GREATER: GRADIENTS OVER REASONING MAKES SMALLER LANGUAGE MODELS STRONG PROMPT OP-TIMIZERS

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ABSTRACT

The effectiveness of large language models (LLMs) is closely tied to the design of prompts, making prompt optimization essential for enhancing their performance across a wide range of tasks. Many existing approaches to automating prompt engineering rely exclusively on textual feedback, refining prompts based solely on inference errors identified by large, computationally expensive LLMs. Unfortunately, smaller models struggle to generate high-quality feedback, resulting in complete dependence on large LLM judgment. Moreover, these methods fail to leverage more direct and finer-grained information, such as gradients, due to operating purely in text space. To this end, we introduce GREATER, a novel prompt optimization technique that directly incorporates *gradient information over taskspecific reasoning*. By utilizing task loss gradients, GREATER enables selfoptimization of prompts for open-source, lightweight language models without the need for costly closed-source LLMs. This allows high-performance prompt optimization without dependence on massive LLMs, closing the gap between smaller models and the sophisticated reasoning often needed for prompt refinement. Extensive evaluations across diverse reasoning tasks including BBH, GSM8k, and FOLIO demonstrate that GREATER consistently outperforms previous state-ofthe-art prompt optimization methods, even those reliant on powerful LLMs. Additionally, GREATER-optimized prompts frequently exhibit better transferability and, in some cases, boost task performance to levels comparable to or surpassing those achieved by larger language models, highlighting the effectiveness of prompt optimization guided by gradients over reasoning. Code of GREATER is available at: <https://github.com/psunlpgroup/GreaTer>.

1 INTRODUCTION

Large Language Models (LLMs) have demonstrated impressive performance across various task domains [\(Brown, 2020;](#page-10-0) [Achiam et al., 2023;](#page-10-1) [Reid et al., 2024\)](#page-11-0). However, these models are known to exhibit prompt sensitivity, a phenomenon where slight variations in input prompts can lead to significant differences in output quality [\(Lu et al., 2021;](#page-11-1) [Madaan & Yazdanbakhsh, 2022;](#page-11-2) [Zhao et al.,](#page-12-0) [2021;](#page-12-0) [Reynolds & McDonell, 2021;](#page-11-3) [Wei et al., 2022;](#page-11-4) [Kojima et al., 2022\)](#page-10-2). Consequently, prompt design has emerged as a critical factor in achieving optimal LLM performance. As the popularity of LLMs has surged, "Prompt Engineering" has become a focal point of attention in the field. Traditionally, this process has been carried out by domain experts who iteratively query expensive LLMs until the desired response is obtained. However, this manual approach is time-consuming and resource-intensive, prompting researchers to explore more efficient alternatives. Recent research has focused on Automated Prompt Engineering [\(Zhou et al., 2022\)](#page-12-1), which aims to systematically search for prompts that improve target task performance. Following this line of research, [\(Pryzant et al.,](#page-11-5) [2023;](#page-11-5) [Ye et al., 2023\)](#page-12-2) improved upon it by resorting to computationally expensive stronger LLMs to reason about failure causes in smaller, efficient LLMs deployed in practical tasks. [Pryzant et al.](#page-11-5) [\(2023\)](#page-11-5) termed this feedback as "textual gradient", since this feedback is leveraged to improve the prompts iteratively.

Figure 1: Comparison of textual feedback-based prompt optimization and GREATER. Left: textual feedback relies entirely on a larger language model's judgments. Right: GREATER avoids external large, proprietary models, using token suggestions from a small model and guiding prompt token selection with loss gradients. GREATER incorporates model reasoning by first generating reasoning, then applying an extraction prompt to obtain answer logits for computing loss gradients. This "gradient over reasoning" approach optimizes using direct signals rather than relying on language model feedback.

Despite showing promising performance, the primary limitation of this category of prompt optimization is the reliance on massive LLMs like GPT-4 for optimizing smaller model performance. Smaller LLMs used in practice rely on large models like GPT-4 for optimization, as these big models generate the "textual gradients" needed to refine and transfer knowledge. [\(Zhang et al., 2024\)](#page-12-3) found that smaller LMs are incapable of generating such optimization feedback, further emphasizing the dependence on large models. Thus, enhancing smaller models depends on the computational power of larger ones. Additionally, the optimization process increases computational costs due to the need for sizeable prompt length due to multiple task samples, and heavy dependence on the optimizer LLM's judgment may result in less reliable outcomes.

To mitigate these issues, we propose GREATER that allows smaller LLMs to optimize prompts using true gradients (i.e., numerical loss gradients) without resorting to larger models. Figure [1](#page-1-0) (right) gives an overview of our approach. GREATER leverages *"gradient over reasoning"* for more accurate prompt improvement direction. GREATER first calculates the forward token probabilities to generate a small number of probable token candidates at the selected position conditioned on the input. Then, it utilizes the LLM to generate the reasoning for problem solution, and extracts the final answer logits for calculating the loss. Finally, we leverage the gradient calculated for the probable token candidates to select the best tokens for optimization. Our technique innovates by tackling token discreteness while integrating reasoning chains, crucial for limited datasets like Big Bench Hard [\(Suzgun et al., 2022\)](#page-11-6), which provide final labels without explicit reasoning paths.

GREATER shows strong prompt optimization performance, where optimized prompt often delivers performance equivalent to larger LLMs in solving the task. In our experiments, we selected Llama-3-8B-Instruct [\(Meta, 2024\)](#page-11-7) and Gemma-2-9B-it [\(Team et al., 2024\)](#page-11-8), two highly popular smaller language models that are proven to be also very useful in solving different tasks. Across a wide variety of selected BBH [\(Suzgun et al., 2022\)](#page-11-6) tasks, mathematical reasoning task GSM8k, and first-order logic task, FOLIO [\(Han et al., 2022\)](#page-10-3), GREATER shows up to 8.9% performance improvement over SOTA prompt optimization technique on average in BBH suite of tasks. Moreover, GREATER optimized prompts perform on par or better than GPT-4 optimized prompts [\(Ye et al., 2023\)](#page-12-2), demonstrating superior performance without resorting to larger proprietary LLMs.

2 RELATED WORK

LLMs as Prompt Optimizers. Recently, significant attention has been brought to the prospect of LLMs as prompt optimizers for less powerful models. This line of work was first proposed by [Zhou](#page-12-1) [et al.](#page-12-1) [\(2022\)](#page-12-1) by prompting LLMs with input-output pairs to infer the instruction. [Pryzant et al.](#page-11-5) [\(2023\)](#page-11-5) formalized the term "textual gradient" to refer to textual feedback based optimization. Here the authors introduced the use of mini-batches of data to create a natural language feedback. These

gradients critique the current prompt, mimicking the role of numerical gradient in optimization. Later, a large body of works has improved upon it by using optimization logic in text space [\(Yang](#page-12-4) [et al., 2023;](#page-12-4) [Yuksekgonul et al., 2024\)](#page-12-5), meta-prompt engineering [\(Ye et al., 2023\)](#page-12-2), agent-based learning and reasoning [\(Wang et al., 2023;](#page-11-9) [Liu et al., 2024;](#page-11-10) [Shinn et al., 2024\)](#page-11-11), external trained model [\(Cheng et al., 2023\)](#page-10-4), evolutionary algorithms [\(Guo et al., 2023;](#page-10-5) [Liu et al., 2024\)](#page-11-10), etc. [Hu](#page-10-6) [et al.](#page-10-6) [\(2024\)](#page-10-6) introduced ZOPO, leveraging Gaussian processes inspired by the Neural Tangent Kernel to systematically explore local optima in prompt optimization using zeroth-order methods. Other approaches like programming model [\(Khattab et al., 2023\)](#page-10-7), editing [\(Prasad et al., 2022\)](#page-11-12), and reinforcement learning [\(Deng et al., 2022\)](#page-10-8) are also notable. These techniques usually rely on reasoning and judgment from larger LMs to improve the performance of smaller LMs. In other words, the larger model can share its knowledge through the optimized prompt which helps smaller models achieve performance uplift. Therefore, to get strong results with smaller, more lightweight language models, prompts must be optimized using powerful, expensive, closed-source models, as smaller models are inadequate at this optimization on their own [\(Zhang et al., 2024\)](#page-12-3).

Prompt Tuning. Prompt-tuning has been explored in prior works as task-specific continuous vectors tuned by gradient-based methods to improve task performance [\(Li & Liang, 2021;](#page-10-9) [Lester et al.,](#page-10-10) [2021;](#page-10-10) [Qin & Eisner, 2021;](#page-11-13) [Gao et al., 2020\)](#page-10-11). Discrete prompts on the other hand involve searching for discrete vocabulary tokens through gradients [\(Shin et al., 2020;](#page-11-14) [Shi et al., 2022\)](#page-11-15). These approaches can be further extended for visual prompt tuning [\(Wen et al., 2024\)](#page-11-16), where the authors optimize hard text based prompts through efficient gradient-based optimization. A fundamental flaw in these methods stems from the fact that these methods are typically only suitable for classification tasks or tasks with fixed input-output structures, as they rely on predefined templates and verbalizers. Reasoning tasks on the other hand require complex analytical reasoning chains, e.g., Big-Bench-Hard [\(Suzgun et al., 2022\)](#page-11-6), which leads to the final output, where using a fixed template verbalizer is incompatible and impractical.

Jailbreaking LLMs. Gradient-based search methods have also been applied to find trigger prompts that bypass LLM alignment-based filtering and generate harmful responses [\(Zou et al.,](#page-12-6) [2023\)](#page-12-6). These methods have been further refined to improve readability and effectiveness by including perplexity regularization and constrained-decoding [\(Guo et al., 2021;](#page-10-12) [Alon & Kamfonas, 2023;](#page-10-13) [Liu et al., 2023;](#page-11-17) [Guo et al., 2024\)](#page-10-14). Similar to prompt tuning, these methods also adhere to a simple input-output structure. The target output typically is an affirmative response *"Sure here is"*, without emphasis on the reasoning chain.

3 PROBLEM DEFINITION

We formally define the problem of prompt optimization to lay the foundation of the optimization target. Given a language model f_{LLM} , and a small representative task dataset, \mathcal{D}_{task} $\{(x_1, y_1), \ldots (x_n, y_n)\}\)$, the goal of prompt optimization is to find a prompt p^* such that:

$$
p^* = \underset{p}{\arg \max} \sum_{(x,y) \in \mathcal{D}_{task}} m\left(f_{\text{LLM}}(x;p), y\right) \tag{1}
$$

where $f_{\text{LLM}}(x; p)$ is the output from task language model f_{LLM} upon channeling the input x with the prompt p, and $m(\cdot)$ is the evaluation function for this task.

Textual Feedback Based Prompt Optimization. As shown in the left part of Figure [1,](#page-1-0) to search for p^* , previous prompt optimization methods based on textual feedback use an optimizer model $f_{\text{optimizer}}$ which is usually substantially larger and more expensive than f_{LLM} [\(Zhou et al., 2022;](#page-12-1) [Ye](#page-12-2) [et al., 2023;](#page-12-2) [Pryzant et al., 2023\)](#page-11-5). Conceptually, $f_{\text{optimizer}}(m(f_{\text{LLM}}(x;p), y)|(x, y) \in \mathcal{D}_{task})$ drives the optimization process by assessing and providing feedback for refining the prompt. Therefore, finding p^* primarily relies on the capabilities of $f_{\text{optimizer}}$ and its hypothesis for prompt refinement.

4 OUR METHOD

While Section [3](#page-2-0) provides the formal explanation of prompt optimization, it's important to understand the role of reasoning in this process. A well-crafted prompt gives clear problem-solving instructions

Figure 2: Overall workflow of GREATER. (i) The language model f_{LLM} generates token candidates by conditioning on input samples. (ii) f_{LLM} uses task input and current prompt to generate reasoning and extract final answer logits. (iii) The logits are used to calculate loss and compute gradient over generated reasoning with respect to the candidate tokens. These gradients determine the selection of candidate token to update the current position of the current prompt.

that guide the language model to think through the problem in a specific way, helping it arrive at a valid answer. Our method, GREATER, is built on this principle. As shown in Figure [2,](#page-3-0) GREATER begins by analyzing task examples to propose potential token candidates, essentially exploring different ways to solve the task. The task input and prompts are then used to generate reasoning steps, from which the final answer and loss are extracted. By applying gradients over the generated reasoning, GREATER refines the candidate selection, ensuring it follows the optimal path for improved performance.

4.1 METHOD OVERVIEW

Given an input x and a prompt $p = [p_1, p_2, p_3, \ldots]$ consisting of several tokens p_i , f_{LLM} generates the reasoning chain, $r \sim f_{\text{LLM}}(x \odot p)$ for the input (⊙ for concatenation). Then, we can extract the final answer from r by prompting f_{LLM} with a formatted extractor prompt p_{extract} , e.g., *"Therefore, the final answer (\$NUMBER\$) is \$"*. Consequently, this produces the final answer logits, $y' =$ $f_{\text{LLM}}(x \odot p \odot r \odot p_{\text{extract}})$. We define our loss function as:

$$
\mathcal{L} = \mathcal{L}_{CE} \bigg(f_{\text{LLM}} \bigg(x \odot p \odot r \odot p_{\text{extract}} \bigg), y \bigg) \tag{2}
$$

In Eq. [2,](#page-3-1) for a fixed p_{extract} and x, only p will affect the loss; therefore we can calculate $\frac{\partial \mathcal{L}}{\partial p}|_{x, p_{\text{extract}}}$ This loss gradient takes the reasoning into account, making it a more direct signal to drive the prompt optimization process. Therefore, this "gradient over reasoning" can be a highly potent alternative to current textual feedback based prompt optimization that entirely relies on massive LLM feedback. Note that, in Eq. [2,](#page-3-1) the entire chain is equivalent to one single forward pass through f_{LLM} , since key, values from reasoning generation can be cached and utilized during logit extraction.

We sequentially apply GREATER optimization in each token position p_i of p. GREATER first employs a *Candidate Proposal* (Section [4.2\)](#page-3-2) stage, where it uses language model-guided forward probabilities to generate potential token candidates for optimized prompt. Subsequently, the current prompt is channeled through LLM, f_{LLM} for solution generation, and then answer logits extraction (Section [4.3\)](#page-4-0). Using these logits, we can calculate the loss and gradient with respect to the small number of prompt token candidates which we use for token selection. (Section [4.4\)](#page-5-0). This process can be applied over all the prompt token positions repeatedly.

In the following subsections, we discuss each stage of GREATER to optimize prompt token p_i at position i. Algorithm [1](#page-4-1) shows all the steps in GREATER. This process is sequentially applied over all the positions repeatedly until convergence.

4.2 PROMPT TOKEN CANDIDATE PROPOSAL

For optimizing prompt token p_i , we first leverage the task language model (LM) f_{LLM} probabilities to propose candidates for the position. For a sample input $x_j \in \mathcal{D}_{task}$, we can calculate the top-k probabilities for candidate token proposals:

$$
\text{cand}_{i,j} = \text{top-}k \left[f_{\text{LLM}}(\cdot | x_j \odot p_1, p_2, \dots, p_{i-1}) \right] \tag{3}
$$

Algorithm 1 GREATER

Therefore, we take top-k tokens from f_{LLM} conditioning on x_j followed by the previous tokens from the optimized prompt. We calculate cand_{i,j} for a randomly sampled set of q inputs, $\mathcal{D}_q \subset \mathcal{D}_{\text{task}}$. Since we want the token candidates to be relevant for all samples in the task, token candidates for position i will incorporate candidates for all samples, so

$$
candidates_i = \bigcap_{x_j \in \mathcal{D}_q} \text{cand}_{i,j} \tag{4}
$$

Equation [4](#page-4-2) gives candidates_i, a set of promising token candidates for position i. Since candidates_i are suggested by LM and conditioned on the inputs, they are representative of the problem domain and more interpretable. Therefore, gradient mass will be calculated only for a small number of promising token candidates, ϵ_i , preventing it from being dispersed over the entire vocabulary.

One-Hot Token Indicators. As shown in Figure [2](#page-3-0) (i), a one-hot token indicator ϵ_i is created for only candidates_i and the current token p_i , with a value of one only for p_i and zeros for all other candidates. Concurrently, from the original LM embedding table, we extract only the rows that correspond to ϵ_i to create a subset of the original embedding table, E. This table is then multiplied by the one-hot indicator ϵ_i , allowing the input to be passed through f_{LLM} .

4.3 REASONING GENERATION AND EXTRACTION

A straightforward way of calculating loss and subsequently taking gradient over it is to only consider the output of $f_{\text{LLM}}(x \odot p)$ and taking cross-entropy loss of the output token to that of the ground truth. However, this completely ignores the role of reasoning as discussed before, whereas modern language models require the generation of a complex reasoning chain to generate correct output [\(Wei et al., 2022\)](#page-11-4). Therefore, simply considering $f_{LLM}(y|x \odot p)$ would give us the wrong objective to optimize, which in turn will give incorrect gradient information.

Consequently, in this stage, we first generate a reasoning $r \sim f_{\text{LLM}}(x \odot p)$. In r, the language model generates reasoning to derive the final answer. To compute the loss accurately, we must extract the answer logits and compare with the ground truth label. A simple way to do that is to get f_{LLM} logits when conditioned on the input, reasoning, followed by a formatted extractor prompt, p_{extract} .

$$
\hat{y} = f_{\text{LLM}}(x \odot p \odot r \odot p_{\text{extract}}) \tag{5}
$$

Equation [5](#page-4-3) results in LM logits that consider the reasoning generated from the current prompt p . Therefore, it better represents the reasoning chain making it suitable for loss calculation.

4.4 GRADIENT OVER REASONING DRIVEN CANDIDATE SELECTION

Equation [5](#page-4-3) gives us the logits \hat{y} that incorporate reasoning chain information originating from current p . Therefore, we can optimize the cross-entropy loss as below. Additionally, we add the perplexity regularization term \mathcal{L}_{perpl} to promote the interpretability of the optimized prompt similar to [\(Zou](#page-12-6) [et al., 2023;](#page-12-6) [Guo et al., 2024\)](#page-10-14).

$$
\mathcal{L}_{\text{CE}} = \text{cross_entropy}(\hat{y}, y), \mathcal{L}_{\text{perpl}} = \exp\left(-\frac{1}{|p|} \sum_{i=1}^{|p|} \log f_{\text{LLM}}(p_i \mid x, p_{\leq i})\right), \mathcal{L} = \mathcal{L}_{\text{CE}} + \lambda \mathcal{L}_{\text{perpl}}
$$
(6)

However, the perplexity term is less important in our case given that we are optimizing only over the top-k candidates suggested by the LM. Consequently, the candidate proposal stage handles most of the interpretability duties.

Upon calculating the loss \mathcal{L} , we can do a backward pass to calculate the gradient over the generated reasoning with respect to one-hot token indicator ϵ_i . As $\frac{\partial \mathcal{L}}{\partial \epsilon_i}$ gives us the gradient directions for each of the token candidates in Equation [4,](#page-4-2) the token replacement at position i is given by:

$$
p_i = \text{token}[\arg \max_{\epsilon_i}(-\frac{\partial \mathcal{L}}{\partial \epsilon_i})]
$$
\n(7)

In practice, we select the top-three candidate tokens with the highest negative gradients and evaluate the token replacement with a forward pass on the training set. This ensures the robustness of the replacement selection process leading to higher performance from optimization.

5 EXPERIMENTS

In this section, we demonstrate that GREATER is highly effective in prompt optimization delivering substantial performance improvement across different tasks. Section [5.1](#page-5-2) describes the experiment setup. Section [5.2](#page-6-0) presents the main results of the GREATER performance with smaller language models. In Section [5.3,](#page-6-1) we compare GREATER prompts optimized by smaller language models against the prompts optimized by larger proprietary language models using state-of-the-art baseline methods. Section [5.4](#page-6-2) performs an ablation study on the effectiveness of gradient over reasoning in GREATER. Section [5.5](#page-7-0) demonstrates the transferability of GREATER prompts. Section [5.6](#page-8-0) shows some case studies.

5.1 EXPERIMENT SETUP

Datasets. To evaluate the efficacy of our approach, we use **GSM8K** [\(Cobbe et al., 2021\)](#page-10-15), **Big-**Bench-Hard (BBH) [\(Suzgun et al., 2022\)](#page-11-6), and FOLIO [\(Han et al., 2022\)](#page-10-3) benchmark datasets for diverse reasoning tasks in mathematics, commonsense, and logical reasoning. For GSM8K, we used the same test split as [\(Cobbe et al., 2021\)](#page-10-15). For BBH, we used the similar split setting as [\(Yuksekgonul](#page-12-5) [et al., 2024\)](#page-12-5). For FOLIO, we evaluate the natural language reasoning with the first-order logic task for the evaluation which also requires complex reasoning capabilities. We used the natural language reasoning task with premises text, conclusion text to infer the labels, and we use the validation set of the updated version of $FOLIO¹$ $FOLIO¹$ $FOLIO¹$. More details about these are given in Appendix [A.1.](#page-12-7)

Models. To demonstrate that our approach can generalize to different backbone language models, we choose two strong and widely-used open-source language models: **Llama-3-8B** [\(Meta, 2024\)](#page-11-7) and Gemma-2-9B [\(Team et al., 2024\)](#page-11-8). For both models, we use the instruction tuned versions 2^3 2^3 .

¹ https://huggingface.co/datasets/yale-nlp/FOLIO

² https://huggingface.co/meta-llama/Meta-Llama-3-8B-Instruct

³ https://huggingface.co/google/gemma-2-9b-it

Table 1: Overall results. GREATER brings substantial performance improvements across different reasoning tasks, demonstrating its efficacy in prompt optimization with smaller models. It considerably outperforms state-of-the-art prompt optimization methods. Detailed prompts and results with breakdown across all the tasks are shown in Appendix [H](#page-16-0) and Appendix [I.](#page-23-0)

Baselines. We compare with state-of-the-art prompt optimization baselines: APE [\(Zhou et al.,](#page-12-1) [2022\)](#page-12-1), APO [\(Pryzant et al., 2023\)](#page-11-5), PE2 [\(Ye et al., 2023\)](#page-12-2), TextGrad [\(Yuksekgonul et al., 2024\)](#page-12-5) where we use them on Llama-3-8B and Gemma-2-9B for optimization. In addition, we also show the efficacy of our approach by comparing against the prompts optimized by massive proprietary LLMs (e.g., GPT-4, PaLM-2-L) using APE, APO, PE2, TextGrad, OPRO [\(Yang et al., 2023\)](#page-12-4), Evo-Prompt [\(Guo et al., 2023\)](#page-10-5).

5.2 OVERALL RESULTS

We evaluate the performance of GREATER in comparison to state-of-the-art baselines, including APE, APO, PE2, TextGrad, and the original zero-shot chain-of-thought approach [\(Kojima et al.,](#page-10-2) [2022\)](#page-10-2), across the GSM8K, BBH, and FOLIO benchmarks. Table [1](#page-6-3) highlights the significant and consistent improvements achieved by GREATER over state-of-the-art prompt optimization methods, especially when optimizing prompts using lightweight language models. Across both Gemma-2-9B and Llama-3-8B, GREATER demonstrates remarkable stability and outperforms the baselines. This is particularly noteworthy given the high variability in performance seen in these textual feedback methods, which tend to be unreliable with smaller models due to increased prompt sensitivity. For instance, while TextGrad performs reasonably well on BBH with Gemma-2-9B, it falters significantly with Llama-3-8B. In contrast, GREATER delivers outstanding results across the board, excelling across diverse tasks. Note that, in the FOLIO dataset, GREATER performs on par with PE2 [\(Ye et al., 2023\)](#page-12-2), suggesting that the model has likely reached its performance ceiling, leaving minimal room for further improvement.

5.3 COMPARISON WITH PROMPTS OPTIMIZED BY LARGER PROPRIETARY MODELS

Besides optimization performance in lightweight language models, we also evaluate the efficacy of GREATER optimized prompt compared with the prompts optimized by massive LLMs. These massive models, like GPT-4 and PaLM-2-L, inherently possess deeper knowledge of complex reasoning tasks and often provide richer guidance in their optimized prompts, making them strong baselines to compare with. In Table [2,](#page-7-1) we compare the performance of GREATER optimized prompt to that of APE (optimized by GPT-4), APO (optimized by GPT-4), PE2 (optimized by GPT-4), OPRO (optimized by PaLM-2-L), EvoPrompt(optimized by GPT-3.5). We use GSM8K, and five randomly selected tasks from BBH to compare the performance of these prompts. We see that in both Llama-3- 8B and Gemma-2-9B, GREATER optimized prompts perform substantially better and robustly compared to the baseline prompts optimized with massive LLMs. The consistency in performance uplift makes GREATER a viable choice to boost task performance in reasoning tasks with lightweight language models.

5.4 ABLATION OF GRADIENT OVER REASONING

As outlined in Section [4.3](#page-4-0) and Section [4.4,](#page-5-0) a core feature of GREATER is the concept of *Gradient Over Reasoning*. Conventional gradient-based optimization methods rely solely on the target answer labels to compute the loss and gradients, overlooking the crucial role that reasoning

Table 2: Comparison of GREATER with prompts optimized by larger proprietary LLMs. GREATER performs on par with or notably better than prompts optimized by GPT 4 and PaLM-2-L across GSM8K and five randomly chosen BBH tasks using Llama-3-8B and Gemma-2-9B. EvoPrompt does not report its prompts on GSM8K. Here, *Target Model: Llama-3-8B* and *Method (Optimized by): APE (GPT-4)* indicates that Llama-3-8B was used for prompt evaluation while the prompt was optimized by GPT-4 with APE.

Target Model	Method (Optimized by)	GSM8K	BBH (5 randomly chosen tasks)						
			movie_rec.	object_count.	tracking_five.	hyperbaton	causal	Average	
	APE (GPT-4)	80.7	50	82	50	76	56	62.8	
æ,	EvoPrompt (GPT-3.5)		48	74	42	68	48	56.0	
	APO (GPT-4)	81.1	56	68	49	75	51	59.8	
L lama -3	PE2 (GPT-4)	81.5	48	82	45	79	49	60.6	
	OPRO (PaLM-2-L)	82.3	60	78	40	70	57	61.0	
	GREATER (Llama-3-8B)	82.6	57	90	70	84	57	71.6	
	APE (GPT-4)	89.2	48	61	83	83	60	67.0	
ą6- Genma-2	EvoPrompt (GPT-3.5)		51	70	82	83	61	69.4	
	APO (GPT-4)	89.3	52	84	72	82	59	69.8	
	PE2 (GPT-4)	89.6	50	65	71	84	64	66.8	
	OPRO (PaLM-2-L)	89.0	50	58	76	81	58	64.6	
	GREATER (Gemma2-9B)	89.4	56	87	85	88	61	75.4	

Llama-3-8B: Impact of Gradient Over Reasoning Gemma-2-9B: Impact of Gradient Over Reasoning

Figure 3: Ablation study on "Gradient Over Reasoning" in GREATER. Gradient calculation without reasoning causes notable performance drops, showing the importance of reasoning for gradients.

plays in this process. To highlight the significance of incorporating reasoning into gradient calculations, we conducted a comparative analysis of GREATER with and without applying *Gradient Over Reasoning*, while keeping all other steps identical. For this experiment, we optimized with both Llama-3-8B and Gemma-2-9B on two BBH tasks: movie recommendation and tracking shuffled objects five objects task. Figure [3](#page-7-2) shows the comparison between with and without *gradient over reasoning*. It clearly demonstrates a substantial performance drop when *Gradient Over Reasoning* is omitted. Fundamentally, from Equation [5,](#page-4-3) removing the reasoning generation part r equates to calculating an incorrect objective function, which will drive gradient-based token selection to diverge from the optimal solution.

5.5 PROMPT TRANSFERABILITY

We conduct further experiments to evaluate the transferability of GREATER optimized prompt. In Section [5.5.1,](#page-8-1) we first evaluate the transferability of GREATER prompt between two smaller language models, Llama-3-8B and Gemma-2-9B, by evaluating the performance of Gemma-2-9B optimized prompts on Llama-3-8B, and vice-versa. Next, in Section [5.5.2,](#page-8-2) we evaluate the transferability of prompts from a smaller model (Llama-3-8B) to a much larger model (Gemma-2-27B).

Target	Method (Optimized by)	BBH (5 randomly chosen tasks)						
Model		movie_rec.	object_count.	tracking five.	hyperbaton	causal_judgement	Average	
		Llama-3-8B \rightarrow Gemma-2-9B						
	TextGrad (Llama-3)	53	78	56	84	63	66.8	
	APO (Llama-3)	53	84	68	84	58	69.4	
	PE2 (Llama-3)	54	84	68	82	60	69.6	
Gemma-2-9B	GREATER (Llama-3)	55	90	85	91	60	76.2	
	APO (GPT-4)	52	84	72	82	59	$\overline{69.8}$	
		Gemma-2-9B \rightarrow Llama-3-8B						
8B	TextGrad (Gemma-2)	35	29	49	65	36	42.8	
Llama-3-	APO (Gemma-2)	54	69	48	71	53	59.0	
	PE2 (Gemma-2)	56	69	49	50	53	55.4	
	GREATER (Gemma-2)	58	87	56	70	52	64.6	
	APO (GPT-4)	36	68	49	75	51	39.8	

Table 3: Transferability of Llama-3-8B optimized prompts to Gemma-2-9B (Upper) and vice versa (Lower). The results demonstrate that prompts produced by GREATER exhibit strong transferability compared with those produced by other state-of-the-art prompt optimization methods.

Table 4: Transferability of Llama-3-8B optimized prompts to Gemma-2-27B. The results demonstrate that GREATER optimized prompts exhibit strong transferability from smaller to larger language models.

Target	Method (Optimized by)	BBH (5 randomly chosen tasks)						
Model		movie_rec.	object_count.			tracking five. hyperbaton causal judgement	Average	
		Llama-3-8B \rightarrow Gemma-2-27B						
27B	PE2 (Llama-3)	59	92	83		54	72.2	
\sim	APO (Llama-3)	53	92	83	72	58	71.6	
	Ours (Llama-3)	59	91	86	82	57	75.0	
	\overline{APO} (GPT-4)	64	92	81		58	74.4	

5.5.1 TRANSFER BETWEEN GEMMA-2 AND LLAMA-3

As shown in Table [3,](#page-8-3) GREATER exhibits exceptional transferability across smaller models compared to other methods. Notably, prompts optimized by GREATER significantly outperform even APO prompts, which were optimized using GPT-4, as reported by [Pryzant et al.](#page-11-5) [\(2023\)](#page-11-5). This distinction is particularly important, as it highlights that GREATER optimized prompts are not only more effective but also better suited for broader, more generalized use across smaller models. These results clearly emphasize the efficacy and versatility of our approach.

5.5.2 TRANSFER TO LARGER MODELS

To assess the transferability of GREATER-optimized prompts to much larger models, we evaluated their efficacy using the Gemma-2-27B model. As demonstrated in Table [4,](#page-8-4) the GREATER-optimized prompts continue to exhibit strong performance when compared to baseline methods. However, a notable observation is that the performance gap between GREATER and the baselines narrows as the model size increases. Additionally, we notice that APO GPT-4 optimized prompts yield similar performance with GREATER across various tasks, often resulting in closely matched outcomes.

Tables [3](#page-8-3) and [4](#page-8-4) reveal that optimized prompts enable smaller models to achieve performance comparable to larger ones, highlighting an efficient approach to maximize model capabilities without relying on resource-intensive models.

5.6 CASE STUDY

One of the key characteristics of GREATER is that the generated prompts tend to be more varied and innovative compared to the textual feedback-based SOTA baselines. As noted in Table [11](#page-0-0) and Table [14,](#page-0-0) the optimized prompts from traditional approaches are often verbose variations of the original query or standard Chain of Thought (CoT) prompts. In contrast, GREATER prompts frequently Table 5: Example prompts (abridged) generated by GREATER and APO. GREATER prompts guide structured ways to solve tasks, leading to improved task performance compared to traditional Chain of Thought (CoT) prompts and their variations often generated by textual feedback-based optimization methods like APO. More examples can be found in the Appendix [H](#page-16-0) and [I.](#page-23-0)

provide highly insightful guidelines that better aid in problem-solving. Table [5](#page-9-0) demonstrates a selection of abridged prompts generated by GREATER and APO. For tasks like formal fallacies and causal understanding, GREATER prompts encourage logical analysis rather than mere languagebased reasoning, which enhances performance. Similarly, in the object counting and navigate tasks, the prompts simplify the original problem by converting it into a more straightforward mathematical task, leading to significant improvements. More interestingly, in the sports understanding task, the prompt promotes agentic behavior, encouraging the model to take an active role in solving the task. Additionally, for multistep arithmetic two, the prompt focuses on parentheses to avoid errors in computation, in date understanding task it instructs to convert into a programming problem (by using Excel formula), and in reasoning about colored objects focuses on logical analysis. These prompts are comparatively more interesting than prompts generated by textual feedback (e.g. APO) where most prompts only show verbose instruction regarding the original question, without any guidance of how to solve the problem. They also demonstrate that GREATER prompts do more than just provide basic instructions—they offer clear and practical strategies tailored to each task. By helping the model think about problems in a more structured and systematic way, GREATER leads to better problem-solving and improved performance compared to traditional methods.

While GREATER generates highly effective and innovative prompts, they may occasionally exhibit minor grammatical issues or a more informal tone compared to standard prompts. For instance, the navigate task and multistep arithmetic two task in Table [5](#page-9-0) reflect such characteristics. However, these issues can be mitigated by adjusting the Top- k parameter in Equation [3.](#page-3-3) Incorporating dynamic Top- k selection could further enhance the naturalness and accuracy of the prompts.

6 CONCLUSION

We present GREATER, a novel gradient-guided prompt optimization technique that enhances performance without relying on massive proprietary LLMs. GREATER proposes token candidates using sample inputs, generates reasoning, and extracts final answer logits to compute loss and gradients. This "Gradient over Reasoning" provides a strong signal for selecting optimal candidates, enabling significant performance gains on tasks like BBH, GSM8K, and FOLIO, outperforming state-of-theart textual feedback-based methods for smaller models. Additionally, GREATER prompts demonstrate notable transferability across smaller models and often match the performance of larger models. Future directions include integrating GREATER with textual feedback-based methods for more robust and effective prompt optimization.

ACKNOWLEDGMENT

This work is supported in part by NSF grant 2338418.

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A BENCHMARK DATASETS, MODELS, AND BASELINES

In this section, we discuss the details of Datasets, Models, and Baselines.

A.1 DATASETS

As discussed in Section [5.1,](#page-5-2) we use GSM8K [\(Cobbe et al., 2021\)](#page-10-15), BBH [\(Suzgun et al., 2022\)](#page-11-6), and FOLIO [\(Han et al., 2022\)](#page-10-3) datasets. For GSM8K, we used 100/100 for train/dev set, and original test set of 1319 size. Then, for BBH datasets, we used 21 selected BBH tasks as in Table [11](#page-0-0) and Table [14.](#page-0-0) This covers almost all types of tasks in BBH dataset. We skip word sorting and dyck languages tasks from our evaluation since we found that the smaller LLM outputs are very difficult to reliably evaluate due to highly inconsistent output pattern. Finally, for logical deduction and tracking shuffled objects, we select five objects tasks as representative of the tasks. For all tasks we use 50/100/100 train/dev/test splits similar to [\(Yuksekgonul et al., 2024\)](#page-12-5).

Finally for the FOLIO dataset, we used the latest version of FOLIO [\(Han et al., 2022\)](#page-10-3) for our evaluation. We use the natural language reasoning task with premises text, conclusion text to infer the labels. The original validation split (203 rows) are used for the evaluation of FOLIO, whereas 50/100 samples are taken for train and dev set respectively out of the original train split.

A.2 MODELS

As described in experimentation setup, we only used Llama-3-8B-Instruct and Gemma-2-9B-it in our experiments due to their smaller footprint and strong performance. However, in several tasks Gemma-2-9B-it shows markedly stronger performance than Llama-3-8B, although the memory requirements for Gemma-2-9B-it is substantially higher. As we have shown, stronger models get lesser benefit from prompt optimization, as good prompts only offset for lower capabilities of weaker models. Across our experiments, we also notice substantial improvement in Llama-3-8B-Instruct, whereas the margin gets narrower for the stronger Gemma-2-9B-it.

A.3 BASELINES

Our primary baselines are APO [\(Pryzant et al., 2023\)](#page-11-5), iterative APE [\(Kojima et al., 2022\)](#page-10-2), PE2 [\(Ye et al., 2023\)](#page-12-2), TextGrad [\(Yuksekgonul et al., 2024\)](#page-12-5). For APO, iterative APE, and PE2 we use the original implementation by [\(Ye et al., 2023\)](#page-12-2) for benchmarking. And we used TextGrad's own library for evaluating their results. Other than that, we also compared against original Zero-Shot CoT [\(Wei](#page-11-4) [et al., 2022\)](#page-11-4), and the larger model optimized reported prompts from APE, APO, PE2, OPRO [\(Yang](#page-12-4) [et al., 2023\)](#page-12-4), EvoPrompt [\(Guo et al., 2023\)](#page-10-5).

B ADDITIONAL EXPERIMENTATION DETAILS

As shown in Algorithm [1,](#page-4-1) we run GREATER for $T = 105$ steps with $k = 10$ for top-k, $q = 5$ and $\lambda = 0.2$ (in Eq. [6\)](#page-5-6). While Algorithm [1](#page-4-1) shows fixed length prompt optimization, we allow dynamic prompt. To attain that, we look for the presence of ending token in the last position. If no ending token is found, we continue the optimization process by adding a placeholder token and optimizing over it. As ending token is encountered we move over to the first position for optimization. We run all our experiments on 2X NVIDIA A100 80GB GPUs.

C PERFORMANCE COMPARISON WITH OTHER GRADIENT-BASED METHODS

GREATER leverages the Gradient Over Reasoning chain to identify the optimal prompt required for enhancing task performance. Previous works, such as [Shin et al.](#page-11-14) [\(2020\)](#page-11-14), utilized gradient-guided search to discover trigger tokens for improving performance in relatively straightforward tasks like sentiment analysis and natural language inference. This concept has also been extended to textto-image tasks by incorporating gradient-based learning in embedding spaces [\(Wen et al., 2024\)](#page-11-16). However, these approaches are limited to simpler tasks and fail to address tasks requiring complex reasoning. As demonstrated in Table [6,](#page-13-0) GREATER-optimized prompts deliver a substantial performance boost compared to prior methods that do not incorporate the reasoning chain.

Table 6: Comparison of performance in movie recommendation and tracking shuffled objects five objects for prompts optimized on Llama-3-8B and Gemma-2-9B. The results demonstrate that prompts optimized by GREATER outperform other methods across both models.

D COMPLEXITY COMPARISON: GREATER VS. TEXT-BASED FEEDBACK **APPROACHES**

Assume each sample contains L input-output tokens on average.

FOR GREATER

- Operations Per Sample:
	- Forward Pass: $O(L^2)$
	- Backward Pass: $O(L^2)$
- Total Complexity:
	- $-$ For N samples, one forward pass, and one backward pass are performed per sample in a single iteration.
	- Total complexity:

$$
N \cdot O(L^2) = O(NL^2)
$$

FOR TEXT-BASED FEEDBACK APPROACHES

• Overview:

- No backpropagation stage.
- $-$ Each iteration involves, evaluating all samples, identifying incorrect samples (n) incorrect samples), and chaining incorrect samples into a single sequence to generate feedback.
- Complexity Breakdown:
	- First Forward Pass:

$$
O(NL^2)
$$

- Feedback Generation:
	- $*$ Incorrect samples (n) are chained together.
	- * Chained length: $n \cdot L$.
	- * Feedback generation complexity:

$$
O((nL)^2) = O(n^2L^2)
$$

• Total Complexity:

$$
O(NL^2) + O(n^2L^2)
$$

- Behavior Based on Task Difficulty:
	- Simple Tasks $(n \rightarrow 0)$:

Total Complexity
$$
\rightarrow O(NL^2)
$$

– Difficult Tasks $(n \rightarrow N)$:

Total Complexity
$$
\rightarrow O(NL^2) + O(N^2L^2) = O(N^2L^2)
$$

COMPARISON

- GreaTer Complexity: $O(NL^2)$ (consistent).
- Text-Based Feedback Complexity: Can scale up to $O(N^2L^2)$.

This complexity difference is also translated into real-world performance. In *movie recommendation task, GREATER is required to be optimized for* \sim 5 hours, whereas TextGrad [\(Yuksekgonul et al., 2024\)](#page-12-5) required a total of ∼14 hours for prompt optimization in our own setup.

E PROMPT OPTIMIZATION VS. FEW-SHOT IN-CONTEXT LEARNING

In-context learning has proven to be highly effective for reasoning tasks in large language models. This raises the question of whether prompt optimization provides any advantages over in-context learning for smaller models. In Figure [4,](#page-14-0) we compare the performance of fiveshot in-context learning with zeroshot reasoning using an optimized prompt from GREATER in Llama-3-8B-Instruct. The results demonstrate that GREATER offers a significant performance improvement over five-shot reasoning. Moreover, using an optimized prompt eliminates the need for repeated

Figure 4: Efficacy of GREATER in zero-shot setting compared to five-shot inference with Llama-3-8B-Instruct.

input-output examples during inference, leading to greater efficiency.

Table 7: Impact of Initialization Prompt. We can see that different initialization has resulted in different optimized prompt, however they offer comparable performance.

Table 8: Performance comparison across selected BBH tasks for Llama-3.2-1B (target model for evaluation) with prompts optimized by different methods. The results demonstrate that prompts optimized by GREATER outperform other optimized prompts.

Method (Optimized By)	movie_rec.	causal_judgement	hyperbaton	tracking_five	object_count.	AVG
APO (GPT4)		40		24		40.8
PE2 (GPT4)		54	69		59	46.0
iAPE (GPT4)		57			41	39.6
GREATER (Llama-3.2-1B)	46	69	62	24	67	53.6

F EFFECT OF INITIALIZATION

For GREATER, we start with a fixed prompt: "Use proper logical reasoning and think step by step. Finally, give the actual correct answer." This fixed initialization is convenient for adapting to various tasks. However, we also explore whether using a different initialization affects performance. To test this, we conduct a small-scale experiment with Llama-3-8B on the BBH-movie-recommendation task. Table [7](#page-15-0) highlights the impact of different prompt initializations on optimization. As shown, a completely misleading initialization leads to a vastly different optimized prompt. However, both prompts result in very similar performance, despite solving the task in different ways. While the default initialization produces a prompt that leverages movie ratings and genre information from databases, the misleading prompt emphasizes concise explanations. Despite these contrasting approaches, both deliver comparable outcomes.

G PROMPT OPTIMIZATION PERFORMANCE IN VERY SMALL LANGUAGE MODEL : LLAMA-3.2-1B-INSTRUCT

While we primarily focused on two popular small language models - Llama-3-8B-Instruct and Gemma-2-9B-it, it is also interesting to see how GREATER perform for even smaller LLM - namely Llama-3.2-1B-Instruct. Given that is one of the smallest modern language models, getting good task performance out of it just by optimizing prompt can be very useful for real world task deployment. As we can see in Table [8,](#page-15-1) GREATER optimized prompts perform significantly better than prompts optimized by GPT-4 with other methods. This clearly shows the efficacy of GREATER in prompt optimization even with very small language models.

Table 9: Optimized Prompts for LLama-3-8B-Instruct on GSM8K dataset.

H PROMPT OPTIMIZATION RESULTS: LLAMA-3-8B-INSTRUCT

H.1 GSM8K AND FOLIO: OPTIMIZED PROMPTS

In Table [9](#page-16-1) and Table [10,](#page-16-2) we first show the optimized prompts with Llama-3-8B-Instruct on GSM8K and FOLIO dataset respectively. As we can see, GREATER performs on par or better than all the baselines in every scenario.

Table 10: Optimized Prompts for LLama-3-8B-Instruct on FOLIO dataset.

H.2 BIG BENCH HARD (BBH): OPTIMIED PROMPTS AND DETAILED RESULTS

Figure [5](#page-17-0) shows that GreaTer outperforms state-of-the-art (SOTA) prompt optimization methods, including APO [\(Pryzant et al., 2023\)](#page-11-5), TextGrad [\(Yuksekgonul et al., 2024\)](#page-12-5), APE [\(Zhou et al., 2022\)](#page-12-1), and PE2 [\(Ye et al., 2023\)](#page-12-2), across 71.4% to 85.% of tasks. A full breakdown of these results is provided in Figure [6.](#page-24-0) Upon closer inspection, it becomes evident that GREATER consistently matches or surpasses the performance of other SOTA methods, highlighting the robustness and reliability of our approach. In contrast, other methods show markedly less consistency due to their sole reliance on LLM judgment.

Figure 5: Win/Draw/Loss Comparison of GREATER and SOTA prompt optimization techniques APO, TextGrad, APE, and PE2 in optimization with Llama-3-8B-Instruct. GREATER maintains a significant winning margin over these methods, highlighting its effectiveness in optimization.

Finally, Table [11](#page-0-0) presents all the optimized prompts generated by the baseline methods and our proposed approach. TextGrad prompts are truncated due to their excessive length, making them challenging to fit on a page, which may also explain their inconsistent performance.

Table 11: List of optimized prompts for BBH tasks by different prompt optimization methods with Llama-3-8B-Instruct.

Continued on next page

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I PROMPT OPTIMIZATION RESULTS: GEMMA-2-9B-IT

I.1 GSM8K AND FOLIO: OPTIMIZED PROMPTS

In Table [12](#page-23-1) and Table [13,](#page-23-2) we first show the optimized prompts with Llama-3-8B-Instruct on GSM8K and FOLIO dataset respectively. As we can see, GREATER performs on par or better than all the baselines in every scenario.

Method	Optimized Prompt	Score
TextGrad	You will answer a mathematical reasoning question. Think step by step.	87.8
APE	Let's think step by step.	88.6
APO	Let's think step by step.	88.6
PE ₂	Let's think step by step.	88.6
GREATER	Use these logical reasoning process steps and explain Step. step. Here is correct answer.	89.4

Table 12: Optimized Prompts for Gemma-2-9B-it on GSM8K dataset

Table 13: Optimized Prompts for Gemma-2-9B-it on FOLIO dataset

I.2 BIG BENCH HARD (BBH): OPTIMIZED PROMPTS AND DETAILED RESULTS

Figure 6: Full performance breakdown across 21 BBH tasks of GREATER and SOTA prompt optimization techniques APO, TextGrad, APE, and PE2 in optimization with Llama-3-8B.

Figure 7: Win/Draw/Loss Comparison of GREATER and SOTA prompt optimization techniques APO, TextGrad, APE, and PE2 in optimization with Gemma-2-9B-it. GREATER maintains winning margin over these methods, highlighting its effectiveness in optimization.

Figure 8: Full performance breakdown across 21 BBH tasks of GREATER and SOTA prompt optimization techniques APO, TextGrad, APE, and PE2 in optimization with Gemma-2-9B.