidelines about their designs. Our work is inspired by the great success of gradient-based optimizers in model optimization, which have been systemically studied in both theory and practice (Sun et al., 2020; Abdulkadirov et al., 2023). Since both optimizers target enhancing model performance through optimization, it is feasible to connect the two different approaches via analogical analysis. In this way, we can borrow the theoretical framework and extensive research of

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gradient-based model optimizers to enhance LLM-based prompt optimizers.

Specifically, in this paper, we take the gradient-based optimization approach from machine learning as reference, and identify two key factors for model parameter learning, namely *update direction* (i.e., gradient calculation) and *update method* (i.e., gradient descent). By analogy, in LLM-based prompt optimizers, the update direction can refer to suitable prompt information informing the LLM about how to produce more effective task prompts, while the update method can refer to how the LLM utilizes such information to improve prompts. By drawing such an analogy, we can develop a more formal framework for LLM-based prompt optimizers and provide guidelines to design more principled meta-prompts.

Furthermore, we develop a capable Gradient-inspired LLM-based **Prompt Optimizer** called **GPO**, with the best configuration from our systematic study. We evaluate its performance across complex reasoning, knowledge-intensive, and common NLP tasks in various evaluation settings. When using Llama-2-7b-chat as the task model, the prompts produced by GPO surpass the instruction “Let’s think step by step” by 18.5% on Big-Bench Hard (BBH) and 7.6% on MMLU. Furthermore, GPO produces an additional improvement of up to 56.8% on BBH and 55.3% on MMLU compared with baseline methods while using fewer tokens.

To the best of our knowledge, it is the first time that a systematic study has been conducted for LLM-based prompt optimizers. More specifically, it has been studied by analogy with gradient-based model optimizers, which we believe is useful to seek theoretical foundations and extend feasible approaches for prompt optimization.

## 2 Related Work

Our work is related to the following two directions.

**Prompt Engineering and Optimization.** Prompt engineering aims to find suitable prompts as the input for LLMs to perform various tasks. To reduce human efforts, researchers have explored automatic prompt optimization, which can be categorized into continuous and discrete optimization methods. Discrete methods (Deng et al., 2022; Xu et al., 2022) directly optimize the natural language prompts through methods like reinforcement learning (Deng et al., 2022; Zhang et al., 2023) and editing (Xu et al., 2022; Prasad et al., 2023). In

contrast, continuous methods perform optimization in the embedding space of LLMs, allowing for optimization through gradient (Li and Liang, 2021; Lester et al., 2021). We focus on discrete methods, especially LLM-based prompt optimizers.

**LLM-based Prompt Optimizers.** Due to the unprecedented capabilities of LLMs, recent work starts to utilize them as prompt optimizers. One line of work (Guo et al., 2023; Yang and Li, 2023) combines LLMs with evolutionary algorithms to perform prompt optimization. Another line of work (Pryzant et al., 2023; Yang et al., 2023) aims to adapt concepts and techniques from gradient-based model optimizers (e.g., gradient (Pryzant et al., 2023) and momentum (Yang et al., 2023)) to LLM-based prompt optimizers. However, no comprehensive guidelines exist for using LLMs as prompt optimizers. We aim to tackle this with a systematic investigation, which is conducted by analogy with gradient-based model optimizers.

## 3 An Analogical Analysis Between Gradient-Based Model Optimizer and LLM-Based Prompt Optimizer

In this section, we present an analogical analysis between model optimization and prompt optimization to build their connections and further improve existing LLM-based prompt optimizers.

### 3.1 Task Formulation

Prompt optimization aims to find the optimal *task prompt*  $p^*$  in the format of natural language that maximizes the performance on a specific task dataset  $\mathcal{D}$  when using an LLM as the task model  $\mathcal{M}_T$ . To perform such optimization, our idea is to develop a prompt optimizer, which can be built upon some search algorithm (e.g., evolutionary algorithms (Guo et al., 2023)) or an LLM (Yang et al., 2023). In this paper, we focus on using an LLM as the prompt optimizer  $\mathcal{M}_O$ . Formally, the problem of prompt optimization can be formulated as:

$$p^* = \arg \max_{p \sim \mathcal{M}_O} \mathbb{E}_{\langle x, y \rangle \in \mathcal{D}} [F(\mathcal{M}_T(x; p), y)], \quad (1)$$

where  $p$  is the prompt generated by the LLM-based prompt optimizer  $\mathcal{M}_O$ ,  $\mathcal{M}_T(x; p)$  represents the output from the task model for input  $x$  conditioned on the prompt  $p$ , and the function  $F(\cdot)$  calculates the task performance based on some measurement.

For the LLM-based prompt optimizer, it requires another prompt to perform the optimization for

the task prompt, which is usually called *meta-prompt* (Yang et al., 2023; Ye et al., 2023). For example, for the mathematical reasoning task, the prompt can be “Let’s solve the problem”, while the meta-prompt may be “Improve the prompt to help a model better perform mathematical reasoning”.

### 3.2 Analogical Analysis for Prompt Optimization

Since both prompt optimizers and model optimizers target enhancing the model performance through some optimization algorithm, in this part, we aim to draw inspiration from the design of gradient-based model optimizers to conduct a systematic analysis of LLM-based prompt optimizers.

#### 3.2.1 Revisiting Gradient-Based Optimizers

Similar to prompt optimization, model optimization aims to find the optimal values of model parameters that minimize the loss function. In model optimization, gradient-based optimizers are the most widely used approaches, which iteratively update model parameters in the direction of the negative gradient of the loss function. To motivate our approach, we take the fundamental optimizer known as *gradient descent* (Boyd and Vandenberghe, 2014) for discussion.

In the basic form of gradient descent, a single optimization step can be formulated as follows:

$$\Theta_{k+1} = \Theta_k - \tau_k g_k, \quad (2)$$

where  $\Theta_k$  and  $\Theta_{k+1}$  are the values of model parameters at the last and current steps,  $\tau_k$  and  $g_k$  are the learning rate and gradient at the current step. Gradient descent can be improved by focusing on two elements in the formula:  $\tau_k$  and  $g_k$ . For  $\tau_k$ , learning rate schedulers (Gotmare et al., 2019) are proposed to dynamically adjust the learning rate. For  $g_k$ , the concept of momentum (Sutskever et al., 2013) is introduced to include historical gradients, and its computation can be expressed as follows:  $v_{k+1} = \beta v_k + g_k = \sum_{i=1}^k \beta^{k-i} g_i$ , where  $\beta$  represents the momentum coefficient.

Despite various gradient-based optimizers, they mainly model two key factors, namely *update direction* (e.g., gradient  $g_k$ ) and *update method* (e.g., direct descent update by subtracting  $\tau_k g_k$ ). Our approach is inspired by the observation that existing LLM-based prompt optimization methods also implicitly employ the two aspects. For example, OPRO (Yang et al., 2023) uses previous task prompts along with their performance to guide the

Factor	Gradient-based model optimizer	LLM-based prompt optimizer
Update direction	Model value Gradient Momentum	Prompt Reflection Trajectory
Update method	Learning rate Descent	Edit distance Editing / Generation

Table 1: Analogy between glossaries in model optimizer and prompt optimizer.

direction of update and utilizes in-context learning based generation as the update method. The comparison between glossaries is shown in Table 1. However, the efforts in existing work only initially explore the design of the two key factors, and we aim to conduct more in-depth and systematic investigations by borrowing the idea of research in gradient-based optimization.

#### 3.2.2 Analogical Prompt Optimization Strategies for “Update Direction”

In prompt optimization, there are no explicit gradients for controlling the update direction. However, we can incorporate the concept of gradient into the design of meta-prompts to improve the prompt optimization process.

**Analogical “Gradient” Forms.** The basic function of the gradient is to inform how the optimization process should adjust according to the model performance. To mimic similar effects, for an LLM with fixed parameters, it is only feasible to design suitable prompting strategies to adjust the output. Here, we consider two analogical forms to implicitly support the gradient-like function.

- *Prompt+performance.* One straightforward method is to include the last-round task prompt and the corresponding model performance into the meta-prompt for LLM-based optimizer  $\mathcal{M}_O$ . It leverages the capacity of LLMs to reason about how to improve prompting optimization.

- *Prompt+performance+reflection.* Another way to solve the barrier of the gradient is to leverage the reflection capability of LLMs (Pryzant et al., 2023). With the reflection mechanism, LLMs can generate feedback from past failures, which can be used to improve performance. Such feedback can be seen as a form of “semantic” gradient signals (Pryzant et al., 2023).

**Analogical “Momentum” Forms.** Inspired by the *momentum* method (Sutskever et al., 2013) in gradi-

ent descent, we consider enhancing the aforementioned basic form of meta-prompt by leveraging the intermediate results accumulated in the prompt optimization process. A straightforward way is to directly include them into the meta-prompt. However, it might be limited by the context length of LLMs and affected by the accumulated noise. To better utilize the optimization trajectory, we propose two alternative methods.

- *Summarization-based trajectory.* One direct approach is to summarize the intermediate results from the optimization trajectory. Specifically, at each step, we use an instruction (e.g., “Your task is to summarize the problems in the previous prompt and the current prompt.”) to let the LLM perform summarization using the summary in the last step and the result in the current step.

- *Retrieval-based trajectory.* Another approach is to dynamically retrieve  $k$  pieces of gradients from the optimization trajectory. Specifically, we consider the following three strategies for selection: (1) recency: selecting  $k$  nearest gradients; (2) relevance: selecting  $k$  most relevant gradients, which are measured by the semantic similarity based on the BGE model (Xiao et al., 2023); (3) importance: selecting  $k$  most important gradients, which is measured by the performance gain.

### 3.2.3 Analogical Prompt Optimization Strategies for “Update Method”

Another important factor to consider is the update method for prompt optimization. In gradient-based model optimizers, the optimization process is controlled by the learning rate and fulfilled by gradient descent on parameters. Accordingly, we explore two analogical aspects: prompt variation control and meta-prompt refinement.

**Prompt Variation Control.** After setting the optimization direction, it is important to adjust the parameter optimization process with a suitable learning rate. This is because using a either too large or too small rate can result in an oscillating or slowly converging optimization process. Similarly, without a suitable control mechanism in prompt optimization, the LLM-based optimizer might overshoot the optimal prompt or oscillate in the optimization process. To mimic the similar effects of learning rate, our idea is to control the variation degree of prompt optimization, which is measured by the *edit distance* between two task prompts at consecutive iterations. Specifically, following Ye

et al. (2023), we add an instruction (i.e., “You are allowed to change up to  $X$  words in the current prompt.”) into the meta-prompt to limit the number of words that can be modified. Accordingly, we propose two control methods as follows:

- *Decay-based constraint.* To avoid overshooting the optimal solution, the decay strategy is proposed to gradually reduce the learning rate (Izmailov et al., 2018). Here, we borrow the idea to control the maximum edit distance and consider gradually reducing its value following either a linear or cosine curve. In addition, following the common practice in training LLMs (Touvron et al., 2023), we reduce the constraint to approximately 20% of its maximum value until convergence.

- *Warmup-based constraint.* To avoid instability in the early stage of optimization, the warmup strategy is proposed to gradually increase the learning rate at the beginning (Goyal et al., 2017). Similarly, we adopt the widely used linear warmup schedule to gradually increase the constraint for the maximum edit distance to its initially set value in the initial 5% steps.

**Prompt Refinement Strategy.** During the optimization process, the task prompt would be iteratively refined, to improve the corresponding model performance. By analogy with the subtraction operation in gradient-based optimizers (i.e.,  $-\tau_k g_k$  in Eq. (2)), we introduce two methods to update the task prompt accordingly.

- *Editing-based refinement.* The first method directly edits the last-round task prompt to improve performance. Specifically, we add an instruction (i.e., “Modify the current prompt and get a new improved prompt”) into the meta-prompt, which requires the LLM to edit the task prompt from the last step according to the update direction. This method allows for effectively exploiting the existing prompt, leading to a gradual performance improvement through a relatively stable optimization process.

- *Generation-based refinement.* In addition to direct edits, we can also leverage the in-context learning capability of LLMs to generate refined task prompts. Specifically, we present the information regarding the update direction in the format of demonstration (e.g., “Below are the previous prompts with their scores. The score ranges from 0 to 100, and a higher score indicates better quality. Prompt: {prompt}. Score: {score}.”). Then, the LLM can follow the demonstration to generate a



Initial prompt: "Let's think step by step." Performance: 31.25					
Gradient form	Momentum form				
	None	S-T	R-T		
			Recency	Relevance	Importance
P+M	41.07	41.03	41.93	<b>42.53</b>	41.84
P+M+R	40.34	40.63	41.55	40.81	39.73

Table 2: The performance comparison between different update directions. "P" denotes prompt, "M" denotes performance, "R" denotes reflection, "S-T" denotes summarization-based trajectory, and "R-T" denotes retrieval-based trajectory.

new task prompt. Compared with the editing-based updating method, the generation-based approach explores a wider range of prompt variations, which has the potential to yield improved performance but also makes the optimization process unstable.

### 3.3 Analogical Analysis Experiments

In this part, we first describe the experiment setting for our analogical analysis, and then detail our findings from the experiment.

#### 3.3.1 Experiment Setup

We select a dataset from each type of task in BBH (Suzgun et al., 2023) to create a lite BBH benchmark for our analysis: i) Navigate (binary choice); ii) Movie Recommendation (multiple choice); iii) Object Counting (numeric response); iv) Word Sorting (free response). We adopt exact match as the metric for performance evaluation. We employ Llama-2-7b-chat (Touvron et al., 2023) as the task model and gpt-3.5-turbo as the prompt optimizer. The initial task prompt is "Let's think step by step." Other details are presented in Appendix B.

#### 3.3.2 Empirical Findings

**Findings For Update Direction.** The results for the update direction of prompt optimization are presented in Table 2. Here are the main findings:

- With regard to the form of gradient, *prompt+performance* achieves better performance than *prompt+performance+reflection*, which brings an improvement of up to 31% compared with the initial task prompt. The substantial improvement brought by prompts can be attributed to their rich semantic information about the task, which can activate the task-specific knowledge of LLMs for optimization. In contrast, LLMs are known to be

Initial prompt: "Let's think step by step." Performance: 31.25			
Variation Control	Refinement strategy	Editing	Generation
	No control	42.53	42.61
	Fixed	42.91	43.09
	+Warmup	41.76	40.08
	Linear decay	42.68	42.86
	+Warmup	41.47	41.12
	Cosine decay	42.95	<b>43.75</b>
	+Warmup	40.19	41.29

Table 3: The performance comparison between different update methods.

limited in their capabilities of reflection (Huang et al., 2023), which may lead to inaccurate updates.

- The analogical concept of momentum can further improve the performance of prompt optimization. Among various designs, *relevance-based trajectory* emerges as the most effective one, which brings an additional 15% improvement. This can be attributed to the fact that LLMs can learn more from prompts that are contextually relevant, while it might be challenging for LLMs to fully understand the signal of recency or importance. By contrast, the summarization-based trajectory proves to be less helpful. This is because summarization only captures common aspects of the trajectory while neglecting details that may be crucial.

**Findings For Update Method.** To investigate the update method for prompt optimization, we conduct experiments using the best configuration found in the previous experiments. The results for the update method of prompt optimization are presented in Table 3. Here are the key findings:

- In general, *generation-based refinement* performs better than editing-based refinement, which brings an improvement of up to 36% compared with the initial task prompt. This may be because LLMs are not specially trained for prompt optimization, and the demonstrations in the generation-based strategy can provide guidance about this task, thus helping LLMs learn to perform better.

- Among various controlling methods for prompt variation, *cosine decay-based constraint* achieves the best performance, bringing an additional 10% improvement. However, unlike gradient-based model optimization, the warmup strategy does not yield improvement. This finding suggests that, at the early stage of prompt optimization, exploration plays a crucial role, while stability becomes more important in the later stage.

## 4 Our Prompt Optimizer: GPO

In this section, we present our novel gradient-inspired LLM-based prompt optimizer called **GPO**, which leverages the insights gained from our systematic study. Our approach proposes a novel design of the meta-prompt, aiming to unleash the potential of LLMs as prompt optimizers.

**Iterative Prompt Optimization.** GPO performs prompt optimization through a multi-step iterative process. At each step, the LLM first generates multiple candidate task prompts based on a meta-prompt. The meta-prompt serves as the input that guides the LLM in optimizing its prompts. Subsequently, the task prompt with the best performance is selected for the next iteration. This iterative process continues until either the performance of the task prompt reaches a plateau or the predefined maximum number of optimization steps is reached.

**The Design of Meta-Prompt.** As the input to the LLM, our meta-prompt consists of two key components: update direction and update method.

- *Update direction.* To determine the update direction, we leverage the retrieval-based optimization trajectory in Section 3.2.2. This trajectory comprises a collection of past task prompts, along with their model performance. They are selected using a relevance-based strategy and are sorted in ascending order based on their performance.

- *Update method.* After the update direction is determined, we further employ the generation-based refinement strategy in Section 3.2.3 to update the task prompt. Specifically, we present the trajectory in the format of demonstration in the meta-prompt. Then, the LLM can follow these demonstrations to generate a new task prompt via in-context learning. Additionally, we implement the cosine-based decay strategy in Section 3.2.3 with an instruction to control the edit distance between task prompts at consecutive iterations, ensuring gradual and controllable changes.

Furthermore, we enhance the meta-prompt by incorporating a few task examples. These examples provide additional context to aid the LLM in understanding the task more effectively. The complete meta-prompt is presented in Appendix C.2.

**Comparison of LLM-Based Prompt Optimizers.** Existing LLM-based prompt optimizers can be divided into two main classes according to the update direction. The first line of research, such

Prompt optimizer	Update direction		Update method	
	Gradient form	Momentum form	Prompt variation	Prompt refinement
APE	P	None	None	Generation
APO	P+R	None	None	Editing
OPRO	P+M	Recency	None	Generation
PE2	P+M+R	Recency	Fixed	Generation
GPO	P+M	Relevance	Cosine	Generation

Table 4: Comparisons of GPO with existing LLM-based prompt optimizers, including APE (Zhou et al., 2023), APO (Pryzant et al., 2023), OPRO (Yang et al., 2023), and PE2 (Ye et al., 2023). “P” refers to prompt, “M” refers to performance, and “R” refers to reflection.

as APO (Pryzant et al., 2023) and PE2 (Ye et al., 2023), leverages the reflection capability of LLMs to produce textual “gradients” as the update direction. Another line of research, such as OPRO (Yang et al., 2023) and APE (Zhou et al., 2023), directly uses task prompts to derive the update direction. Our approach is based on the systematic investigation of the update direction as well as the update method. In particular, we propose several novel designs for the meta-prompt: relevance-based trajectory as the update direction and decay-based constraint for edit distance in the update method. Table 4 presents a detailed comparison.

## 5 Experiments

In this section, we first set up the experiments and then report the results and detailed analysis.

### 5.1 Experimental Setup

**Tasks and Datasets.** We select datasets from three groups of tasks for the experiment: Big-Bench Hard (BBH) (Suzgun et al., 2023) and GSM8K (Cobbe et al., 2021) for complex reasoning tasks, MMLU (Hendrycks et al., 2021) for knowledge-intensive tasks, and WSC (Levesque et al., 2012) and WebNLG (Gardent et al., 2017) for common NLP tasks. Due to computational limitations, we sample a subset from each dataset for the main experiment. In addition, we use the lite BBH benchmark in Section 3.3.1 for detailed analysis. Other details are presented in Appendix C.1.

**Baselines.** We select several representative methods for comparison, including existing LLM-based prompt optimizers and one adapted from gradient-based model optimizers. (1) *SGDM* (Sutskever et al., 2013) is a momentum-based model optimizer. We adapt it for prompt optimization using

the summarization-based trajectory and the editing-based refinement strategy. (2) *APE* (Zhou et al., 2023) utilizes LLMs to generate semantically similar variants of task prompts and selects one with the best performance. (3) *APQ* (Pryzant et al., 2023) first uses reflection to obtain the gradient and then edits the task prompt accordingly. (4) *OPRO* (Yang et al., 2023) incorporates historical prompts with their scores into the meta-prompt. (5) *PE2* (Ye et al., 2023) adds historical prompts and reflection into the meta-prompt and controls the edit distance with a fixed constraint. In addition, we consider the baseline without an instruction (“Empty”) and the instruction “Let’s think step by step.” from chain-of-thought prompting (“CoT”) (Kojima et al., 2022) for performance comparison.

**Evaluation Metrics.** We report the average accuracy of all the subtasks for BBH and MMLU following Suzgun et al. (2023) and Hendrycks et al. (2021), accuracy for GSM8K following Cobbe et al. (2021), ROUGE-L (Lin, 2004) for WSC and WebNLG following Wang et al. (2022).

**Implementation Details.** For the task model, we use both the base model (*i.e.*, Llama-2-7b) and the instruction-tuned models (*i.e.*, Llama-2-7b-chat, GPT-3.5-turbo, and GPT-4). For the prompt optimizer, we use GPT-3.5-turbo and GPT-4. Unless otherwise specified, we use Llama-2-7b-chat as the task model and GPT-3.5-turbo as the prompt optimizer throughout experiments. For the initial task prompt, we use the original ones from Hendrycks et al. (2021) for MMLU, “Let’s think step by step.” from Kojima et al. (2022) for GSM8K and BBH, and “Let’s solve the problem.” from Yang et al. (2023) for WSC and WebNLG. We repeat all the experiments three times and report the average of the results. Other details are presented in Appendix C.2.

## 5.2 Main Results

Table 5 and Table 6 present the results of different methods for prompt optimization across various tasks and evaluation settings.

First, when only considering the task prompt, we can see that trajectory-based methods (*i.e.*, SGDM, OPRO, PE2, and GPO) perform very well. One possible reason is that the trajectory helps the prompt optimizer pay more attention to the important information instead of the noise in the current step. Furthermore, our prompt optimizer GPO achieves the best performance across all tasks.

Task	Complex reasoning task		Knowledge intensive task	Common NLP task	
Dataset	BBH	GSM8K	MMLU	WSC	WebNLG
Empty	30.51	22.00	35.96	60.67	32.14
CoT	29.91	24.00	36.36	59.33	31.11
SGDM	33.30	27.33	37.30	64.00	38.01
APE	32.94	25.00	37.53	62.00	36.49
APQ	32.97	25.33	37.75	62.00	34.92
OPRO	33.29	26.67	37.88	63.33	37.89
PE2	33.43	25.33	38.15	62.67	39.10
GPO	<b>35.43</b>	<b>28.33</b>	<b>39.14</b>	<b>65.33</b>	<b>42.51</b>

Table 5: Performance comparison using only the task prompts obtained from different methods.

Task model	Llama-2-7b	Llama-2-7b-chat	
Setting	Inst. + Demo.	Inst.	Inst. + Demo.
Empty	40.28	32.29	36.63
CoT	36.46	31.25	34.20
SGDM	42.19	40.63	35.77
APE	42.54	42.01	36.29
APQ	42.19	40.34	36.29
OPRO	42.02	42.14	36.46
PE2	42.88	42.01	36.81
GPO	<b>45.48</b>	<b>43.75</b>	<b>38.02</b>

Table 6: Performance comparison under different evaluation settings. “Inst.” denotes instruction and “Demo.” denotes demonstration.

Our relevance-based trajectory provides semantically similar demonstrations that can be effectively learned by the LLM, while the cosine-based decay strategy can control the optimization process in a fine-grained manner through edit distance.

Second, under various evaluation settings for the lite BBH benchmark, it can be observed that GPO not only excels in the “Instruction” setting but also yields substantial gains in the “Instruction + Demonstration” setting for both the base model and the instruction-tuned variant. Even in the scenario that is challenging for baselines (*i.e.*, Llama-2-7b-chat with “Instruction + Demonstration”), our approach still demonstrates strong improvement over the empty prompt. This showcases the versatility of our approach in both zero-shot and few-shot evaluation settings.

## 5.3 Detailed Analysis

Next, we conduct a detailed analysis of our prompt optimizer GPO from the following aspects.

**The Impact of Model Selection.** To confirm the effectiveness of GPO across different models, we explore the impact of model selection. Specifically, for the prompt optimizer, we

Prompt optimizer	Task model	Accuracy (before / after)
GPT-3.5-turbo	Llama-2-7b-chat	31.25 / 43.75
	GPT-3.5-turbo	62.15 / 67.02
	GPT-4	73.61 / 76.56
GPT-4	Llama-2-7b-chat	31.25 / 44.97
	GPT-3.5-turbo	62.15 / 67.80
	GPT-4	73.61 / 78.65

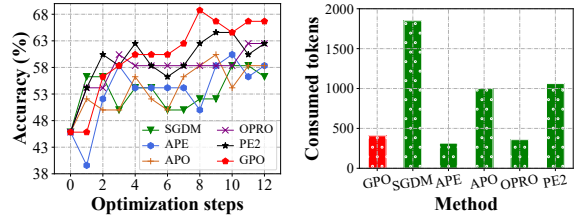
Table 7: The performance before/after prompt optimization with different models as the prompt optimizer and the task model.

Initial prompt		Accuracy (before / after)
Default	Let’s think step by step.	31.25 / 43.75
Instructive	Let’s think about this logically. First,	32.64 / 44.40
	Let’s solve this problem by splitting it into steps.	33.85 / 43.15
Misleading	Don’t think. Just feel.	29.34 / 39.59
	Let’s think step by step but reach an incorrect answer.	26.22 / 41.15
	Let’s count the number of “a” in the question	26.73 / 36.11
Irrelevant	By the way, I found a good restaurant nearby.	30.03 / 34.89
	AbraKadabra!	29.69 / 35.42
	It’s a beautiful day.	30.55 / 38.02

Table 8: The performance before/after prompt optimization with different initial prompts.

employ GPT-3.5-turbo and GPT-4, while for the task model, we utilize Llama-2-7b-chat, GPT-3.5-turbo and GPT-4. Table 7 presents the results on the lite BBH benchmark. In general, GPO demonstrates remarkable capabilities for prompt optimization across various scenarios, including strong-to-weak optimization, self-optimization, as well as weak-to-strong optimization. This indicates the versatility of our framework. In particular, GPT-4 can consistently find better task prompts than GPT-3.5-turbo, which suggests the need for a capable model as the prompt optimizer.

**The Impact of Initial Prompts.** In our main experiment, we take “Let’s think step by step.” as the initial prompt. In this part, we aim to explore the impact of initial task prompts. Specifically, we consider prompts from three categories (instructive, misleading, and irrelevant) and select three prompts from each category following Kojima et al. (2022). Table 8 presents the results on the lite BBH benchmark. In general, GPO can consistently boost performance across various initial prompts. This observation underscores the versatility of GPO as



(a) Optimization curve

(b) Token consumption

Figure 1: The efficiency of our approach GPO w.r.t. optimization steps and token consumption.

a prompt optimizer. Furthermore, the efficacy of optimization is more pronounced with relevant initial prompts (*i.e.*, instructive and misleading). It means that prompt initialization is still important, especially in conveying task-specific information.

**The Efficiency of Optimization.** LLM-based prompt optimization requires multiple interactions with the LLM. In this part, we investigate the efficiency of GPO from the optimization curve and token consumption. First, Figure 1a shows that on the movie recommendation dataset, GPO exhibits rapid enhancement of the task prompt in the early stage, followed by consistent performance improvement in the later stage of optimization. Second, as depicted in Figure 1b, the average token consumption of GPO on the lite BBH benchmark is much lower than SGDM, APE, and PE2, and comparable to APR and OPRO. Since GPO only utilizes task prompts to derive the update direction and performs fine-grained control over the variation, it can achieve better performance with high efficiency.

## 6 Conclusion

We present **GPO**, a novel gradient-inspired LLM-based prompt optimizer. It utilizes LLMs to automatically optimize prompts, drawing inspiration from gradient-based model optimization techniques. By identifying the two crucial aspects of *update direction* and *update method* in model optimization, we enhance prompt optimizers by incorporating concepts from gradient-based model optimizers. Through extensive experiments, GPO demonstrates remarkable capabilities for prompt optimization across diverse tasks, models, and initial prompts. Moreover, it surpasses competitive baselines while consuming fewer tokens.

In future work, we will explore more guidelines to further enhance the effectiveness and efficiency of LLM-based prompt optimizers.



## 7 Limitations

In this work, we improve the design of LLM-based prompt optimizers by drawing an analogy with the most widely used gradient-based optimizers in model optimization (e.g., gradient descent). More advanced model optimizers like Newton’s method (Boyd and Vandenberghe, 2014) and the corresponding improvement for meta-prompts remain to be investigated. In addition, due to the computational and budget limitations, we only conduct experiments on representative tasks and models.

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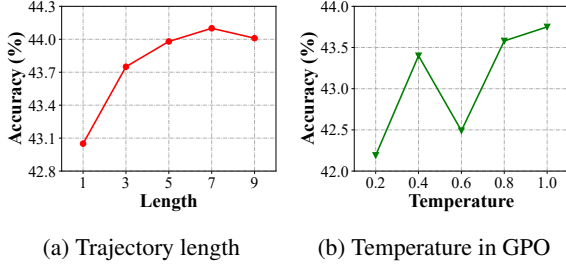


Figure 2: Performance comparison w.r.t. the temperature of the LLM in GPO and the length of the trajectory.

## A Hyper-Parameter Analysis

GPO includes a few hyper-parameters to tune. Here, we report the tuning results of two hyper-parameters on the lite BBH benchmark: the temperature of the prompt optimizer and the length of the trajectory. The performance curve depicting these results is illustrated in Figure 2. We can see that GPO achieves the best performance when setting the length of the trajectory to 7. A trajectory that is too short does not provide sufficient context for the LLM to engage in effective in-context learning. Conversely, a long trajectory may introduce excessive noise, negatively impacting performance. In addition, the performance shows an upward trend as temperature increases, reaching its peak at 1.0. It suggests the significance of exploration in optimizing task prompts.

## B Additional Details for the Setup of Analogical Analysis

**Tasks and Metrics.** Following Yang et al. (2023), we utilize Big-Bench Hard (BBH) (Suzgun et al., 2023) for evaluation. BBH is a suite of 23 challenging BIG-Bench tasks (Srivastava et al., 2022) that covers various kinds of reasoning capabilities. Due to the constraints of computational resources, we select a dataset from each type of task in BBH to create a lite benchmark for our analysis: i) Navigate (Binary choice); ii) Movie Recommendation (Multiple choice); iii) Object Counting (Numeric response); iv) Word Sorting (Free response). For each dataset, we split it into train/valid/test sets with a ratio of 2:2:6. Following Suzgun et al. (2023), we adopt the exact match as the metric for performance evaluation.

**Implementation Details.** Following Crispino et al. (2023), we select Llama-2-7b-chat (Touvron et al., 2023) as the task model and set its tem-

perature to 0 to make the output as deterministic as possible. For the prompt optimizer, we employ gpt-3.5-turbo, which is the underlying model of ChatGPT. We set its temperature to 1.0 to encourage the generation to be more diverse. To help the prompt optimizer understand the downstream task, following Yang et al. (2023), we randomly sample 3 examples from the dataset and fill them into the meta-prompt of the prompt optimizer. In the process of optimization, we take the instruction “Let’s think step by step.” as the initial prompt and insert it at the end of the question to obtain better performance following Suzgun et al. (2023). At each step, we first prompt the optimizer to generate 8 candidate task prompts, and then select the best-performing one as the task prompt for the next iteration following Yang et al. (2023); Ye et al. (2023). The optimization process lasts for at most 3 epochs with a batch size of 8. We repeat all the experiments three times and report the average of the results. The meta-prompts we used are detailed in Appendix D.1.

## C Additional Details for the Setup of Experiment

### C.1 The Statistics of Datasets

As mentioned in Section 5.1, we sample a subset of the dataset for efficient evaluation. For BBH and MMLU, we split the entire dataset into training, validation, and test sets with a ratio of 2:2:6. For GSM8k and WebNLG, we randomly sample 100 examples as the training set, 100 for the validation set, and 300 for the test set. For WSC, we randomly sample 50 examples as the training set, 50 for the validation set, and 150 for the test set.

### C.2 Implementation Details

For the task model, we use both the base model (*i.e.*, Llama-2-7b) and the instruction-tuned models (*i.e.*, Llama-2-7b-chat, GPT-3.5-turbo, and GPT-4). The temperature is 0. For the prompt optimizer, we use GPT-3.5-turbo and GPT-4. The temperature is 1.0. Unless otherwise specified, we use Llama-2-7b-chat as the task model and GPT-3.5-turbo as the prompt optimizer throughout experiments. In the meta-prompt, we include 3 task examples and 7 historical task prompts. For the initial task prompt, we use the original ones from Hendrycks et al. (2021) for MMLU, “Let’s think step by step.” from Kojima et al. (2022) for GSM8K and BBH, and “Let’s solve the problem.”



from Yang et al. (2023) for WSC and WebNLG. At each step, the optimizer generates 8 candidates, and the best-performing one is selected. The optimization lasts for at most 3 epochs with a batch size of 8. We repeat all the experiments three times and report the average of the results. The meta-prompts are detailed in Appendix D.2.

## D Meta-Prompt

### D.1 Analogical Analysis

Here are the meta-prompts we used in Section 3.

- *Prompt+performance.*

Below is the current prompt with its score. The score ranges from 0 to 100, and higher score indicates better quality.

Prompt: {current prompt}

Score: {current prompt score}

- *Prompt+performance+reflection*

Your task is to point out the problems with the current prompt based on the wrong examples.

The current prompt is:

{current prompt}

But this prompt gets the following examples wrong.

You should analyze the differences between wrong predictions and ground truth answers, and carefully consider why this prompt led to incorrect predictions.

Below are the task examples with Question, Wrong prediction, and Ground truth answer.

{error demonstrations}

Give a reason why the prompt could have gotten these examples wrong.

Wrap the reason with <START> and <END>.

- *Summarization-based trajectory*

Your task is to integrate the problems in the previous prompt and the current prompt.

Below are the problems that arose from the previous prompts.

{previous problems}

Below are the problems of the current prompt.

{current problem}

You should integrate the problems of the previous prompt and the current prompt.

Wrap the integrated problems with <START> and <END>.

- *Retrieval-based trajectory*

Below are the previous prompts with their scores. The score ranges from 0 to 100, and higher scores indicate better quality.

Prompt: {prompt1}

Score: {score1}

Prompt: {prompt2}

Score: {score2}

Prompt: {prompt3}

Score: {score3}

...

- *Editing-based refinement*

Your task is to modify the current prompt to replace <Prompt>.

Below is the current prompt with its score. The score ranges from 0 to 100, and higher score indicates better quality.

Prompt: {current prompt}

Score: {current prompt score}

The current prompt is:  
{current prompt}

The following exemplars show how to apply the prompt: you replace <Prompt> in each input with your new prompt, then read the input and give an output. We say your output is wrong if it is different from the given output, and we say your output is correct if they are the same.

{task examples}

Modify the current prompt and get a new improved prompt to replace <Prompt> {prompt position description} in the task examples.

Wrap the modified prompt with <START> and <END>.

- *Generation-based refinement*

Your task is to write a prompt to replace <Prompt>.

Below is the current prompt with its score. The score ranges from 0 to 100, and higher score indicates better quality.

Prompt: {current prompt}

Score: {current prompt score}

The current prompt is:  
{current prompt}

The following exemplars show how to apply the prompt: you replace <Prompt> in each input with your new prompt, then read the input and give an output. We say your output is wrong if it is different from the given output, and we say your output is correct if they are the same.

{task examples}

Write a new improved prompt to replace <Prompt> {prompt position description} in the task examples.

Wrap the new prompt with <START> and <END>.

## D.2 Experiment

Here are the meta-prompts we used in Section 5.

- *SGDM*

The meta-prompt for gradient

Your task is to point out the problems with the current prompt based on the wrong examples.

The current prompt is:  
{current prompt}

But this prompt gets the following examples wrong.

You should analyze the differences between wrong predictions and ground truth answers, and carefully consider why this prompt led to incorrect predictions.

Below are the task examples with Question, Wrong prediction, and Ground truth answer.

{error demonstrations}

Give a reason why the prompt could have gotten these examples wrong.  
Wrap the reason with <START> and <END>.

The meta-prompt for momentum

Your task is to integrate the problems in the previous prompt and the current prompt.

Below are the problems that arose from the previous prompts.  
{previous problems}

Below are the problems of the current prompt.  
{current problem}

You should integrate the problems of the previous prompt and the current prompt.  
Wrap the integrated problems with <START> and <END>.

The meta-prompt for update

Your task is to modify the current prompt to replace <Prompt>.

Below is the current prompt with its score.  
The score ranges from 0 to 100, and higher score indicates better quality.

Prompt: {current prompt}  
Score: {current prompt score}

The current prompt is:  
{current prompt}

Below are the problems with this prompt.  
{problems}

The following exemplars show how to apply the prompt: you replace <Prompt> in each input with your new prompt, then read the input and give an output. We say your output is wrong if it is different from the given output, and we say your output is correct if they are the same.

{task examples}

Modify the current prompt and get a new improved prompt to replace <Prompt> {prompt position description} in the task examples.  
Wrap the modified prompt with <START> and <END>.

- *APE*

#### The meta-prompt for update

Your task is to write a prompt to replace <Prompt>.

Below is the current prompt with its score. The score ranges from 0 to 100, and higher score indicates better quality.

Prompt: {current prompt}

Score: {current prompt score}

The current prompt is:

{current prompt}

The following exemplars show how to apply the prompt: you replace <Prompt> in each input with your new prompt, then read the input and give an output. We say your output is wrong if it is different from the given output, and we say your output is correct if they are the same.

{task examples}

Write a new improved prompt to replace <Prompt> {prompt position description} in the task examples.

Wrap the new prompt with <START> and <END>.

- *APO*

#### The meta-prompt for gradient

Your task is to point out the problems with the current prompt based on the wrong examples.

The current prompt is:

{current prompt}

But this prompt gets the following examples wrong.

You should analyze the differences between wrong predictions and ground truth answers, and carefully consider why this prompt led to incorrect predictions.

Below are the task examples with Question, Wrong prediction, and Ground truth answer.

{error demonstrations}

Give a reason why the prompt could have gotten these examples wrong.

Wrap the reason with <START> and <END>.

#### The meta-prompt for update

Your task is to modify the current prompt to replace <Prompt>.

Below is the current prompt with its score. The score ranges from 0 to 100, and higher score indicates better quality.

Prompt: {current prompt}

Score: {current prompt score}

The current prompt is:

{current prompt}

Below are the problems with this prompt.

{problems}

The following exemplars show how to apply the prompt: you replace <Prompt> in each input with your new prompt, then read the input and give an output. We say your output is wrong if it is different from the given output, and we say your output is correct if they are the same.

{task examples}

Modify the current prompt and get a new improved prompt to replace <Prompt> {prompt position description} in the task examples.

Wrap the modified prompt with <START> and <END>.



- *OPRO*

The meta-prompt for update

Your task is to write a prompt to replace <Prompt>.

Below are the previous prompts with their scores. The score ranges from 0 to 100, and higher scores indicate better quality.

Prompt: {prompt1}

Score: {score1}

Prompt: {prompt2}

Score: {score2}

Prompt: {prompt3}

Score: {score3}

...

The current prompt is:

{current prompt}

The following exemplars show how to apply the prompt: you replace <Prompt> in each input with your new prompt, then read the input and give an output. We say your output is wrong if it is different from the given output, and we say your output is correct if they are the same.

{task examples}

Carefully analyze the previous prompts and their scores, and write a new improved prompt to replace <Prompt> {prompt position description} in the task examples.

Wrap the new prompt with <START> and <END>.

- *PE2*

The meta-prompt for gradient

Your task is to point out the problems with the current prompt based on the wrong examples.

The current prompt is:

{current prompt}

But this prompt gets the following examples wrong.

You should analyze the differences between wrong predictions and ground truth answers, and carefully consider why this prompt led to incorrect predictions.

Below are the task examples with Question, Wrong prediction, and Ground truth answer.

{error demonstrations}

Give a reason why the prompt could have gotten these examples wrong.

Wrap the reason with <START> and <END>.

### The meta-prompt for update

Your task is to write a prompt to replace <Prompt>.

Below are the previous prompts with their scores. The score ranges from 0 to 100, and higher scores indicate better quality.

Prompt: {prompt1}  
Score: {score1}

Prompt: {prompt2}  
Score: {score2}

Prompt: {prompt3}  
Score: {score3}  
...

The current prompt is:  
{current prompt}

Below are the problems with this prompt.  
{problems}

The following exemplars show how to apply the prompt: you replace <Prompt> in each input with your new prompt, then read the input and give an output. We say your output is wrong if it is different from the given output, and we say your output is correct if they are the same.

{task examples}

Carefully analyze the previous prompts and their scores, and write a new improved prompt to replace <Prompt> {prompt position description} in the task examples.

You are allowed to change up to {modified word number} words in the current prompt.

Wrap the new prompt with <START> and <END>.

### • GPO

#### The meta-prompt for update

Your task is to write a prompt to replace <Prompt>.

Below are the previous prompts with their scores. The score ranges from 0 to 100, and higher scores indicate better quality.

Prompt: {prompt1}  
Score: {score1}

Prompt: {prompt2}  
Score: {score2}

Prompt: {prompt3}  
Score: {score3}  
...

The current prompt is:  
{current prompt}

The following exemplars show how to apply the prompt: you replace <Prompt> in each input with your new prompt, then read the input and give an output. We say your output is wrong if it is different from the given output, and we say your output is correct if they are the same.

{task examples}

Carefully analyze the previous prompts and their scores, and write a new improved prompt to replace <Prompt> {prompt position description} in the task examples.

You are allowed to change up to {modified word number} words in the current prompt.

Wrap the new prompt with <START> and <END>.

## E Prompts Optimized by Different Methods

Here, we present the prompts optimized by all the methods on the lite BBH benchmark. Prompts on the other tasks can be seen at <https://github.com/RUCAIBox/GPO>.

Methods	Optimized prompt
SGDM	Based on your current facing direction and any changes in direction, will following these step-by-step instructions, with explicit reference to direction and orientation, lead you back to the starting point?
APE	Will following the given set of instructions result in returning to the starting point?
APO	Based on the provided instructions, including the starting direction and the changes in direction throughout the sequence, determine if the person will return to the starting point.
OPRO	Think systematically and consider each step to determine the correct answer.
PE2	Carefully analyze the given instructions step by step and determine if you will return to the starting point.
GPO	Analyze the given step-by-step instructions in detail and determine if they will guide you back to the starting point. Carefully evaluate each instruction and vividly imagine the movements to make your decision.

Table 9: Prompts optimized by different methods on the Navigate task.

Methods	Optimized prompt
SGDM	What specific aspects of storytelling style, narrative structure, plot structure, character development, and narrative techniques should be considered when finding a movie similar to films like Pulp Fiction, Forrest Gump, Dances with Wolves, and The Usual Suspects? Analyze these elements in each movie’s construction and compare them against the given list to determine similarity. Focus on shared storytelling elements rather than thematic or genre similarities. Keep in mind that the most important factor in determining similarity might not be the overall theme or genre. Provide a single letter as your answer.
APE	Which of the following movies is most similar to the given movies based on their genre, themes, and plot elements? Choose the best option from the following choices:
APO	Which movie from the following options is most similar to the given movies, taking into account specific themes, plot, genre, characters, setting, tone, and style? Please provide a ranked list of the relevant elements mentioned above in determining similarity between movies. Consider the highest ranked element as the primary criteria and subsequent elements as secondary criteria in determining similarity. Additionally, consider the overall popularity and critical acclaim of the movies when making your selection. This will help ensure more accurate predictions.
OPRO	Which of the given movies is most similar to the listed options? Consider the movies Batman, The Usual Suspects, The Silence of the Lambs, and Jurassic Park. Choose the option that closely matches the given movies.
PE2	Select the movie option that is most closely related to the given list of movies after conducting a meticulous analysis.
GPO	Thoroughly analyze the themes, genres, and narrative elements of each film to identify the movie that best aligns with the provided options. Make a well-informed decision based on your comprehensive evaluation.

Table 10: Prompts optimized by different methods on the Movie Recommendation task.

Methods	Optimized prompt
SGDM	Count the number of items
APE	Develop a systematic approach to accurately determine the total number of items by counting each individual item separately and recording their corresponding quantities.
APO	What is the total count of mentioned items, considering each item individually without categorization and counting duplicates as separate items? Please provide the correct count as your output.
OPRO	How can we solve the problem by breaking it down step by step?
PE2	By employing a systematic and thorough approach, meticulously analyze each item in a step-by-step manner to precisely determine the total count.
GPO	Let's break down the problem systematically by deconstructing it into individual steps and accurately computing the total number of objects.

Table 11: Prompts optimized by different methods on the Object Counting task.

Methods	Optimized prompt
SGDM	Sort the given words, alphabetically, in case-sensitive order, considering the entire word, including all characters. The sorting should be done in ascending order based on the lowercase versions of the words, while preserving the original case and considering the entire word.
APE	How would you sort the given list of words in alphabetical order, considering both uppercase and lowercase letters?
APO	Sort the given list of words in lowercase alphabetical order, taking into account all characters including special characters and numbers. Ensure that the sorting process is case-insensitive and considers all characters, including special characters and numbers. Convert all letters to lowercase before sorting. Consider special characters and numbers in the sorting process.
OPRO	Arrange the given words in alphabetical order by considering only the first letter of each word and exclude punctuation or special characters.
PE2	Analyze the given words and provide a sorted list in alphabetical order.
GPO	Arrange the following words in alphabetical order:

Table 12: Prompts optimized by different methods on the Word Sorting task.