Divide, Optimize, Merge: Fine-Grained LLM Agent Optimization at Scale

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Abstract

LLM-based optimization has shown remarkable potential in enhancing agentic systems. However, the conventional approach of prompting LLM optimizer with the whole training trajectories on training dataset in a single pass becomes untenable as datasets grow, leading to context window overflow and degraded pattern recognition. To address these challenges, we propose Fine-Grained Optimization (FGO), a scalable framework that divides large optimization tasks into manageable subsets, performs targeted optimizations, and systematically combines optimized components through progressive merging. Evaluation across ALF-World, LogisticsQA, and GAIA benchmarks demonstrate that FGO outperforms existing approaches by 1.6-8.6% while reducing average prompt token consumption by 56.3%. Our framework provides a practical solution for scaling up LLM-based optimization of increasingly sophisticated agent systems. Further analysis demonstrates that FGO achieves the most consistent performance gain in all training dataset sizes, showcasing its scalability and efficiency.

1 Introduction

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Large Language Models (LLMs) have emerged as powerful optimizers for LLM systems, capable of analyzing execution trajectories and refining system modules like prompts (Yang et al., 2024; Zhou et al., 2022; Khattab et al., 2023; Opsahl-Ong et al., 2024), tools (Qian et al., 2023; Zhang et al., 2024c,b; Wang et al., 2024a). These agentic systems have shown promising results in enhancing agent performance across various domains, including reasoning (Cheng et al., 2024; Zelikman et al., 2023), software engineering (Jimenez et al., 2023; Pan et al., 2024), data analysis (Hu et al., 2024b; Jing et al., 2024), computer using (Wang et al., 2025; Xie et al., 2025; Abuelsaad et al., 2024).



Figure 1: Agent optimization approaches. (a) Basic agent execution process. (b) Traditional all-at-once optimization faces context overflow and inferior performance with large trajectory data. (c) Our method: divide-and-conquer optimization with progressive merging enables scalable processing of large datasets.

However, due to the increasing volume of data required for optimizing LLM agentic systems autonomously, directly applying LLM-based optimization approaches encounters a fundamental scalability issue. Existing methods typically concatenate all execution trajectories on the training data and perform optimization in an all-at-once manner, feeding the entire dataset into the LLM optimizer in a single prompt. While this approach works for optimization tasks with small-scale data, it becomes problematic as the data grows. For instance, in the GAIA benchmark (Mialon et al., 2023), agents normally rely on external tools to col042

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lect real-world information and generate lengthy execution traces for subsequent optimization, which 056 is filled with raw documents and complex intermediate reasoning steps, even challenge for human to parse. This increasing complexity leads to two critical limitations: (1) The concatenated trajectories exceed LLM context windows, forcing truncation 061 of valuable optimization signals. (2) Even when content fits within context windows, LLMs struggle with analyzing long-range dependencies in exten-064 sivecorpus (Bai et al., 2024; Liu et al., 2024; Ni et al., 2024; Ravaut et al., 2024), making it hard for the LLM optimizer to capture subtle patterns 067 and relationships between execution traces. As a result, such approaches can produce suboptimal solutions, particularly in complex scenarios where understanding the intricate relationships between different execution trajectories is crucial for improving agent performance. 073

> To address these scalability challenges, we introduce FGO, a framework that enables efficient optimization of LLM-based agentic systems with largescale data. Specifically, FGO operates through three components: (1) Task division that breaks down the large training dataset into more manageable subsets, (2) Fine-grained optimization enabling efficient processing of each subset, and (3) Progressive module merging that adaptively combines optimized modules while preserving crucial insights from each subset. This design allows FGO to effectively handle larger optimization tasks while maintaining high-quality results.

We evaluate FGO by optimizing two agent modules: instruction prompts and tools agent could access. Across diverse tasks including ALF-World (Shridhar et al., 2020), LogisticsQA, and GAIA (Mialon et al., 2023). Agent trained with FGO produces significant performance gains across all datasets, ranging from 8.3% to 38.1%, outperforming other optimization methods by 1.6%-8.6%. Further analysis reveals that FGO maintains superior performance across varying training dataset sizes, highlighting its scalability and stability. Notably, FGO achieves these improvements while reducing prompt token consumption by 56.3% and increasing optimization efficiency by 7.6% compared to conventional all-at-once optimization.

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Our contributions are threefold: (1) We identify and analyze the scalability limitations in current LLM-based optimization approaches for agentic systems. (2) To address the scalability limitation, we propose FGO, a scalable optimization framework that effectively handles large-scale agent op-
timization through task division and progressive107merging. (3) We demonstrate FGO's effectiveness108across diverse tasks and provide insights into its110scalability advantages through comprehensive em-
pirical analysis.111

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2 Preliminary

2.1 Problem Setup

LLM Agent Optimizable Modules Agentic systems exhibit complex behavioral patterns emerging from multiple factors. A critical insight in designing such systems lies in the decomposition of the agent's parameter space into *modules* that can be independently optimized (Anthropic, 2024a). This decomposition enables targeted optimization of specific functional aspects while maintaining global system coherence. Denote the parameter space of agentic system as Θ , which partitions into trainable modules $\{\Theta_i\}_{i=1}^n$ governing distinct behavioral dimensions. Each module must satisfy two key properties to qualify as a modular unit. First, the trainability property requires that each module can meaningfully influence the agent's policy gradients when exposed to specific queries. This ensures the module is sufficiently responsive to reward signals during optimization. Second, the orthogonality property mandates that parameter gradients across different modules exhibit minimal directional alignment during optimization. Such orthogonality constraint ensures modules encode non-redundant functionalities while guaranteeing each contributes uniquely to performance optimization.

Agentic System Optimization An agent interacts with an environment \mathcal{E} by generating a sequence of actions in response to a query. Given parameters θ , the agent's policy determines actions based on the current state of interaction and observation. These actions along with the observations form a trajectory τ that represents the agent's solution attempt for the given query.

$$a_t \sim \pi(\cdot | a_{1:t}, o_{1:t}; \theta), \ o_{t+1} \sim \mathcal{E}(\cdot | a_t), \ \forall t \in [T]$$

$$\tau = \mathcal{A}(q; \theta) = (o_1, a_1, \dots, o_T, a_T)$$
(1)

The performance is quantified through a loss function \mathcal{L} . Given a distribution \mathcal{D} over query-label pairs (q, y), we aim to find optimal agent parameters that minimize expected loss across the task

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2.2 Motivation

In LLM-as-optimizer setting, we assume the numeric value of the policy gradient is not accessiblein Eq. 2. This constraint emerges from a practical reality in modern LLM agent systems - the increasing reliance on proprietary Large Language Models like GPT-4 (OpenAI, 2023) and Claude (Anthropic, 2024b), where internal parameters are inaccessible.

distribution. The optimization objective is:

 $\theta^* = \arg\min_{\theta \in \Theta} \mathbb{E}_{(q,y) \sim \mathcal{D}} \left[\mathcal{L}(\mathcal{A}(q;\theta), y) \right]$

ules provides a unified abstraction for analyzing

performance-critical factors in agentic system de-

sign. In practice, the modules include prompt for

task handling (Wen et al., 2024; Wu et al., 2024b),

long term memory (Zhang et al., 2024e), the avail-

able toolbox (Zhang et al., 2024c), the weights of

backbone LLM (Zeng et al., 2024; Ma et al., 2024).

This formulation of optimization via tuning mod-

Current approaches that leverage LLM as optimizer typically follow a two-step iterative process: first evaluating modules on training data to collect trajectories and losses, then prompting the LLM optimizer with this information to generate improved modules. While these methods have shown promising results (Yang et al., 2024; Zhang et al., 2024c; Cheng et al., 2024), they face fundamental scalability challenges that limit their practical applications.

Context window limit. The inherent constraint 181 of LLM context windows is a critical bottleneck in 182 optimization. As training samples grow, the con-183 catenated trajectories and module-loss pairs can exceed the context capacity of even the most ca-186 pable LLMs. This limitation becomes particularly acute in complex tasks where individual trajecto-187 ries contain extensive reasoning steps or multi-turn 188 interactions. In such scenarios, even a modest number of samples can overwhelm the context window, 190 severely limiting the LLM optimizer's ability to 191 process comprehensive training data. 192

Insufficient context utilization. Even when the
 content fits within context limits, LLMs can face
 significant challenges in effectively processing and
 discovering patterns across extensive collections
 of trajectories (Ni et al., 2024). Recent bench marks on long-form text comprehension and sum marization tasks have consistently demonstrated
 that LLM's performance deteriorates significantly

with increasing text length, particularly in processing complex dialogues and lengthy documents (Bai et al., 2024; Wu et al., 2024a; Ni et al., 2024; Song et al., 2024; Zhang et al., 2024d). In the context of LLM based optimizers, optimization requires grasping long-range dependencies and analyzing fine-grained details to capture subtle patterns across multiple lengthy samples. This inherent limitation of LLMs can lead to suboptimal module updates that fail to capture the full complexity of the optimization problem, especially in real-world applications where performance depends on understanding both broad patterns and fine-grained details across diverse samples. 201

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3 Methods

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3.1 Overview

The overall pipeline of FGO is illustrated in Figure 2. The core concept behind our proposed framework is to divide the large task set into smaller, more manageable subsets and optimize them independently. After we obtain the optimal modules trained on each subsets, we develop an algorithm to progressively merge them into an optimal module.

3.2 Fine-Grained LLM Agent Optimization

Basic Module Optimization We begin with describing how we perform agent optimization. The pipeline is illustrated in Algorithm 1. In each epoch, the agent undergoes a three-phase cycle: exploration, evaluation, and optimization. During exploration, the agent interacts with the given task with the current module, generating the solution trajectories. The evaluation phase introduces a post-hoc LLM based evaluator that analyzes these trajectories to determine correctness, identify failures, patterns as well as potential areas for improvement based on the ground truth and trajectory. The evaluations serve as textual gradients to guide the direction for updating the instruction toward better performance. The optimization phase then leverages these insights by feeding the trajectories, textual gradients into an LLM based optimizer, which synthesizes this information to generate an updated module.

Divide As the number and complexity of task set scales, the length and number of the trajectories can quickly increase, posing challenge to LLM based optimization. To address the issue, we propose a divide-and-conquer based strategy that decomposes the training dataset D into N disjoint



Figure 2: Illustration of FGO's optimization pipeline. The system operates in three stages: (1) Divide: the full dataset is split into manageable subsets, (2) Optimize: parallel optimization is performed on each subset using LLM-based optimization with multiple iterations, and (3) Merge: optimized modules are progressively combined using recursive clustering to produce the final optimal agent system.

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Algorithm 1 Module	Optimization
Input: Task set \mathcal{D} , 1	number of epochs E
Output: Optimized	module θ
$\theta \leftarrow \phi$	▷ Start from scratch
for $e \leftarrow 1$ to E do	
$\mathcal{H} \leftarrow \{\}$	▷ Empty trajectory history
for $(q,y)\in \mathcal{D}$ d	0
$ au \leftarrow \mathcal{A}(q; \theta)$	⊳ Eq. 1
$r \leftarrow \text{Evaluat}$	e(au,y)
$\mathcal{H}.append((a))$	(au,r))
end for	
$\theta \leftarrow \text{LLM}_{\text{optim}}($	\mathcal{H}, θ > Update module
end for	
return θ	

subsets $\{D_i\}_{i=1}^N$, and perform optimization on the subsets independently. By operating on smaller, focused subsets, the intuition is to capture subtle patterns and requirements that might be overlooked in global optimization. The process yields N distinct module-loss pairs, each specialized for its respective subset's characteristics.

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Progressive Merging While decomposition addresses the immediate scalability constraints, it introduces the challenge of integrating N independently optimized modules while preserving

gorithm 2 Progressive Module Merging
Input: List $\mathcal{M} = \{(\theta_i, \mathcal{T}_i, p_i)\}$ containing mod-
ules, their tasks, and performances
Output: Optimized module θ^*
function ProgressiveMerge(\mathcal{M}, t)
if $ \mathcal{M} \leq t$ then
$\theta, p \leftarrow Merge(\mathcal{M}) \triangleright Base: Direct Merge$
return $ heta$
end if
$C \leftarrow KMeans(S, \sqrt{ \mathcal{M} }) \triangleright Adaptive cluster$
for each cluster $c_i \in C$ do
$\theta_i, p_i \leftarrow \text{ProgressiveMerge}(c_i, t)$
end for
return Merge($\{\theta_i, p_i\}$)
end function
return ProgressiveMerge(\mathcal{M}, t)

their specialized insights. The straightforward approach would be to directly prompt an LLM with all module-performance pairs and generate an updated module. However, such all-at-once merging struggles to effectively process and synthesize patterns across many modules simultaneously, potentially losing the specialized optimizations gained through divided optimization. We propose progressive merging, implemented as a recursive algorithm that controls merging granularity through a cluster

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size threshold. Algorithm 2 shows the process of 271 progressive merging. For a given list of module-272 performance pairs, we first check if the list size 273 exceeds the threshold. For larger lists, we partition it into $k = |\sqrt{n}|$ clusters based on similarities, where n is the number of modules. Each resulting 276 cluster then undergoes recursive merging. When a 277 cluster's size falls below the threshold, we merge 278 its modules by prompting an LLM with the mod-279 ule contents and their corresponding performance statistics. After each merge operation, we evaluate 281 the merged module's performance through validating on the combined task set from all constituent modules. The recursive process naturally builds a 284 bottom-up merging tree, where each internal node 285 represents a validated merge of its children's modules. This controlled, progressive approach ensures that each merge operation stays within LLM context limits while capturing intricate relationships between similar modules, ultimately enabling efficient optimization of large-scale agentic systems.

4 Evaluations

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4.1 Experiment Setup

We evaluate FGO by optimizing two different modules of the agentic system: instructions and tools.
With proper instructions on the guidelines for the tasks, the agent can comprehend the scenario and solve it with ease (Fu et al., 2024; Chen et al., 2024; Wu et al., 2024b; Zhao et al., 2024). The tools expand the action space available to the agent, functioning as specialized modules that enable specific capabilities. Optimizing the tool configuration directly impacts the agent's ability to execute complex tasks efficiently and accurately.

Datasets We conduct experiments on three different benchmarks to study the performance of FGO.

306 • ALFWorld (Shridhar et al., 2020) is a text-based 307 benchmark in which the agent is tasked with performing household tasks. Given a high-level objective, the agent needs to interact with the virtual 310 environment and perform actions through natural language to finish the task. We randomly select 312 60 tasks from the training datasets (10 for each 313 task type), and use the unseen set containing 134 314 tasks as test set. The benchmark contains 6 types 315 316 of tasks, we set the number of agent optimizers to 6, with each agent optimizer optimizing 317 each type of task. We report the success rate on different types of tasks and the overall success rate. 320

• LogisticsQA is our own curated benchmark. The dataset consists of UBL format shipping invoice documents from real world scenarios. The agent is tasked to understand and extract the transport reference number from the document. The dataset contains 267 document instances. For further details of the dataset, please refer to Appendix B. We randomly select 48 documents for training, the remaining 219 for testing. We set the number of agent optimizers to 8, each performs optimization on randomly split 6 tasks. A task is considered successful if the agent's answer is an exact match with the ground truth.

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• GAIA (Mialon et al., 2023) is a benchmark designed to test the capability of agents as general assistants. It encompasses tasks from different domains such as file browsing, web searching and scraping, making it a perfect testbed for benchmarking agent's tool usage capability as well as the quality of the toolbox. We utilize 36 tasks from the training set and evaluate on 60 tasks. The optimization is distributed across 4 optimizers, each handling a distinct subset of tasks.

Baselines for Comparison. We compare performance with different agent optimization methods: (1) **All-at-once** optimization represents the conventional approach of performing agent optimization on the whole training set using the algorithm illustrated in Section 3.2; (2) **Batch-wise** optimization employs a fixed-size batching strategy, splitting the training dataset into predetermined chunks and performing optimization sequentially on each task batch within an epoch; (3) **Bootstrapping** optimization implements a stochastic approach, sampling task batches from the training dataset with replacement.

Implementation details. We optimize the instructions for the agent on ALFWorld and LogisticsQA, and optimize the tools on GAIA. For ALF-World, we leverage gpt-4o-mini as the backbone for the agent and evaluator, and gpt-4o for optimization and merging. For LogisticsQA and GAIA, we use gpt-4o in the whole process. For a fair comparison, all methods use the same number of optimization steps.

4.2 Main Results

Finding 1: FGO demonstrates superior optimization performance across multiple domains. We present the optimized agent's performance on different bencmarks in Table 1. For the majority of

Mathada	ALFWorld					LogisticOA	CAIA		
Methods	Pick	Clean	Heat	Cool	Look	Pick Two	Average	LogisticQA	GAIA
Vanilla Agent	69.4	50.5	65.2	20.6	31.5	21.6	45.5	36.3	15.0
All-at-once	90.2	72.6	78.3	78.6	66.7	55.9	75.0	52.1*	21.7*
Batch-wise	77.1	71.0	67.4	64.3	86.1	73.5	72.8	55.7	10.0
Bootstrapping	91.7	77.4	73.9	74.6	87.0	41.2	75.6	62.6	20.0
FGO	90.2	83.8	87.0	88.9	86.1	62.7	83.6	64.8	23.3

Table 1: Performance of the optimized agent using different optimization methods on ALFWorld, LogisticQA and GAIA. The best results are in bold. * denotes that we encounter context window exceeded error during optimization and have to trim the number of trajectory reward pairs sent to the LLM optimizer.

371the tasks, the agent demonstrates performance gain372in most cases after optimization. This highlights373how targeted prompt and tool refinement can sig-374nificantly enhance LLM agent capabilities. Among375the optimization methods, FGO achieves the most376performance boost in all cases, with gains rang-377ing from 8.3% to 38.1% compared to the vanilla378agents.

379 Finding 2: Progressive merging effectively preserves task-specific patterns while achieving global optimal. The superior performance of 381 FGO can be attributed to its divide-and-conquerbased methodology. The All-at-once approach pro-383 384 cesses the entire training dataset simultaneously, requiring the LLM optimizer to learn from trajectories across the complete dataset. This leads to 386 suboptimal performance due to the optimizer's difficulty in processing complex patterns in long corpus, as evidenced by the suboptimal performance on ALFWorld subtasks. Alternative methods like boot-390 strapping optimization and batch-wise optimization demonstrate strong performance in specific categories, but fail to maintain consistent performance across the task spectrum. Their batch-wise optimization approach introduces instability in the training process, as the LLM optimizer encounters 396 different data distributions in successive iterations, potentially compromising previously learned pat-398 terns. In contrast, FGO overcomes these limitations through its systematic merging of independently 400 optimized instructions and tools. By first optimiz-401 402 ing subset-specific instructions and tools and then progressively merging them, FGO can preserve 403 task-specific patterns while building toward global 404 optimization. We further examine the implication 405 of merging on FGO performance in Section 4.4. 406

80 Success Rate (%) 70 60 Batch-wise All-at-once 50 Bootstrapping FGO 40 0 12 24 48 60 Training Data Size

Figure 3: Analysis of the number of training tasks. We run optimization on varied training dataset sizes and plot the performance. FGO achieves best performance in all training settings, and demonstrate a steady increase as the training taskset size increases.

Finding 3: FGO demonstrates extraordinary scalability. We evaluated how training data volume affects optimization performance on ALF-World. As shown in Figure 3, FGO maintains stable performance across all dataset sizes, with consistent improvements as training samples increase. While batch-wise optimization shows similar training accuracy in low-data settings, it yields lower performance compared to bootstrapping optimization, indicating poorer generalization. This aligns with established machine learning principles where bootstrapping enhances generalization (Breiman, 1996). Additionally, All-at-once optimization proves impractical for LogisticsQA and GAIA due to their extensive document lengths (>3,000 tokens) and complex solution trajectories exceeding LLM context windows, validating the need for our scalable approach.

Finding 4: FGO achieves an optimal balance between token cost, efficiency and performance. We visualize the relationship between prompt to-

407 **4.3** Further Analysis

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Figure 4: Comparison of prompt token efficiency across different optimization methods on ALFWorld, LogisticsQA, and GAIA. Each panel plots the trained agent's performance against the total prompt tokens consumed during optimization. Circle diameters are proportional to the optimization token consumption, with crosses (+) indicating circle centers.

ken used for optimization and the performance after training with different optimization methods in Figure 4, and outline the time to train and performance in Figure 5. In terms of token cost, FGO requires larger number of prompt tokens compared to Batchwise optimization and Boostrapping optimization. This is because the merging process requires evaluating on the combined task set from all the constituent modules. This is a sacrifice in exchange for accurately modeling the merged module's capability in order to generate more accurate modules in the merging process. In contrast, All-at-once prompts the LLM optimizer with the whole list of trajectories and losses, leading to the largest token consumption requirements than other methods. In terms of efficiency, FGO can perform optimization in parallel and gather the optimized modules at once, which is an unique advantage compared to the sequential training methods.

4.4 Ablation Study

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We investigate the following questions to understand the impact of different components and hyperparameters in FGO:

How does progressive merging and choice of 452 clustering algorithm affect performance? То 453 analyze the impact of progressive merging and eval-454 uate different clustering algorithms in the merging 455 process, we conduct experiments on the ALFWorld 456 benchmark. We first establish a baseline by remov-457 ing the progressive merging entirely, and instead 458 prompting an LLM to generate the final module di-459 rectly from the module-performance pairs obtained 460 461 from divided optimization. We then evaluate the effect of different clustering algorithms by fixing 462 the independently optimized modules and chang-463 ing the clustering method to Spectral clustering and 464 Bisect K-Means. We report the average and best of 465

Methods	Cluster	ALFWorld	
	Algorithm	Avg of 3	Best of 3
Vanilla	-	45.5	61.9
FGO	None	73.1	84.3
	Spectral	81.6	89.6
	Bisect K-Means	80.1	91.0
	K-Means	83.6	89.6

Table 2: Ablation study on the effects of clustering algorithms used. "None" means we skip the clustering step and directly merge the optimized modules.

three runs in Table 2. Without progressive merging, the method achieves a 73.1% average success rate, demonstrating that even basic merging provides substantial improvement over the vanilla agent. In comparison, the introduction of progressive merging significantly boosts performance. Regardless of the clustering algorithm employed during merging, the final performances all demonstrate consistent improvement to no merging. This consistency suggests that the progressive nature of the merging strategy, rather than the specific clustering algorithm, is the key driver of improvement. 466

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Does the division of training data affect performance? To examine the robustness of FGO, we compare our default category-based partitioning against random partitioning of training tasks in ALFWorld. As shown in Table 3, while random partitioning shows a slight performance drop, the system still maintains strong performance thanks to the progressive merging process, which effectively combines optimization insights across partitions. This demonstrates that FGO's performance remains robust even with suboptimal partitioning strategies.

How does the number of divided subsets affect performance? To answer this question, we conduct ablation study on the number of independent

Dortition	ALFWorld		
Partition	Avg of 3	Best of 3	
Random	80.3	88.1	
Category	83.6	89.6	

Table 3: Ablation on the data partitioning strategy. 'Category' denotes we partition the training data according to the task type.



Figure 5: Ablation study on the number of divided subsets. Most parameter settings achieve similar performance, with varying time for optimization.

agent optimizers. We trained agents on LogisticsQA and set the number of divided subsets to 3, 4, 6, 8, 12. Due to the high cost in running gpt-40, we sampled 100 tasks from the test set and validate the optimized agent's performance respectively. We plot the relationship between performance and training time in Figure 5. The results suggest that the choice of agent number primarily impacts computational efficiency rather than optimization quality.

How does performance change with respect to backbone LLM? Finally, to ensure FGO well generalizes to different backbones, we change the optimizer backbone to o3-mini and observe the metrics. We report the token consumption for training, wall-clock time, and performance in Table 4. In line with the main results, FGO maintains strong performance while reaching most efficiency, with slightly overhead in token consumption.

Method	# Tokens (107)	Time (s)	Avg of 3	Best of 3
All-at-once	8.15	7583	87.8	93.3
Batch-wise	1.59	2969	83.1	92.3
Bootstrapping	1.34	2521	88.8	95.0
FGO	1.97	2142	89.3	95.5

Table 4: Ablation on the optimizer backbone. We leverage o3-mini as the backbone for optimization, and report the metrics. Best result is in bold.

5 Related Work

LLM as Optimizer. LLMs are increasingly used as a blackbox optimizer for different LLM systems. In prompt optimization, LLM is leveraged to automously maximizing LLM's performance to novel tasks without expensive model tuning (Zhou et al., 2022; Pryzant et al., 2023; Cheng et al., 2023; Prasad et al., 2022; Opsahl-Ong et al., 2024; Khattab et al., 2024). In the realm of in-context learning (Min et al., 2021; Dong et al., 2022; Brown, 2020), by automatically retrieving demonstrations from training set (Zhao et al., 2021; Lu et al., 2021; Liu et al., 2021) or from adaptively annotated samples by LLM (Zhang et al., 2023; Wu et al., 2022; Su et al., 2022), prompt with autonomously selected in-context examples can reach performance better can human crafted prompts. LLM based optimizers are also used as a meta-optimizers to improve an LLM based system (Zelikman et al., 2023; Yin et al., 2024).

Automated Agentic System Design. There has been efforts in exploring inference time performance boost since the emergence of Large Language Models (Shinn et al., 2024; Madaan et al., 2024; Yao et al., 2023, 2024; Wei et al., 2022; Guo et al., 2024). Recent works have extended this paradigm to agentic systems. Some works represent and learn the optimal workflow of agentic systems in the form of complex graphs (Zhuge et al., 2024; Wu et al., 2024c), code (Hu et al., 2024a), and trees (Zhang et al., 2024a) to improve the system's performance on complex tasks, while others learns reusable tools (Zhang et al., 2024c; Cai et al., 2023; Qian et al., 2023; Yuan et al., 2023) and experience (Zhao et al., 2024; Wang et al., 2024b) for agentic systems.

6 Conclusion

In this paper, we addressed the scalability challenges in LLM-based agent optimization by introducing FGO, a framework that effectively processes large-scale execution trajectories through task division, fine-grained optimization, and progressive module merging. Our evaluation across multiple dataset demonstrates consistent performance improvements. FGO reaches an optimal balance between performance, efficiency and token consumption.

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The merging process introduces computational overhead, as it requires to back test the merged module on the merged training dataset, resulting in larger token cost compared to Batch-wise optimization and Bootstrappingoptimization. In future works, we attempt to leverage LLM to predict the performance of the merged module using incontext learning, or approximate the performance using Bayesian methods.

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A More Experiments

How is the efficiency of FGO in terms of optimizing time consumption? In this section, we present the time for optimization on each method. Ours are the most efficient thanks to the parallel implementation.

How does the trained agent perform after different optimization methods? We plot the token consumption for inferencing on the dataset with the modules trained with different methods. As shown in Table 6, 7, 8,FGO can reach competent performance with reasonable token consumption overhead.

B LogisticQA Dataset

B.1 Background

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We evaluate our system on a collection of realworld Universal Business Language invoice documents, developed in cooperation with one of the world's largest logistics companies. The primary task is to extract transport reference numbers from these documents. The reference numbers exist in these invoice documents in a non-fixed pattern. It typically requires human effort to extract it manually during real-world business operations. AI agents that can effectively understand the context and extract reference numbers can make the business workflow more efficient. The LogisticQA dataset shows LLMs' ability to achieve such a goal. It contains 267 valid invoice documents and transport reference pairs. It can also reflect LLM's instruction-learning capability in real-world document understanding tasks.

The dataset presents several challenging characteristics that make it an ideal testbed for evaluating the instruction learning capabilities. First, it requires specialized domain knowledge of business documents and terminology not commonly found in general language model training. Second, the hierarchical structure of UBL documents and

-	-		-
Methods	ALFWorld	LogisticQA	GAIA
all	8372	3600	7400
batch	2975.67	2550	4798
bootstrap	2567.72	2621	3957
FGO	1998	2434.0691	5906

Table 5: Performance comparison across different methods on ALFWorld, LogisticQA and GAIA datasets.

Method	Tokens	Performance
All-at-once	8,856,145	75.0
Batch-wise	9,018,478	72.8
Boostrapping	8,172,052	75.6
FGO	7,594,598	83.6

Table 6: Inference cost and performance for ALFWorld.

Method	Tokens	Performance
All-at-once	6,483,562	52.1
Batch-wise	6,872,656	55.7
Boostrapping	5,703,318	62.6
FGO	6,287,424	64.8

Table 7: Inference cost and performance for Logistic-sQA.

the significant variability in format and identification patterns pose substantial extraction challenges. Additionally, as a novel benchmark without prior literature coverage, this dataset offers unique opportunities to assess agents' adaptive learning abilities in a practical, high-stakes business context. 921

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B.2 Dataset Statistics

The analysis of our XML business document dataset demonstrates strong alignment with realworld business documentation patterns, as shown in Figure 6. The document length distribution peaks between 200-500 lines, while the XML structure complexity with most documents containing 100-400 tags. The token distribution centered around 2,000-4,000 tokens indicates a long-context understanding challenge for LLMs. Notably, the language distribution across documents (Turkish: 39.5%, English: 29.6%, Spanish: 22.0%, Italian: 8.9%) reflects a realistic multinational business environment, particularly common in European and Mediterranean operations where English serves as a lingua franca alongside regional languages.

B.3 Dataset Example

Here is an example XML business document in the dataset. The ground truth extraction is 847 5321 9084. The named and loations in the dataset are all anonymized.

<?xml version="1.0" encoding="UTF-8"?>
<Invoice xmlns="urn:oasis:names:specification:ubl:schema:xsd:
 Invoice-2"
 xmlns:cac="urn:oasis:names:specification:ubl:schema:
 xsd:CommonAggregateComponents-2"
 xmlns:cbc="urn:oasis:names:specification:ubl:schema:
 xsd:CommonBasicComponents-2">
 <cbc:UBLVersionID>2.1



Figure 6: Statistical analysis of XML business documents. Top left: Distribution of document lengths showing typical business document sizes. Top right: Distribution of XML tags indicating document structure complexity. Bottom left: Token distribution demonstrating the long context challenge for LLM. Bottom right: Language distribution across documents reflects business documents' multinational nature.

Method	Tokens	Performance
All-at-once	527,551	21.7
Batch-wise	436,337	10.0
Boostrapping	877,283	20.0
FGO	787,921	23.3

Table 8: Inference cost and performance for GAIA.

<pre><cbc:customizationid>urn:cen.eu:en16931:2017#compliant#urn: fdc:peppol.eu:2017:poacc:billing:3.0CustomizationID></cbc:customizationid></pre>
<cbc:id>rmCMsB6Km6J40p2a</cbc:id>
<pre><cbc:issuedate>2023-10-11</cbc:issuedate></pre>
<cbc:invoicetypecode>Invoice</cbc:invoicetypecode>
<cbc:documentcurrencycode>TRY</cbc:documentcurrencycode>
<cbc:note>SALE</cbc:note>
HADIMKOY BRANCH 847 5321 9084
No withholding tax applies when not self-owned according to law
This invoice must be paid by: 01/08/24
PLEASE INDICATE THE VEHICLE PLATE NUMBER AND INVOICE NUMBER IN THE DESCRIPTION OF YOUR BANK TRANSFER RECEIPT
For invoices not paid by due date, late payment interest will
be charged according to the Law on Collection Procedure
of Public Receivables (AATUHK).
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<cac:accountingsupplierparty></cac:accountingsupplierparty>	
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<pre><cbc:name>S.S 350 COOPERATIVE AIRPORT CARGO TERMINAL LOGISTICS SERVICES MOTOR CARRIERS </cbc:name></pre>	
<cac:postaladdress></cac:postaladdress>	
<pre><cbc:streetname>Cargo Terminal Cooperative Service</cbc:streetname></pre>	
<cbc:cityname>Springfield</cbc:cityname>	
<cbc:postalzone>None</cbc:postalzone>	
<cac:country></cac:country>	
<pre><cbc:identificationcode>TR</cbc:identificationcode></pre>	
IdentificationCode>	
<cac:accountingcustomerparty></cac:accountingcustomerparty>	
<cac:party></cac:party>	
<cac:partyname></cac:partyname>	
<pre><cbc:name>GLOBAL LOGISTICS SOLUTIONS LTD.Name></cbc:name></pre>	
<cac:postaladdress></cac:postaladdress>	
<pre><cbc:streetname>INDUSTRIAL DISTRICT SPRINGFIELD< /cbc:StreetName></cbc:streetname></pre>	
<cbc:cityname>None</cbc:cityname>	
<pre><chc.postalzone>None</chc.postalzone></pre>	

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1023	This invoice must be paid by: 01/08/24
1024	PLEASE INDICATE THE VEHICLE PLATE NUMBER AND INVOICE NUMBER IN
1025	THE DESCRIPTION OF VOUR DANK TRANSFER DESCRIPT
1023	THE DESCRIPTION OF YOUR DANK TRANSFER RECEIPT
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1051	<pre><cbc:invoicedquantity unitcode="EA">1.0</cbc:invoicedquantity></pre>
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1057	<pre><cbc:description>THY-NEWTOWN transportation fee-78</cbc:description></pre>
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1059	<pre><cbc:name>IHY-NEWIOWN transportation fee-/8XYZ432</cbc:name></pre>
1060	chc:Name>
1000	
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1062	<cac:price></cac:price>
1062	
1003	<pre><cbc:priceamount currency1d="IRY">2243.26</cbc:priceamount></pre>
1064	PriceAmount>
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1069	C Complexity Analysis

In this section, we analyze the computational complexity of the recursive clustering in the progressive merging process.

C.1 Clustering Tree Depth

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At each recursive step, the number of module is reduced by taking the square root:

$$n_{i+1} = \sqrt{n_i}, \quad \text{with } n_0 = N.$$
 (3)

The recursion stops when the number of items sat-1077 isfies: 1078 $(1, \infty)$

$$n_D = N^{(1/2)^D} \le t.$$
 (4)

Taking logarithms on both sides gives:

$$(1/2)^D \cdot \log N \le \log t.$$
 (5) 1081

Solving for D yields:

$$D = O\left(\log \log N\right). \tag{6}$$

Backtesting Complexity C.2

Each merge operation performs a backward testing 1085 over all tasks contributing to the merged module. 1086 Since tasks are merged without duplication, the 1087 total number of unique tasks remains T throughout 1088 the process. As every level of the clustering tree 1089 processes T tasks and the depth of the tree is D =1090 $O(\log \log N)$, the overall complexity of testing is: 1091

> $O(T \cdot \log \log N)$. (7)

This demonstrates that the overhead introduced by backward testing is modest as N scales. 1094

D Prompt 1095

ALFWorld **D.1**

Perform actions and interact with a 1098 household to solve a task. At the 1099 beginning of your interactions, you 1100 will be given the detailed 1101 description of the current 1102 environment and your goal to 1103 accomplish. The environment only 1104 accept certain format of actions. 1105 Here are two examples, learn the 1106 pattern carefully. 1107

D.2 LogisticsQA

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Task background 1110 Read the content of a xml file which 1111 contains a shipment invoice document 1112 in UBL format. You are tasked to 1113 understand the content and extract 1114 the transport reference number from 1115 it. 1116 When you reach a conclusion, format your 1117 answer as "final answer: [extracted 1118 reference number]" 1119

D.3 GAIA

1121	
1122	# Task
1123	You need to solve the question below
1124	given by a user. When you are
1125	building tasks, explicitly consider
1126	where the task can benefit from web
1127	navigation capability.
1128	
1129	# Task
1130	{task}
1131	11 11 11