

Beyond Elicitation: Provision-based Prompt Optimization for Knowledge-Intensive Tasks

Yunzhe Xu, Zhuosheng Zhang, Zhe Liu

Abstract—While prompt optimization has emerged as a critical technique for enhancing language model performance, existing approaches primarily focus on elicitation-based strategies that search for optimal prompts to activate models’ capabilities. These methods exhibit fundamental limitations when addressing knowledge-intensive tasks, as they operate within fixed parametric boundaries rather than providing the factual knowledge, terminology precision, and reasoning patterns required in specialized domains. To address these limitations, we propose Knowledge-Provision-based Prompt Optimization (KPPO), a framework that reformulates prompt optimization as systematic knowledge integration rather than potential elicitation. KPPO introduces three key innovations: 1) a knowledge gap filling mechanism for knowledge gap identification and targeted remediation; 2) a batch-wise candidate evaluation approach that considers both performance improvement and distributional stability; 3) an adaptive knowledge pruning strategy that balances performance and token efficiency, reducing up to 29% token usage. Extensive evaluation on 15 knowledge-intensive benchmarks from various domains demonstrates KPPO’s superiority over elicitation-based methods, with an average performance improvement of ~6% over the strongest baseline while achieving comparable or lower token consumption. Code at: <https://github.com/xyz9911/KPPO>.

Index Terms—Prompt optimization, large language models, natural language processing

I. INTRODUCTION

Large Language Models (LLMs) have achieved unprecedented performance across diverse natural language processing tasks through sophisticated prompt engineering techniques [1]. The field has evolved from manual prompt design approaches [2], [3] to automated optimization frameworks [4]–[7], where optimizer LLMs iteratively refine prompts to maximize task performance. These automated approaches, collectively termed *elicitation-based optimization*, operate under the fundamental assumption that optimal prompts can unlock latent capabilities within pre-trained model parameters through strategic reformulation of instructions, exemplars, or reasoning templates. However, elicitation-based optimization encounters fundamental limitations when applied to knowledge-intensive domains that require specialized expertise beyond the model’s parametric knowledge. Consider tasks in specialized scientific domains, emerging technologies, or domain-specific applications where factual accuracy, terminology precision, and specialized reasoning patterns are paramount. In such contexts, the assumption that optimal prompts can elicit non-existent knowledge becomes untenable.

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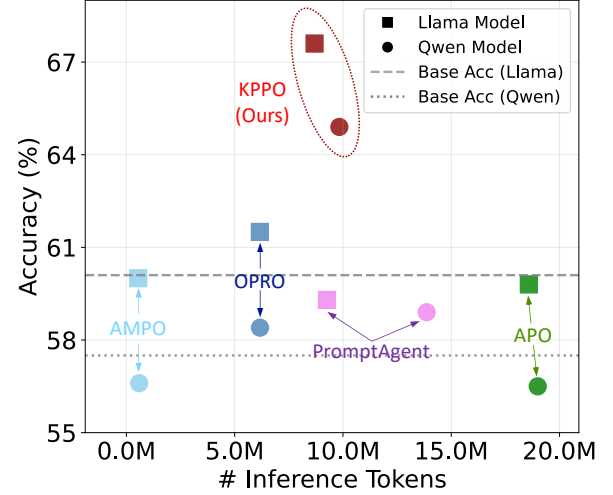


Fig. 1. Comparative analysis of prompt optimization performances on 15 knowledge-intensive tasks from various domains. Traditional elicitation-based methods achieve marginal or even negative improvements, while KPPO demonstrates substantial improvements (average +6%) while achieves comparable or enhanced efficiency.

We analyze the performance of traditional methods across 15 knowledge-intensive question-answering benchmarks spanning multiple domains. As demonstrated in Figure 1, traditional methods achieve marginal or even negative improvements when a clear task instruction is provided. Figure 2 reveals that elicitation-based optimization fails to address underlying knowledge gaps, instead producing shallow improvements that do not resolve the fundamental knowledge deficiencies. Our systematic analysis of this phenomenon reveals two critical deficiencies: **1) Knowledge Poverty**: optimized prompts lack sufficient domain-specific information to address knowledge gaps, instead focusing on superficial reformulations that fail to provide substantive content. **2) Optimization Ineffectiveness**: even when prompts incorporate relevant information, the optimization process lacks effective validation mechanisms to ensure the knowledge gap is mitigated.

To address these fundamental deficiencies, we must shift from elicitation to provision by directly integrating domain-specific knowledge rather than attempting to activate non-existent parametric knowledge. However, this introduces three challenges: How can we identify missing domain knowledge and generate targeted prompts to fill these gaps? How can we ensure selected prompts reliably address knowledge gaps rather than achieving spurious validation score? How can we balance comprehensive knowledge provision with token efficiency constraints as knowledge accumulates iteratively?

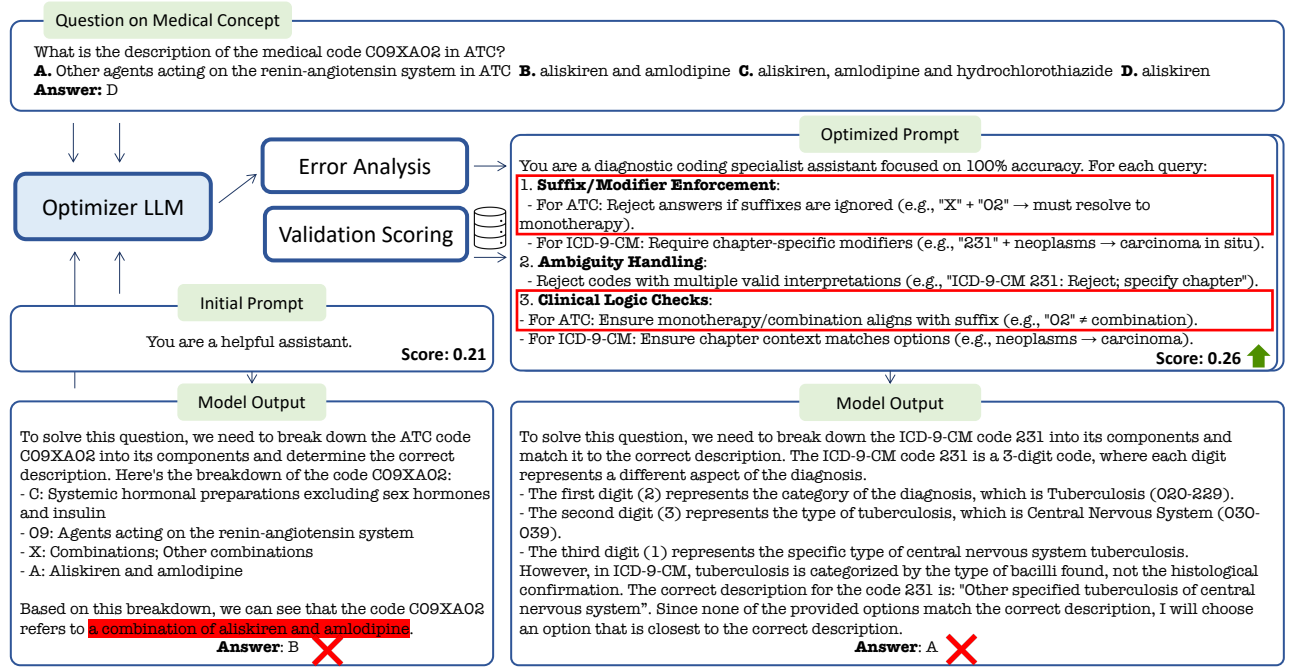


Fig. 2. Visualization of the failure of elicitation-based prompt optimization to fill LLM’s knowledge gap in specific domains. Despite achieving improved accuracy on the validation split, the optimized prompt fails to provide sufficient domain knowledge, resulting in continued errors on the original failure cases. The optimized prompts capture surface-level patterns rather than providing the substantive domain knowledge required to resolve the failure cases.

We propose **Knowledge-Provision-based Prompt Optimization (KPPO)**, a principled framework that addresses these challenges through three corresponding innovations. Rather than attempting to elicit non-existent knowledge through linguistic manipulation, KPPO explicitly provides the factual content, terminology, and reasoning patterns required for task success. First, an analysis framework examines failure cases to identify specific knowledge deficiencies and generates candidate prompts incorporating targeted domain content. Second, we introduce batch-wise dual-objective evaluation that jointly optimizes for performance improvement on recent failures and distributional stability, inspired by trust region methods [8]. Third, we design an adaptive pruning mechanism that identifies structural inefficiencies through local degree and global balance constraints, maintaining essential domain information while reducing token consumption.

Extensive evaluation across 15 knowledge-intensive benchmarks demonstrates KPPO’s effectiveness. Our method achieves average improvements of 6.1% and 6.0% on Llama 3.1 [9] and Qwen 2.5 [10] respectively, compared to the strongest baselines. Notably, the pruning variant significantly reduces token usage by up to 29% while outperforming baselines. These results establish a new direction for prompt optimization research, extending beyond the parametric boundaries of pre-trained models to systematically incorporate external knowledge. This paradigm shift has significant implications for deploying LLMs in specialized domains where tuning approaches are computationally prohibitive or data-limited, opening new avenues for practical knowledge-intensive applications. The contributions of this work are threefold:

- We propose KPPO, a framework that systematically inte-

grates domain-specific knowledge into prompts, achieving significant improvements across knowledge-intensive tasks spanning various domains.

- The technical innovations include: knowledge gap filling with targeted gap identification, dual-objective batch-wise evaluation ensuring both performance gains and optimization robustness, and adaptive pruning that maintains effectiveness while reducing token consumption.
- We establish provision-based optimization as a viable paradigm for knowledge-intensive applications, addressing knowledge poverty and optimization ineffectiveness of traditional methods and providing an alternative for domain-specific tasks.

II. RELATED WORKS

A. Prompt Optimization

Prompt engineering has emerged as a critical technique for enhancing LLM performance, with research spanning multiple optimization dimensions including prompt design [2], [3], exemplar selection [11], [12], and exemplar ordering [13]. Early approaches relied on manual prompt crafting [14], but recent work has shifted toward automated optimization to reduce engineering effort. One direction focuses on test-time prompt modification [15]–[18], which refines user inputs to improve task understanding, either through auxiliary models [19]–[21] trained for prompt rewriting or through direct optimization. In contrast, automatic prompt optimization operates without auxiliary models during inference, employing only an optimizer LLM [5], [22]–[24] for iterative prompt refinement, offering greater practical efficiency. Current approaches primarily focus on comprehensive search algorithms, employing beam

search [4], [24], Monte Carlo tree search [6], and evolutionary algorithms [25], [26] to generate diverse mutations [27], [28] with bandit-based selection on validation sets [29]. These methods collectively constitute elicitation-based optimization, seeking optimal prompts to unlock latent model capabilities. Recent extensions have broadened the scope to multi-turn scenarios [30], label-free optimization [31], exemplar-focused refinement [32]–[34], and advanced techniques incorporating multi-agent learning [35], meta-learning [36], and probabilistic optimization [37]. While these approaches effectively improve prompt quality through strategic reformulation, they fundamentally operate within parametric boundaries by seeking to elicit latent capabilities rather than augmenting the model’s knowledge base with external domain expertise. Our work diverges from this elicitation paradigm by systematically integrating domain-specific knowledge.

B. Self-Evolution in Large Language Models

LLMs have demonstrated potential for self-improvement through mechanisms that identify and rectify errors without external supervision [38], [39]. Initial approaches focus on single-turn refinement through self-reflection techniques [40], [41], where models analyze their own reasoning traces to detect inconsistencies and improve response quality. This verification process can be augmented by invoking external tools [42], [43] to ensure factual consistency and logical coherence. More recent work extends self-evolution to multi-turn scenarios, learning from direct environmental feedback [44], [45] to iteratively improve task performance through experience accumulation and reflection in sequential decision-making contexts for language agents. TextGrad [7] bridges self-evolution with prompt optimization by enabling textual gradients derived from self-reflection to backpropagate through prompts. However, when models lack domain-specific knowledge, self-reflection mechanisms cannot bridge this gap. In contrast, our approach directly addresses knowledge gaps by systematically integrating external domain content into prompts, transcending the parametric boundaries that constrain self-evolution methods. While self-evolution improves how models use existing knowledge, KPPO expands what knowledge is available to the model during inference.

III. PILOT EXPERIMENTS

This section defines prompt optimization for knowledge-intensive tasks and provides diagnoses for elicitation-based prompt optimization that motivates our approach.

A. Problem Formulation

Given a dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ where each instance (x_i, y_i) represents an input-output pair requiring specialized domain knowledge, we define a system prompt p as a structured natural language construct containing both domain-specific knowledge and procedural guidance for task execution. The inference process combines the prompt p , task input x , and standardized task instruction ℓ to produce a prediction $\hat{y} = \text{LLM}_{\text{task}}(p, x, \ell)$ from the target language model. The

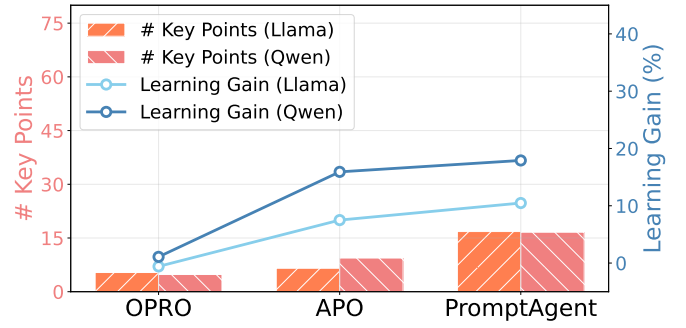


Fig. 3. Analysis of key points within the optimized prompt and learning gain across knowledge-intensive tasks.

optimization objective seeks to identify the optimal prompt p^* that maximizes expected task performance:

$$p^* = \arg \max_p \mathbb{E}_{(x,y) \sim \mathcal{D}} [f(p, x, y)],$$

$$f(p, x, y) = \begin{cases} 1, & \text{if } \text{LLM}_{\text{task}}(p, x, \ell) = y \\ 0, & \text{otherwise,} \end{cases} \quad (1)$$

where $f(\cdot)$ evaluates prediction correctness.

B. Analysis of Elicitation-based Methods

We evaluate three representative prompt optimization methods: OPRO [5], APO [4], and PromptAgent [6] on Llama 3.1 and Qwen 2.5. For each optimized prompt, we employ DeepSeek-V3 [46] as an evaluator to identify and quantify domain-specific key points through prompt analysis. We introduce the **learning gain** metric to quantify optimization effectiveness, capturing the model’s ability to resolve previously failed cases through knowledge acquisition:

$$\frac{1}{|P|} \sum_{i=1}^{|P|} \frac{1}{|\mathcal{B}_i|} \sum_{(x,y) \in \mathcal{B}_i} [f(p_i, x, y) - f(p_{i-1}, x, y)], \quad (2)$$

where P represents the optimization trajectory and \mathcal{B}_i is the training batch for step i . Figure 3 presents our empirical findings, revealing two critical deficiencies in current approaches:

1) Knowledge Poverty: All evaluated methods demonstrate remarkably low key points counts (<15), indicating optimization is not focusing on substantive knowledge integration.

2) Optimization Ineffectiveness: Learning gains remain substantially low ($<20\%$) across all methods, revealing that existing methods lack effective mechanisms to ensure that knowledge gaps have been effectively addressed. Prompts may achieve improved validation accuracy through pattern matching while failing to resolve underlying knowledge deficiencies.

These findings motivate our approach, which transcends elicitation-based limitations through systematic knowledge integration that directly fill knowledge gaps and improves optimization effectiveness.

IV. METHOD

Overview

Our proposed framework addresses the limitations of elicitation-based approaches by integrating domain-specific

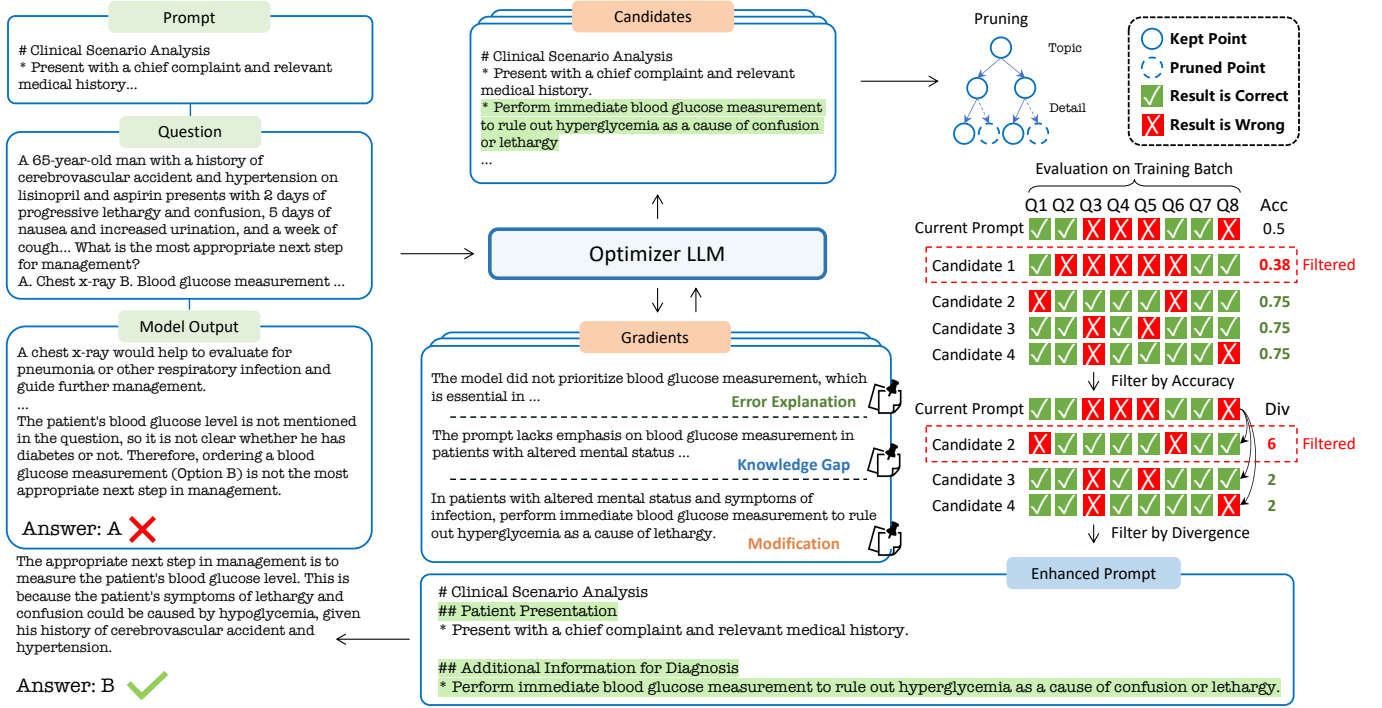


Fig. 4. Overview of KPPO. Given task mistakes, the optimizer LLM generates “gradients” by analyzing the original prompt’s limitations, producing explanations of failures, identifying knowledge gaps, and suggesting targeted modifications. The framework then integrates these gradients to generate candidate prompts, which undergo an alternative pruning procedure to avoid over-lengthened prompt. Prompt candidates are filtered with a batch-wise dual-objective evaluation that jointly considers performance improvement on recent training instances and distribution stability to ensure robust knowledge integration.

knowledge into prompt structures. As illustrated in Figure 4, KPPO employs an optimizer LLM (LLM_{opt}) to iteratively enhance prompts through targeted knowledge provision. The framework maintains a beam of optimized prompts \mathcal{C} that are refined based on failure case analysis. At each iteration t , the system samples a training batch \mathcal{B}_t from the dataset, identifies failure cases \mathcal{E}_t , and generates improved prompts through analysis and candidate filtering. The optimization process is detailed in Algorithm 1.

A. Knowledge Gap Filling

Our approach identifies knowledge deficiencies that cause prediction errors, moving beyond surface-level pattern recognition to address knowledge gaps. Given a current prompt p and failure cases $\mathcal{E} = \{(x, y) \in \mathcal{B}_t : LLM_{task}(p, x, \ell) \neq y\}$, the system employs LLM_{opt} to analyze each failure from three critical perspectives: **1) Error Explanation:** Analyzes the underlying reasons why the current prompt leads to incorrect predictions, examining flaws in LLM’s response. **2) Knowledge Gap Analysis:** Identifies specific domain knowledge missing from the current prompt that is required to resolve the failure cases. **3) Modification:** Suggests targeted improvements and specific knowledge pieces that should be integrated into the prompt structure. This analysis represents the “gradients” g that provide guidance for prompt improvement. Based on these gradients g , LLM_{opt} generates M candidate prompts per iteration, each incorporating targeted knowledge to address identified deficiencies. To ensure systematic knowledge integration, KPPO organizes the incorporated domain information

Algorithm 1: KPPO

Input : Initial prompt p_0 , Training set \mathcal{D}_{train} , Window size K , Iteration limit T , Validation set \mathcal{D}_{val} , New prompts per step M

Output: Optimized knowledge prompt p^*

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1 Initialize beam  $\mathcal{C} \leftarrow \{p_0\}$  and bank  $\mathcal{Q} \leftarrow \emptyset$ 
2 for step  $t = 1$  to  $T$  do
3   Initialize candidate set  $cand \leftarrow \emptyset$ 
4   Sample batch  $\mathcal{B}_t \subset \mathcal{D}_{train}$ 
5   Update instance bank:  $\mathcal{Q} \leftarrow \mathcal{Q} \cup \mathcal{B}_t$ 
6   Get  $K$  recent instances:  $\mathcal{Q}_K \leftarrow \{q_i \in \mathcal{Q} : i > |\mathcal{Q}| - K\}$ 
7   Get failure cases:  $\mathcal{E} \leftarrow \{(x, y) \in \mathcal{B}_t : f(p, x, y) = 0\}$ 
8   for  $p \in \mathcal{C}$  do
9      $cand \leftarrow cand \cup \{(p, p)\}$ 
10     $issues \leftarrow \emptyset$ 
11    if pruning then
12       $issues \leftarrow ViolationDetect(p)$ 
13    for  $i = 1$  to  $M$  do
14      Generate gradients:  $g_i \leftarrow LLM_{opt}(p, \mathcal{E})$ 
15      Generate candidate:
16         $p'_i \leftarrow LLM_{opt}(p, \mathcal{E}, g_i, issues)$ 
17         $cand \leftarrow cand \cup \{(p'_i, p)\}$ 
18     $\mathcal{C} \leftarrow CandidateFilter(cand, \mathcal{Q}_K)$ 
19 return  $\arg \max_{p \in \mathcal{C}} \mathbb{E}_{(x, y) \sim \mathcal{D}_{val}} [f(p, x, y)]$ 

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within each prompt using a structured knowledge hierarchy represented as a directed acyclic graph $\mathcal{T} = (V, E)$. The vertex set V is partitioned into two disjoint subsets: **topic nodes** V_t that represent conceptual categories, and **note nodes** V_n that contain specific domain facts.

Algorithm 2: Candidate Evaluation

Input : Candidate pairs $cand$, Recent examples \mathcal{Q}_K , Beam width W
Output: Selected prompts B

```

1 Initialize  $ranking \leftarrow \emptyset$ 
2 for  $(p', p) \in cand$  do
3   Calculate  $\Delta s \leftarrow \Delta S(p', p)$  using eq. (4)
4   if  $\Delta s > 0$  then
5     Calculate  $d \leftarrow D(p', p)$  using eq. (5)
6      $ranking \leftarrow ranking \cup \{(\Delta s, d)\}$ 
7 Sort  $ranking$  by  $(\Delta s, -d)$ 
8 return Top  $W$  prompts from  $ranking$ 

```

B. Batch-Wise Candidate Evaluation

The newly generated prompt candidates require systematic evaluation to filter out ineffective variants and ensure optimization robustness. Traditional prompt optimization relies on full validation set evaluation, which is computationally expensive and may not effectively validate knowledge integration quality. we introduce a batch-wise evaluation mechanism that operates on recent training instances \mathcal{Q}_K to improve efficiency and robustness. However, accuracy-based batch-wise validation may lead to instability as the evaluation instances are limited to a fixed window K , and we cannot fully ensure that prompt changes will generalize well to other instances.

To address this challenge, we propose a principled filtering mechanism inspired by trust region policy optimization [8] that considers both learning gains and output stability. Let $p(y|x)$ and $p'(y|x)$ denote output distributions under the current and candidate prompt respectively. We formulate the prompt update objective as:

$$\arg \max_{p'} \mathbb{E}_{(x,y) \sim \mathcal{Q}_K} \left[\frac{p'(y|x)}{p(y|x)} A(p', p, x, y) \right], \quad (3)$$

where the ratio $\frac{p'(y|x)}{p(y|x)}$ measures distribution change and $A(p', p, x, y) = f(p', x, y) - f(p, x, y)$ represents the advantage of the new prompt over the current one. We approximate this objective through discrete metrics that can be efficiently computed. The performance improvement on recent instances \mathcal{Q}_K is formulated as:

$$\Delta S(p', p) = \sum_{(x,y) \in \mathcal{Q}_K} A(p', p, x, y). \quad (4)$$

The distribution ratio is approximated through correctness divergence:

$$D(p', p) = \sum_{(x,y) \in \mathcal{Q}_K} \mathbb{I}[f(p', x, y) \neq f(p, x, y)], \quad (5)$$

where $\mathbb{I}[\cdot]$ is the indicator function. We implement this objective by selecting candidates with positive Δs and ranking them by performance improvement and divergence $(\Delta s, -d)$, as detailed in Algorithm 2. This lexicographic ranking considers distribution stability, ensuring prompt updates maintain consistency with existing knowledge while incorporating targeted improvements. The approach provides two key benefits: reduced computational cost compared to full validation set

Algorithm 3: Violation Detection

Input : Prompt p , Max children C , Max factor F
Output: $issues_{local}$: Nodes with local degree violations,
 $issues_{global}$: Nodes with global balance violations

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1 Parse prompt:  $\mathcal{T} = (V, E) \leftarrow \text{Parse}(p)$ 
2 Initialize  $issues_{local} \leftarrow \emptyset, issues_{global} \leftarrow \emptyset$ 
3 for  $v \in V$  in pre-order traversal do
4    $\mathcal{T}_v \leftarrow$  subtree rooted at  $v$ 
5   Calculate  $\text{bf}(\mathcal{T}_v)$  using eq. (8)
6   if  $\text{outdeg}(v) > C$  then
7      $issues_{local} \leftarrow issues_{local} \cup \{v\}$ 
8   if  $\beta(v) > F$  then
9      $issues_{global} \leftarrow issues_{global} \cup \{v\}$ 
10 return  $(issues_{local}, issues_{global})$ 

```

evaluation, and conservative prompt updates that limit the risk of degradation on unseen instances.

C. Adaptive Knowledge Pruning

While systematic knowledge integration improves performance, the iterative knowledge provision can lead to excessively long prompts that exceed practical token limits. To address this challenge, we introduce a pruning mechanism by detecting structural inefficiencies in the hierarchy and providing guidance to LLM_{opt} for targeted knowledge reduction. We define two types of structural constraints to identify pruning opportunities:

Local Degree Constraint: Limits excessive branching at individual nodes:

$$\forall v \in V_t : \text{outdeg}(v) \leq C, \quad (6)$$

where C is the maximum children for topic node.

Global Balance Constraint: Ensures hierarchical efficiency by detecting nodes with excessive branching relative to their subtree structure:

$$\forall v \in V_t : \beta(v) = \frac{\text{outdeg}(v)}{\text{bf}(\mathcal{T}_v)} \leq F, \quad (7)$$

where the branching factor of subtree \mathcal{T}_v is:

$$\text{bf}(\mathcal{T}_v) = \frac{\sum_{u \in V_t(\mathcal{T}_v)} \text{outdeg}(u)}{|V_t(\mathcal{T}_v)|}, \quad (8)$$

and F controls the maximum allowed deviation from average branching patterns. A high $\beta(v)$ indicates that node v has excessive direct children relative to the organizational patterns in its subtree. The detected nodes with violations provide explicit instructions to LLM_{opt} in candidate prompt generation for performing targeted pruning. The violation detection procedure is detailed in Algorithm 3. This constraint-guided approach ensures that pruning maintains essential domain information while resolving organizational inefficiencies.

V. EXPERIMENTS**A. Datasets**

To comprehensively evaluate KPPO's effectiveness on knowledge-intensive tasks, we curate a diverse benchmark suite of 15 tasks spanning multiple specialized domains where domain expertise and terminology precision are critical.

Our selection criteria prioritize tasks that require substantial domain-specific knowledge beyond general language understanding. The selected benchmarks are organized into three domain categories:

Financial Domain. We employ FiQA [47], a challenging aspect-based sentiment analysis task requiring models to identify specific financial entities and classify sentiments toward multiple hierarchical aspects. This task demands deep understanding of financial terminology where context dramatically shifts sentiment.

Legal Domain. From the LexGLUE benchmark [48], we select the Case Hold task evaluating models’ ability to identify correct legal holdings from court decisions. Each instance presents an excerpt from a court decision with a masked holding statement, requiring the model to select the correct holding from five candidates.

Medical Domain. We incorporate three complementary medical benchmarks that collectively assess different facets of medical knowledge:

- **MedQA** [49]: A large-scale dataset containing professional medical board examination questions. These questions present clinical vignettes that require integrating patient symptoms, test results, and medical knowledge to identify correct diagnoses, treatments, or procedures.
- **MedConceptsQA** [50]: A specialized benchmark focusing on medical coding and terminology interpretation across diagnoses, procedures, and pharmacological concepts. This dataset tests precise understanding of standardized medical classification systems where subtle distinctions in terminology directly impact clinical documentation and billing accuracy.
- **MedMCQA** [51]: A comprehensive multiple-choice dataset containing questions from medical entrance examinations, covering 2,400 healthcare topics across 21 medical specialties. We select 11 representative specialties for our evaluation: Anatomy, Dental, Gynecology & Obstetrics, Medicine, Microbiology, Pathology, Pediatrics, Pharmacology, Physiology, Social & Preventive Medicine, and Surgery. Each specialty tests distinct domain knowledge, enabling fine-grained analysis of knowledge provision across medical subdomains.

B. Baselines

We evaluate our proposed framework against several well-established prompt optimization methods:

Base Prompt: We establish a minimal baseline using the system prompt “You are a helpful assistant” without any domain-specific content or task-specific instructions.

OPRO [5]: An algorithm that maintains a trajectory of historical prompts with their corresponding validation scores, using this meta-information to guide the generation of improved prompt candidates to maximize validation performance.

APO [4]: An approach that analyzes errors to generate “gradients” describing prompt deficiencies, guiding iterative prompt refinement. We evaluate two variants: the original implementation and an iteration-aligned variant matching our optimization budget for fair comparison.

AMPO [24]: A multi-branched prompt optimization method that iteratively develops prompts with multiple branches to handle diverse patterns in complex tasks. This multi-branched design is particularly relevant for knowledge-intensive domains where tasks exhibit heterogeneous question types requiring different knowledge components.

PromptAgent [6]: A planning-based framework that formulates prompt optimization as sequential decision-making, employing Monte Carlo Tree Search (MCTS) to systematically explore the prompt space. We evaluate two variants: the original implementation and an iteration-aligned variant matching our optimization budget for fair comparison.

C. Implementation Details

We employ Llama 3.1-8B [9] and Qwen 2.5-7B [10] as target language models and DeepSeek-V3 [46] as the optimizer LLM, with inference conducted using vLLM under a specific seed for deterministic evaluation. Training instances are selected via sentence embedding similarity [52] to evaluation samples, ensuring semantic relevance for knowledge provision. Each task employs approximately 150 training samples, 50 validation samples, and 100 test samples; datasets lacking standard splits use validation sets as test sets. Optimization hyperparameters are: batch size $B = 5$, recent instance window $K = 10$, training iterations $T = 60$, candidate prompts per step $M = 4$, and beam width $W = 2$. For the pruning variant, we set maximum children per topic node $C = 16$ and maximum balance factor $F = 8.0$ to detect structural violations while preserving essential knowledge. Iteration-aligned baseline variants (APO*, PromptAgent*) match our 60-iteration budget for fair comparison, while original implementations use default settings.

D. Quantitative Results

Table I presents comprehensive performance comparisons across all 15 knowledge-intensive benchmarks. KPPO demonstrates substantial improvements over elicitation-based baselines, achieving average accuracy gains of 6.1% on Llama 3.1 and 6.0% on Qwen 2.5, with particularly strong gains on tasks requiring specialized factual knowledge such as MedConceptsQA medical coding (+18.4% and +3.3%) and MedMCQA Anatomy (+4.9% and +6.5%). In contrast, traditional elicitation-based methods exhibit inconsistent and marginal performance: OPRO achieves only +1.4% and +0.9% improvements over base prompts, while APO, AMPO, and PromptAgent frequently underperform the minimal baseline (e.g., APO +1.0% on Llama but -1.6% on Qwen), confirming that elicitation-based methods struggle when clear task instructions are provided. The iteration-aligned variants yield suboptimal results and reveal architecture-dependent dynamics: extended iterations modestly improve baselines on Qwen 2.5 (APO*: +0.4%, PromptAgent*: +1.4%) but degrade performance on Llama 3.1 (APO*: -0.2%, PromptAgent*: -1.5%), suggesting overfitting to superficial patterns without genuine knowledge acquisition. These results validate our hypothesis that provision-based optimization transcends parametric boundaries by directly augmenting models’ effective

TABLE I
PERFORMANCE COMPARISON (ACCURACY %) OF PROMPT OPTIMIZATION METHODS ACROSS 15 TASKS FROM VARIOUS DOMAINS.

Method	FiQA	Case	Med	MedC	Anat	Dent	G&O	Medn	Mic	Path	Ped	Phar	Phys	S&P	Surg	AVG
Results on Llama 3.1																
Base	73.2	49.0	69.0	28.3	61.3	47.0	65.1	63.4	61.0	71.3	62.1	76.9	66.7	53.9	53.0	60.1
OPRO [5]	73.2	55.0	70.0	30.0	63.7	50.3	58.9	64.9	53.3	72.4	69.7	76.9	62.5	64.1	57.6	61.5
APO [4]	73.2	52.0	65.0	35.0	61.3	45.9	61.2	63.4	59.7	71.3	65.2	74.6	66.7	61.5	60.6	61.1
APO* [4]	73.2	55.0	63.0	33.3	66.1	51.4	57.4	63.4	58.4	71.3	57.6	73.1	62.5	53.9	56.8	59.8
AMPO [24]	73.2	49.0	65.0	28.3	60.5	45.3	62.8	63.4	61.0	72.4	66.7	76.2	60.4	53.9	62.1	60.0
PromptAgent [6]	73.2	51.0	65.0	28.3	55.7	39.8	62.8	64.1	67.5	74.7	65.2	76.2	69.8	64.1	54.6	60.8
PromptAgent* [6]	73.2	45.0	65.0	28.3	65.3	45.3	54.3	61.8	59.7	71.3	64.4	74.6	61.5	60.3	59.9	59.3
KPPO (Ours)	77.3	55.0	70.0	51.7	71.0	58.6	69.0	68.7	61.0	75.9	69.7	80.8	71.9	69.2	63.6	67.6
Results on Qwen 2.5																
Base	74.2	61.0	60.0	35.0	54.0	44.8	53.5	56.5	57.1	69.0	56.8	68.5	61.5	62.8	47.7	57.5
OPRO [5]	73.2	54.0	59.0	35.0	52.4	47.0	54.3	58.0	66.2	74.7	57.8	72.3	67.7	52.6	51.5	58.4
APO [4]	75.3	62.0	55.0	30.0	54.8	45.9	50.4	53.4	57.1	64.4	53.0	71.5	63.5	55.1	47.7	55.9
APO* [4]	76.3	57.0	64.0	35.0	55.7	45.3	58.1	53.4	53.3	63.2	53.8	66.2	61.5	59.0	46.2	56.5
AMPO [24]	75.3	61.0	64.0	20.0	58.1	44.8	53.5	54.2	57.1	65.5	53.0	69.2	65.6	55.1	52.3	56.6
PromptAgent [6]	76.3	60.0	61.0	31.7	53.2	40.9	56.6	61.1	57.1	77.0	52.3	73.1	64.6	61.5	49.2	58.4
PromptAgent* [6]	76.3	60.0	58.0	50.0	52.4	48.6	51.2	58.8	64.9	66.7	55.3	68.5	61.5	52.6	58.3	58.9
KPPO (Ours)	77.3	61.0	65.0	53.3	60.5	56.4	58.9	66.4	66.2	80.5	59.9	80.8	66.7	62.8	57.6	64.9

Abbreviations: Case = Case Hold, Med = MedQA, MedC = MedConceptsQA, Anat = Anatomy, Dent = Dental, G&O = Gynaecology & Obstetrics, Medn = Medicine, Mic = Microbiology, Path = Pathology, Ped = Pediatrics, Phar = Pharmacology, Phys = Physiology, S&P = Social & Preventive Medicine, Surg = Surgery. '*' denotes methods with optimization iterations aligned to our framework.

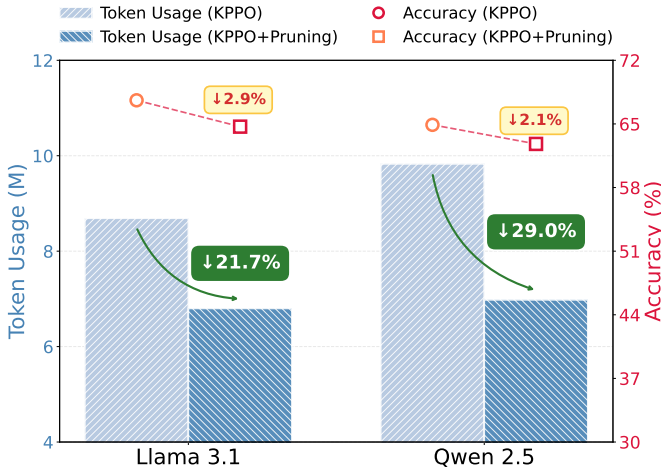


Fig. 5. Inference token efficiency vs. performance trade-off of adaptive knowledge pruning on 15 tasks.

knowledge bases, while elicitation-based approaches cannot overcome fundamental knowledge deficiencies.

E. Ablation Studies

Effect of Adaptive Knowledge Pruning. Figure 5 illustrates the efficiency-performance trade-off of adaptive pruning across all benchmarks. The pruning mechanism substantially reduces

inference token consumption by 21.7% for Llama 3.1 and 29.0% for Qwen 2.5, decreasing average usage from 9.26M to 6.89M tokens. The corresponding accuracy drops are modest: 2.9% for Llama 3.1 and 2.1% for Qwen 2.5, demonstrating that our constraint-guided mechanism effectively identifies and removes organizational redundancy while preserving essential domain knowledge. Notably, Qwen 2.5 exhibits greater token reduction with smaller performance degradation, revealing architecture-dependent sensitivity to prompt structure and knowledge organization. Critically, the pruned variant maintains substantial superiority over all baseline methods, with margins of 3.2% over the strongest competitor for Llama 3.1 and 3.9% for Qwen 2.5. This validates our pruning strategy's ability to balance comprehensive knowledge provision with token efficiency, a critical consideration for practical deployment where token costs directly impact inference expenses.

Token Efficiency Analysis. Figure 6 illustrates inference token utilization across optimization methods and KPPO variants. Full validation evaluation that evaluates all candidates on the complete validation set (Val Acc) consumes substantially more tokens than elicitation-based methods due to provision-based prompts creating longer inputs and conducting comprehensive validation, with maximum disparity reaching 157M versus 20M tokens on Anatomy with Qwen2.5. KPPO with batch-wise validation demonstrates significantly lower consumption compared to full evaluation, establishing batch-

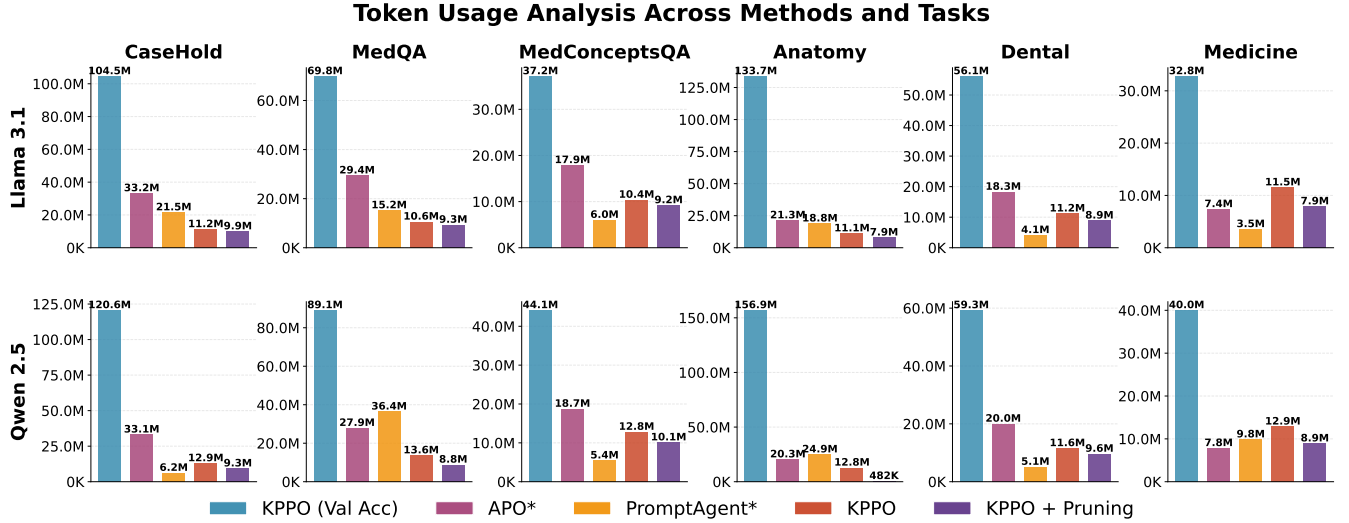


Fig. 6. Token consumption analysis across optimization methods and KPPO variants. The ‘Val Acc’ variant represents full validation set evaluation. ‘*’ denotes baselines with optimization iterations aligned to our framework.

TABLE II
ABLATION ON CANDIDATE EVALUATION.

Filtering	Case	Med	MedC	Anat	Dent	Medn
Results on Llama 3.1						
Val Acc	50.0	70.0	36.7	71.8	49.2	59.5
Batch Acc	<u>53.0</u>	69.0	<u>40.0</u>	66.1	<u>54.7</u>	<u>61.8</u>
Batch Acc + Div	55.0	70.0	51.7	<u>71.0</u>	58.6	68.7
Results on Qwen 2.5						
Val Acc	63.0	<u>59.0</u>	45.0	54.0	<u>49.2</u>	59.5
Batch Acc	54.0	56.0	<u>51.7</u>	<u>58.9</u>	48.6	<u>61.8</u>
Batch Acc + Div	<u>61.0</u>	65.0	53.3	60.5	56.4	66.2

Abbreviations: Case = Case Hold, Med=MedQA, MedC = MedConceptsQA, Anat = Anatomy, Dent = Dental. Medn=Medicine.

wise evaluation as both effective and efficient. Compared to baselines, batch-wise KPPO exhibits competitive efficiency with PromptAgent and better efficiency than APO, despite the substantial improvement. The adaptive pruning mechanism further reduces token consumption across all tasks, achieving approximately 2M additional savings per task beyond batch-wise evaluation, demonstrating that our constraint-guided approach successfully balances knowledge provision with computational efficiency, a critical requirement for practical deployment where token costs scale linearly with prompt length.

Candidate Evaluation Analysis. Table II evaluates our dual-objective batch-wise evaluation mechanism against two alternatives: simple accuracy-based batch evaluation without divergence consideration (Batch Acc) and full validation evaluation (Val Acc). Our dual-objective approach (Batch Acc + Div) consistently outperforms simple batch-wise evaluation, achieving average improvements of 5.1% on Llama 3.1 and

5.2% on Qwen 2.5, demonstrating that maintaining distributional stability during prompt updates is critical for robust knowledge integration. Notably, full validation evaluation, despite its computational expense, often underperforms batch-wise methods. On MedConceptsQA, it falls 15.0% and 8.3% below dual-objective batch-wise evaluation for Llama 3.1 and Qwen 2.5 respectively. This substantial gap reveals that full validation optimization can encourage superficial pattern matching that improves global validation metrics without genuinely addressing knowledge gaps, whereas batch-wise evaluation better validates knowledge integration by focusing on resolving recent failure cases. The dual-objective criterion effectively prevents overfitting to spurious patterns by penalizing excessive distributional changes, ensuring that selected prompts provide generalizable domain knowledge rather than instance-specific adjustments. These results validate our design choice to prioritize targeted knowledge gap remediation over global validation performance maximization.

Prompt Knowledge Analysis. Figure 7 presents quantitative analysis of knowledge content in optimized prompts across three categories: domain knowledge points, reasoning instructions, and output specifications. KPPO integrates substantially more domain knowledge than elicitation-based methods, averaging 56.8 points on Llama 3.1 (26.2× more than OPRO and 7.4× more than PromptAgent), directly addressing the knowledge poverty limitation of elicitation approaches. The adaptive pruning mechanism effectively reduces knowledge points by 30-50% across tasks while maintaining essential information, demonstrating successful identification of organizational redundancy. Critically, full validation evaluation consistently yields lower domain knowledge content than even the pruned variant, with particularly dramatic differences on knowledge-intensive tasks like MedConceptsQA (19 vs. 38 points) and Medicine (10 vs. 24 points), revealing that optimizing for global validation metrics does not encourage substantive knowledge integration. This misalignment explains

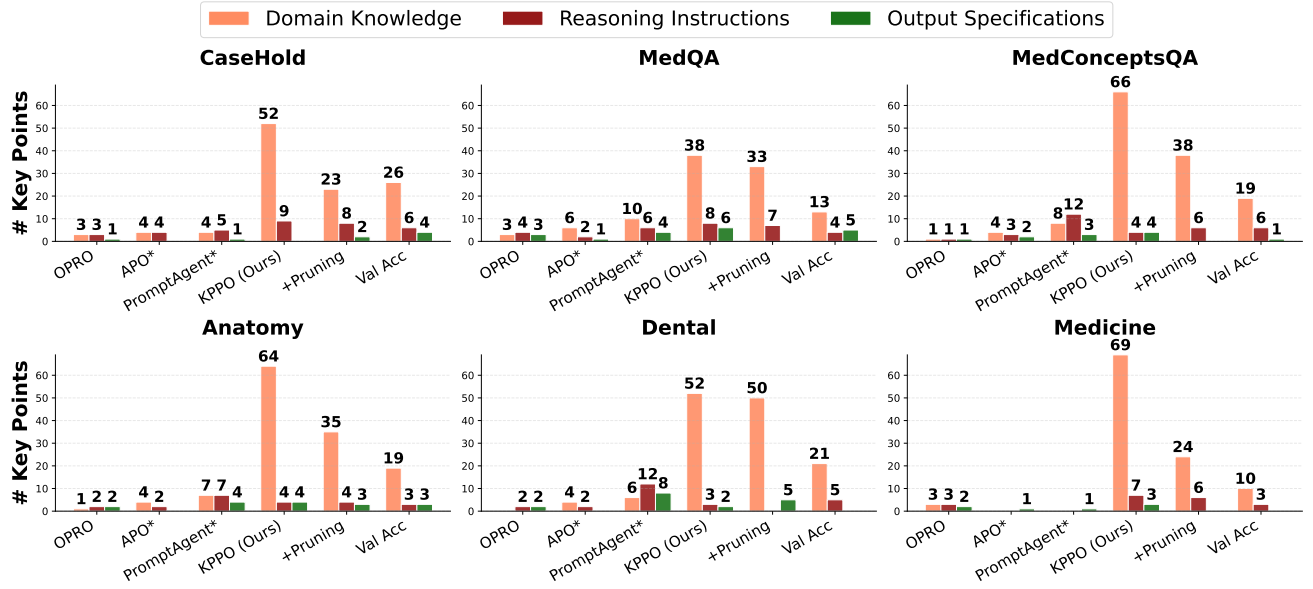


Fig. 7. Quantitative analysis of knowledge content in optimized prompts across six tasks on Llama 3.1, categorized into domain knowledge, reasoning instructions, and output specifications.

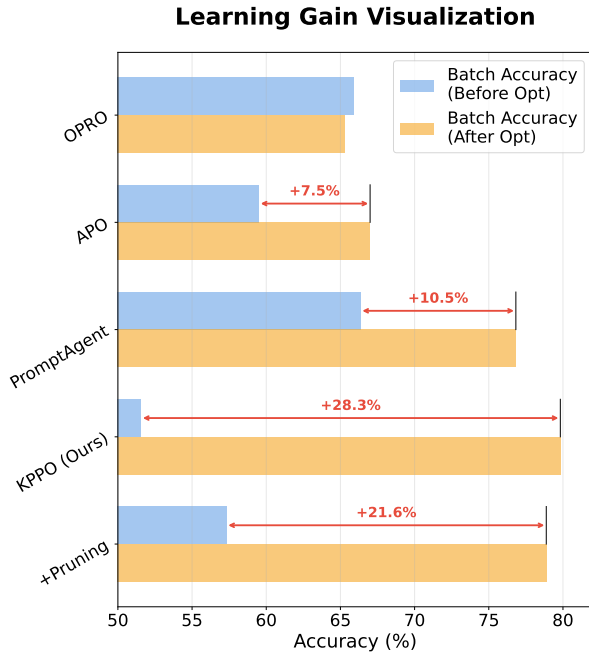


Fig. 8. Learning gain comparison across optimization methods with Llama model.

why full validation often underperforms batch-wise evaluation despite greater computational cost. It rewards pattern exploitation rather than genuine knowledge provision. These findings validate our batch-wise evaluation design, which prioritizes failure case resolution over validation accuracy maximization, ensuring that optimization genuinely expands the model’s effective knowledge base.

Optimization Effectiveness Analysis. Figure 8 presents optimization effectiveness across methods through the learning gain metric, which measure the proportion of previous fail-

ure cases successfully resolved during optimization. KPPO achieves 28.3% learning gain, substantially outperforming elicitation-based baselines: $3.8\times$ higher than APO (7.5%) and $2.7\times$ higher than PromptAgent (10.5%). The pruning variant maintains 21.6% learning gain, still exceeding all baselines by substantial margins. These results demonstrate KPPO’s superior capability in addressing knowledge gaps through targeted knowledge provision rather than superficial pattern adjustments. KPPO also exhibits lower initial batch accuracy compared to baselines, which we attribute to the introduction of provisional knowledge that may initially introduce noise; however, through rigorous iterative refinement and batch-wise validation, this provisional knowledge converges to reliable domain expertise that systematically resolves failure cases.

F. Qualitative Results

To understand how prompts evolve through iterative refinement, we trace the longitudinal development of specific knowledge components across optimization steps.

Knowledge Provision. Figure 9 illustrates monotonic knowledge expansion through the evolution of periodontal surgical procedures across six optimization checkpoints. The trajectory demonstrates three key characteristics of effective knowledge provision: hierarchical expansion from isolated procedural descriptions to comprehensive taxonomically-organized collections encompassing multiple surgical modalities; dimensional augmentation that introduces orthogonal clinical aspects such as procedural mechanisms (Step 20), flap type classifications (Step 25), and structured taxonomies with contraindications (Step 35-55); and specificity refinement evident in evolution from general statements (“indicated for edematous pockets”) to precise clinical specifications (“indicated exclusively for edematous pockets”). This accumulation pattern is particularly valuable for protocol-driven domains where systematic

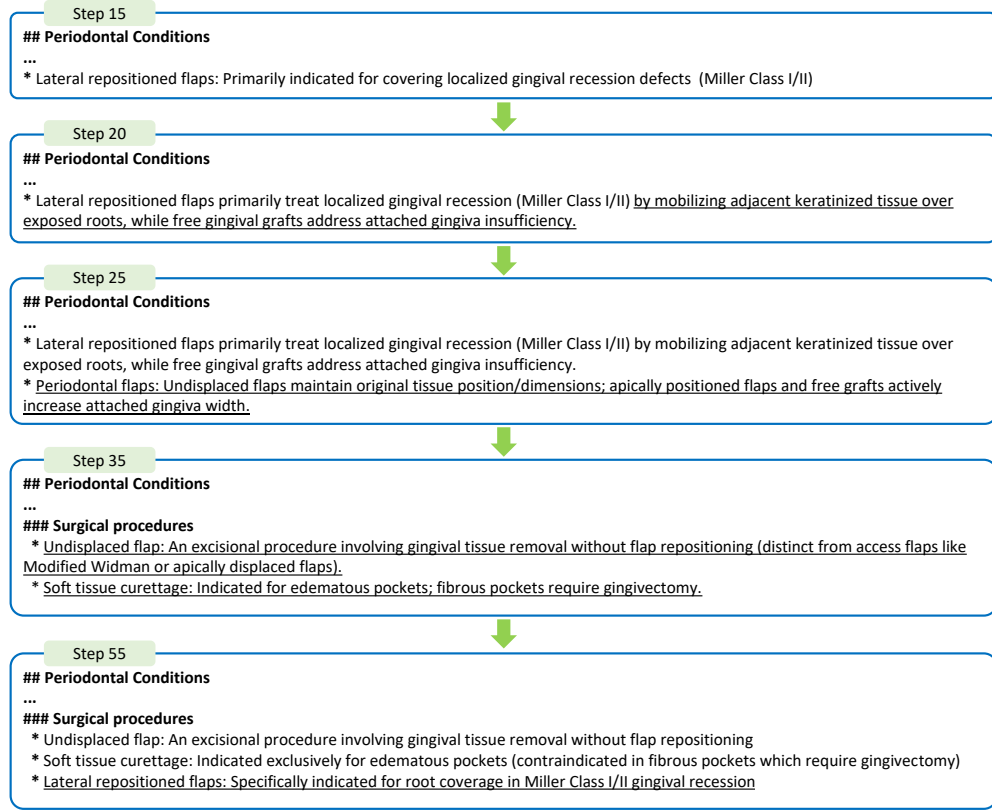


Fig. 9. Progressive knowledge accumulation in periodontal surgical procedures across six optimization steps. Each panel shows incremental additions (marked with underline) to the knowledge base. This pattern exemplifies monotonic knowledge growth typical of well-structured domain ontologies.

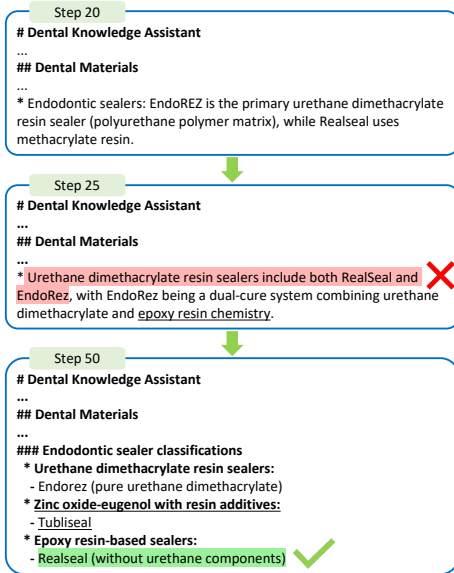


Fig. 10. Self-correction trajectory in endodontic sealer classification demonstrating non-monotonic accuracy evolution. Step 25 introduces a taxonomic error (red highlighting). Step 50 implements systematic correction through structured taxonomy and explicit negative specifications (green highlighting).

knowledge expansion occurs through iterative gap-filling based on failure case feedback, enabling comprehensive coverage without disrupting previously validated content.

Self-Correction. In contrast to monotonic accumulation, Fig-

ure 10 reveals KPPO’s capacity for self-diagnosis and rectification of domain-specific misconceptions through endodontic sealer classification evolution. The trajectory exhibits non-monotonic accuracy dynamics: Step 20 correctly identifies EndoREZ as urethane dimethacrylate-based, Step 25 paradoxically introduces taxonomic error by incorrectly grouping RealSeal with urethane-based sealers despite RealSeal being epoxy resin-based, and Step 50 implements systematic correction through structured taxonomy with explicit negative specifications (“RealSeal: epoxy resin-based, without urethane components”). This self-correction pattern demonstrates two critical insights: iterative knowledge provision can temporarily degrade accuracy when integrating unfaithful content, as the optimizer explores knowledge space based on limited failure cases; however, through continued refinement across diverse training batches, contradictions surface and the framework converges to faithful representations that resolve both original and newly-encountered failure cases.

Baseline Comparison. Figure 11 provides qualitative comparison between PromptAgent and KPPO on a medical code interpretation task from MedConceptsQA. The baseline prompt offers generic guidance (“analyze prefixes, suffixes, and their implications”) that fails to address specific knowledge gaps, resulting in incorrect interpretation of ICD10PROC code 03190Z. In contrast, KPPO integrates precise domain knowledge about ICD10PROC coding conventions, specifically that “the suffix ‘0Z’ indicates ‘No Device’ used in the procedure.” This case exemplifies how KPPO addresses deficiencies

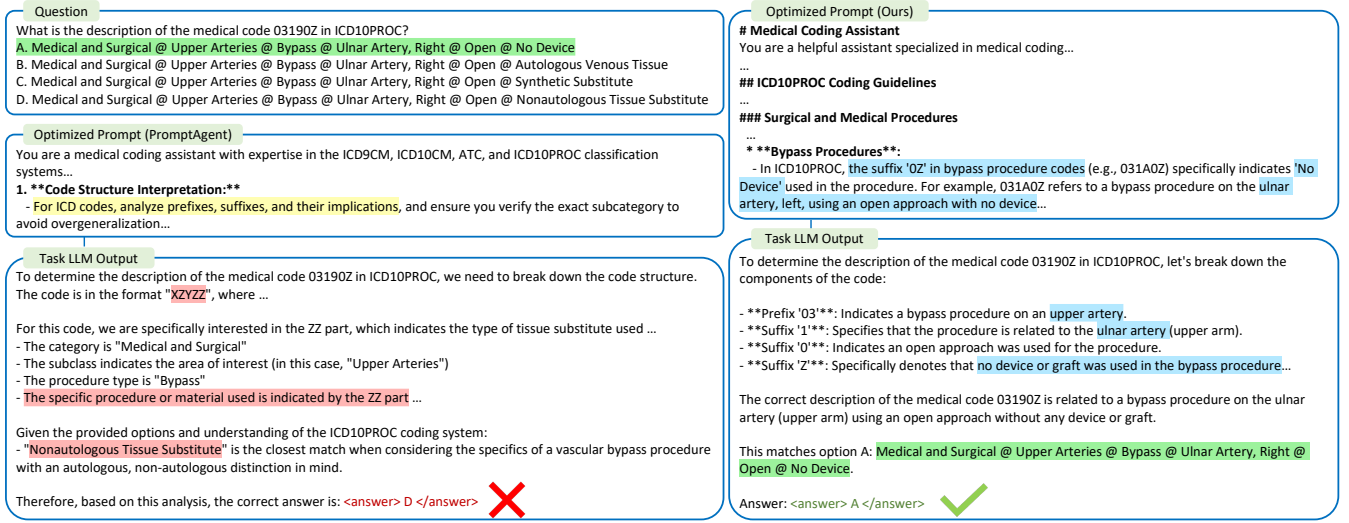


Fig. 11. Qualitative comparison between PromptAgent and KPPO on medical code interpretation task. PromptAgent provides generic analytical guidance (yellow highlighting) that fails to address the specific knowledge gap, resulting in incorrect code interpretation (red answer). KPPO integrates domain knowledge about ICD10PROC conventions (blue highlighting), enabling accurate identification that suffix '0Z' indicates 'No Device', leading to the correct answer (green).

through knowledge provision rather than superficial instruction reformulation. The qualitative analysis demonstrates KPPO's fundamental advantage: rather than hoping that better instructions can elicit non-existent knowledge, our framework directly provides the domain-specific information required for accurate task performance.

VI. CONCLUSION

This paper addresses a fundamental limitation in automated prompt optimization: the inability of elicitation-based methods to transcend parametric knowledge boundaries in knowledge-intensive domains. We introduce KPPO, a principled framework that reformulates prompt optimization as systematic knowledge integration through three technical innovations: knowledge gap filling via gradient-based failure analysis, batch-wise dual-objective evaluation ensuring robust integration over superficial pattern matching, and adaptive pruning optimizing computational cost through structural constraint guidance. Extensive evaluation across 15 benchmarks in financial, legal, and medical domains demonstrates KPPO's substantial improvements of approximately 6% over strongest elicitation-based baselines, with the pruning variant achieving 21.7-29.0% token reduction. These results establish provision-based optimization as a viable paradigm for deploying LLMs in specialized domains where task success fundamentally depends on domain expertise beyond parametric knowledge, providing an efficient alternative when traditional fine-tuning is computationally prohibitive or data-limited.

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APPENDIX

This appendix provides the complete prompt templates and formatting structures used throughout our KPPO framework to ensure reproducibility of our experimental results. The templates are organized according to the three main components of our optimization pipeline: task execution, gradient generation, prompt candidate generation and pruning procedure.

{question}

Solve the question above. Provide a thorough explanation of your reasoning. After your explanation, on a new line, write 'Answer:' followed by only the letter of the correct option enclosed within <answer> and </answer> tags, using this exact format: <answer> {letter} </answer>.

Fig. 12. Task instruction template for target language models to produce answers.

Example <{index}>:
 <question>{question}</question>
 <model_response>{response}</model_response>
 Correct Label: {label}
 Model Prediction: {prediction}

Fig. 13. Template for formatting task failure cases provided to the optimizer.

I'm enhancing a prompt to improve a language model's performance by addressing knowledge gaps.

The current prompt is:

<prompt>
 {prompt}
 </prompt>

But this prompt gets the following examples wrong:
 {example_string}

Analyze each error using the following XML structure:

<example>
 <examination> Examine why the the model's output is wrong and how it fails to capture the correct answer. </examination>
 <gap> Identify the specific knowledge missing or misunderstanding from the prompt that led to this error. </gap>
 <modification> Provide a concise, factual statement to add to the prompt that directly addresses the identified gap. Avoid general or vague suggestions. </modification>
 </example>

Focus on concise, high-impact information that can be easily incorporated into a prompt to enhance the model's accuracy across diverse scenarios. Avoid outputting auxiliary content other than the XML structures.

Fig. 14. Template for optimizer LLM to generate gradients based on current prompt and failure cases.


```

<error>
  <instance>{index}</instance>
  <question>{question}</question>
  <model_response>{response}</model_response>
  <labels>
    <correct>{label}</correct>
    <predicted>{prediction}</predicted>
  </labels>
  <analysis>
    <examination>The model's error: {examination}</examination>
    <gap>Knowledge gap or misunderstanding: {problem}</gap>
    <modification>Suggested prompt modification to address the gap:
    {modification}</modification>
  </analysis>
</error>

```

Fig. 15. Combined template showing task failure cases with corresponding gradients.

Enhance the prompt for a QA task by integrating factual information from the error analysis.

Current Prompt:

```

<prompt>
{prompt}
</prompt>

```

Error analysis and current prompt assessment:

```
{gradient}
```

Instructions:

Create an improved, comprehensive prompt that:

1. Integrates all factual information provided in the <modification> tags from the error analysis seamlessly. This is crucial for addressing identified knowledge gaps.
2. Remains general and applicable to various contexts (questions), avoiding mention of specific instances.
3. Structures all content using a logical hierarchy with headers (#) and bullet points (*). Minimize redundancy and avoid contradictions.
4. Maximizes conciseness and clarity. Group related concepts and use precise language to convey complex ideas efficiently.
5. Retains all correct information from the current prompt, optimizing structure to coherently incorporate new information.

Formatting:

Enclose the new prompt within <prompt> and </prompt> tags.

Example:

```

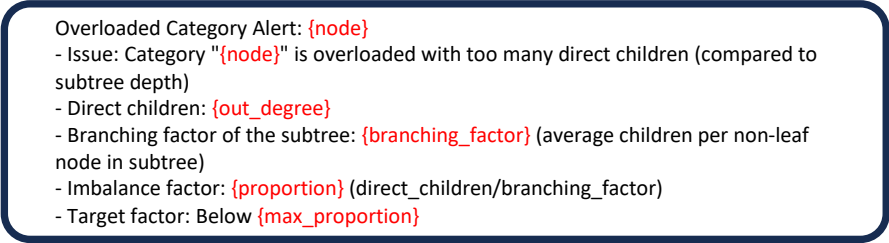
<prompt>
...
</prompt>

```

IMPORTANT: You must not include any meta-information about the task itself in the new prompt. Ensure the prompt is directly usable by a language model without further interpretation.

Output:

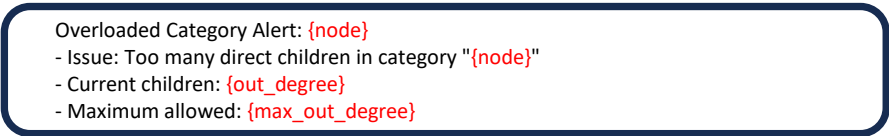
Fig. 16. Template for optimizer LLM to generate new prompt candidates based on current prompt, failure cases, and analyzed gradients.



Overloaded Category Alert: {node}

- Issue: Category "{node}" is overloaded with too many direct children (compared to subtree depth)
- Direct children: {out_degree}
- Branching factor of the subtree: {branching_factor} (average children per non-leaf node in subtree)
- Imbalance factor: {proportion} (direct_children/branching_factor)
- Target factor: Below {max_proportion}

Fig. 17. Template for formatting balance constraint violations.



Overloaded Category Alert: {node}

- Issue: Too many direct children in category "{node}"
- Current children: {out_degree}
- Maximum allowed: {max_out_degree}

Fig. 18. Template for formatting degree constraint violations.

Enhance the prompt for a QA task by integrating factual information from the error analysis and selectively pruning content to address structural issues.

Current Prompt:

```
<prompt>
{prompt}
</prompt>
```

```
{issue_string}
```

Pruning strategy:

- For each overloaded category listed above, remove or consolidate enough children to meet the specified requirements
- Prioritize removing or consolidating children that are least relevant to the error analysis findings
- Keep all children not selected for removal

Error analysis and current prompt assessment:

```
{gradient}
```

Instructions:

Create an improved, comprehensive prompt that:

1. Integrates all factual information provided in the <modification> tags from the error analysis seamlessly. This is crucial for addressing identified knowledge gaps.
2. Remains general and applicable to various contexts (questions), avoiding mention of specific instances.
3. Structures content using a logical hierarchy with headers (#) and bullet points (*). Minimize redundancy and avoid contradictions.
4. Maximizes conciseness and clarity. Group related concepts and use precise language to convey complex ideas efficiently.
5. Retains all correct information from the current prompt, optimizing structure to coherently incorporate new information.

Pruning decision process:

- For each alert, identify which children are least critical based on:
 - * Relevance to the error analysis modifications
 - * Frequency of use in typical questions
 - * Redundancy with other content
- Remove or consolidate only the minimum number of children needed to satisfy the alert requirements
- Preserve all other children and the overall logical structure

Formatting:

Enclose the new prompt within <prompt> and </prompt> tags.

Example:

```
<prompt>
...
</prompt>
```

IMPORTANT: You must not include any meta-information about the task itself in the new prompt. Ensure the prompt is directly usable by a language model without further interpretation.

Output:

Fig. 19. Template for optimizer LLM to generate pruning-aware prompt candidates, incorporating detected violations from pruning analysis.