# Let Large Language Models Find the Data to TRAIN THEMSELVES

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#### ABSTRACT

The current iterative development process for large language models (LLMs) is heavily data-centric, relying on human researchers and engineers to manually analyze model performance and determine what data to acquire for further training. However, this human-supervised approach is costly and may fail to identify optimal training signals. Its scalability is further limited as models become increasingly capable and may eventually exceed human intelligence. To address these issues, we propose an automated framework that enables models to autonomously discover and strategically acquire the most valuable training data to enhance their performance. It establishes a self-improving framework where models can invoke APIs to crawl and/or generate tailored datasets from various resources and environments, and retrain themselves. The data selection decisions are shaped by reinforcement feedback signals that reward performance gains while penalizing computational overhead. This formulation incentivizes models to develop selfknowledge about their strengths and areas for improvement in order to efficiently select training data. Empirical results demonstrate that LLMs operating within our framework are able to autonomously and strategically acquire valuable training data to enhance their performance across a variety of skills in 1,000 diverse in-house test tasks and three public benchmarks.

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#### 1 INTRODUCTION

Large language models (LLMs) (Zhao et al., 2023) have seen remarkable progress in various do-031 mains and tasks with extensive training on massive data. Currently, one of the most important 032 aspects of developing LLMs is *data engineering*, which typically involves teams of researchers 033 and engineers meticulously examining model outputs, identifying shortcomings, and then collecting 034 and curating next-iteration training data from various sources to refine model performance (Achiam et al., 2023; Anil et al., 2023; Dubey et al., 2024). While this method has yielded impressive results, it is not without inherent limitations. The human-driven nature of this process introduces poten-037 tial biases and inefficiencies, as it relies heavily on the intuition and expertise of the development 038 team (Wang et al., 2023; Sun et al., 2024). Furthermore, as these AI models continue to evolve in complexity and capability, there is a growing concern that they may soon exceed human intelligence in certain domains, which raises questions about the long-term viability and scalability of current 040 development practices (Burns et al., 2024). 041

In this work, we conceptualize and prototype an ACTIVE DATA SEARCH (ADS) framework that fa cilitates LLMs to automatically acquire training data from external environments for training them selves, without human supervision. In ADS, existing data collection and curation methods are
 encapsulated into APIs and the LLMs themselves determine when and how they use these APIs for
 data acquisition. The APIs may involve a wide range of data crawling, filtering, cleaning, refine ment, synthesis, and manual annotation techniques to obtain tailored training data. The data sources
 are also varied, from raw texts extracted via web searches to documents sourced across various
 platforms, as well as supervised demonstrations generated by AI assistants.

We achieve the above automatic process through development of an optimizer that generates these
 APIs sequentially based on the target task. Specifically, the optimizer first analyzes the required
 capabilities for successful task completion, then strategically invokes appropriate API calls to collect
 training data for performance improvement. To facilitate the optimizer's decision-making process in
 obtaining optimal training data, we propose a reinforcement learning strategy for optimizer training,

leveraging feedback reward signals from the policy to maximize task performance while minimizing computational costs by iterative rejection sampling (RS) (Bai et al., 2022a) and direct preference optimization (DPO) (Rafailov et al., 2024). This refinement process fosters the development of self-knowledge regarding the model's strengths and weaknesses, enabling more efficient training data discovery and utilization. Compared to recent studies (Lozhkov et al., 2024; Wettig et al., 2024; Zhou et al., 2024a) that focus on improving the quality of training data agnostically, a unique characteristic of our framework is its model- and task-specific nature for data acquisition, enabling more tailored and targeted performance enhancement.

062 In our experiments, we build on top of two popular open-source LLMs: Qwen-2-7B-Instruct (Yang 063 et al., 2024a) and Gemma-2-9B-Instruct (Riviere et al., 2024), and establish three distinct types of APIs for knowledge acquisitions, utilization, and enhancement. Experimental results across 064 1,000 in-house test tasks with both reward model (RM) and GPT-4 evaluation demonstrate that 065 the LLM equipped with ADS presents consistent performance improvements, achieving a win rate 066 of more than 80% in RM judgment compared to the initial baseline. Moreover, in three public 067 benchmarks: AlpacaEval 2.0 (Dubois et al., 2024), Arena-Hard (Li et al., 2024), and MT-Bench 068 (Zheng et al., 2024), ADS exhibits generalized performance enhancement, even enabling the rel-069 ative smaller 7B/9B LLMs to compete with the larger 72B/27B counterparts. It is worth noting that across tasks of varying categories and complexities, ADS typically improves performance in 071 knowledge, reasoning, and challenging tasks. To sum up, we highlight our contributions as follows:

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• We pioneer the idea of automating the data search process for training LLMs, a task currently handled by expert human efforts, making a further step towards fully automated self-improving AI systems capable of continuous learning and adaptation.

- We propose the ACTIVE DATA SEARCH (ADS) framework, which encapsulates existing data collection and synthesis methods into APIs, enabling LLMs to generate optimal API calls for efficient data discovery through interactions with diverse environments.
- We showcase the effectiveness of ADS by conducting comprehensive experiments on 1,000 diverse in-house test tasks and three public benchmarks. Our results demonstrate that LLMs equipped with ADS exhibit substantial performance improvements. Furthermore, we provide an in-depth analysis of the underlying factors contributing to the efficacy of ADS.
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## 2 Related Work

LLM as an Optimizer With the progressive advancement of LLMs, LLM-as-an-optimizer (i.e., 087 maximizing a downstream metric of an AI system using LLMs without human intervention) has emerged as a new paradigm, where the input optimization task and the output solution are described 880 in natural language and processed by an LLM. This approach has been pioneered in automatic 089 prompt engineering (Pryzant et al., 2023; Zhou et al., 2023; Wang et al., 2024; Guo et al., 2024; 090 Yang et al., 2024b; Xiao et al., 2024), pipeline optimization of LLM-based agents (Zhang et al., 091 2024; Khattab et al., 2024; Yuksekgonul et al., 2024; Zhuge et al., 2024; Zhou et al., 2024b), and new 092 algorithm discovery (Liu et al., 2024a; Lu et al., 2024). Our research distinguishes itself from these previous studies as our optimization goal is to enhance the fundamental capabilities of LLMs through 094 automated data collection and curation, which is very important given that data is the (perhaps most) 095 major power engine for today's LLMs. Moreover, existing work simply prompts off-the-shelf LLMs 096 for optimization, which can lead to sub-optimal performance as these LLMs have not been explicitly 097 trained to do so. Conversely, we develop methods to fine-tune the optimizer models.

098 **Synthetic Data Generation** Synthetic data, which leverages the generation capability of LLMs 099 for data construction, has become crucial components across various stages in LLMs develop-100 ment (Long et al., 2024), including pre-training (Gunasekar et al., 2023; Li et al., 2023; Ben Allal 101 et al., 2024), supervised fine-tuning (Taori et al., 2023; Mukherjee et al., 2023; Xu et al., 2023), 102 and preference learning (Rafailov et al., 2024; Dubey et al., 2024; Adler et al., 2024). Instead of 103 contributing to the booming spectrum by proposing yet another data synthesis method, we introduce 104 a meta-optimization framework, which aims to integrate different data synthesis techniques and de-105 velop the best strategy (our optimizer) to leverage them. More recently, there is also a growing interest in targeted data synthesis for enhancing the model's particular weaknesses (Lee et al., 2024; 106 BAAI, 2024; Cheng et al., 2024). Nevertheless, these approaches require extensive evaluation to 107 spot the weaknesses, which sometimes necessitates expert-level knowledge for test set design and



Figure 1: Overview of ACTIVE DATA SEARCH (ADS) framework. Upper: The optimizer is developed to generate optimal API calls and execute them in the environment for training data acquisition. The policy is then updated using the collected training data. Bottom: To make effective and efficient data-collecting decisions, the optimizer is iteratively refined through reinforcement learning.

result analysis. In contrast, our work strives to develop self-knowledge capabilities; the AI system
 knows its strengths and areas for improvement without any external feedback or guidance. Specifically, given only a small set of representative task queries, the optimizer introspects and identifies
 potential capability gaps that prevent the policy from completing the target task, and strategically
 generates optimal API calls to collect training data for addressing the identified gaps.

132 **Self-Improving of LLMs** Developing an autonomous self-improving system has been a major focus of current LLM research. Conventional reinforcement learning from human feedback (RLHF) 133 methods (Ziegler et al., 2019; Stiennon et al., 2020; Ouyang et al., 2022; Dong et al., 2024; Liu et al., 134 2024b; Rosset et al., 2024) train a reward model from human preference data and subsequently use 135 this model to fine-tune LLMs via reinforcement learning. The reliance on human preference data of 136 course can be removed for scenarios where the correctness of output can be validated automatically 137 and unambiguously (Zelikman et al., 2022; Gulcehre et al., 2023; Singh et al., 2023). For general 138 instruction following, recent studies have built upon the success of LLM-as-a-judge (Zheng et al., 139 2024) and leverage AI feedback for self-improvement, an approach also known as RLAIF (Bai et al., 140 2022b; Lee et al., 2023). Yuan et al. (2024) and Wu et al. (2024) have further advanced this concept 141 by employing LLMs to provide self-rewarding feedback on their own generated outputs. Unlike 142 previous work that constrains the system from leveraging external signals, our framework allows 143 for information inflow from external environments through the interactions of API calls, potentially 144 elevating the upper bounds of self-improving.

## 146 3 SELF-IMPROVING VIA ACTIVE DATA SEARCH

147 The primary objective of our ACTIVE DATA SEARCH (ADS) framework is to endow AI systems 148 with the capability to acquire valuable training data from external environments for retraining them-149 selves, thereby facilitating self-improvement with minimal human supervision. As illustrated in 150 Figure 1, we develop an *optimizer* model for a *policy* model. The optimizer model is designed to 151 discover tailored training datasets to improve the policy by generating textual API calls to inter-152 act with various resources and environments. In this section, we start with a brief introduction to 153 the problem formulation, followed by an overall description of policy optimization and optimizer 154 refinement processes. We defer the details of our prototype implementations in Section 4.

156 3.1 PROBLEM FORMULATION

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Given a target task T and a policy model  $\mathcal{M}^p$ , the goal of ADS is to maximize the performance of the policy model on T through active search for optimal training data. The data search process is conducted by an optimizer model  $\mathcal{M}^o$  and a set of pre-defined APIs. Each API requires some input parameters and returns output data gathered from various environments. These APIs can be implemented through a variety of established methods, which may encompass but are not limited to data crawling, filtering, cleaning, refinement, synthesis, and manual annotation. The resultant data can also be sourced from a broad spectrum, such as internet search engines, LLM-based AI assistants, or crowdsourcing annotation services. To mitigate excessive and unnecessary API invocations, we assign varying costs to different APIs according to their practical complexities. Following common practice, each target task is represented by a set of instructions Q, which serve as input for the optimizer model. The output of this model is an action trajectory A, comprising multiple API calls.

#### 168 3.2 POLICY OPTIMIZATION

The system optimizes its policy model  $\mathcal{M}^p$  for a given target task T through the following steps. First, the optimizer model  $\mathcal{M}^o$  is instructed to conduct a comprehensive analysis of the instructions Q, identifying the essential required capabilities. Following this,  $\mathcal{M}^o$  performs an introspective assessment of its own proficiencies and deficiencies on these identified capabilities, and generates sequential API calls  $A = [a_1, a_2, ..., a_K]$  for data acquisition, where K is the number of API calls and is determined on-the-fly. Notably, the above process is completed by the optimizer as free-form text generation, enabling seamless incorporation of any pre-defined APIs.

176 Next, we execute each API call  $a_k$  in the environment  $\mathcal{E}$ , and collect the returned data to obtain a 177 training dataset D, which may include a variety of data types such as raw documents, supervised 178 demonstrations, and preference data, following the best practice of current LLM training. Finally, 179 we train the original  $\mathcal{M}^p$  on the tailored training dataset to update its knowledge and capacities, 180 resulting in an updated policy model  $\hat{\mathcal{M}}^p$ .

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182 3.3 Optimizer Refinement

To make efficient data-collecting decisions, the optimizer model  $\mathcal{M}^o$  should be aware of the strengths and weaknesses of the policy model  $\mathcal{M}^p$ . Therefore, we propose an iterative training process for optimizer refinement. First of all, we assume a set of training tasks  $\mathcal{T} = \{T\}$ , where reliable performance measurements are available. It is important to note that we *do not* make this assumption at test-time since the evaluation of arbitrary real-world tasks can be complex and resource-intensive. Instead, we posit that the self-knowledge developed for the optimizer during the training phase can be effectively generalized to novel test tasks.

190 We then employ reinforcement learning and consider both performance gains and API costs in re-191 ward design. The training is conducted iteratively. At each iteration, we sample multiple API trajectories  $\mathcal{A} = \{A\}$  for each training task T. We then execute the data acquisition and policy 192 training processes accordingly and collect the corresponding performance gain S(A) and API cost 193 C(A). To avoid potential data leakage, we partition the instruction set Q of T into an observed set 194  $Q^o$  and another held-out set  $Q^h$ . The optimizer can only see the examples in the observed set and 195 the performance gains are measured based on the held-out set. This results in a set of quadruple 196  $\mathcal{B} = \{(T, A, S, C)\}$ . We then optimize  $\mathcal{M}_{t}^{o}$  to  $\mathcal{M}_{t+1}^{o}$  on  $\mathcal{B}$  with reinforcement learning algorithms 197 such as rejection sampling (Bai et al., 2022a) and direct preference optimization (Rafailov et al., 198 2024). The complete process of optimizer refinement is described in Algorithm 1. 199

Re	<b>quire:</b> Training tasks $\mathcal{T}$ , policy model $\mathcal{M}^p$ , optimizer model $\mathcal{M}^o$ , environment $\mathcal{E}$
1:	for iteration $t$ in $N$ do
2:	Initialize optimizer buffer $\mathcal{B} = \{\}$ .
3:	for task $T$ in $\mathcal{T}$ do
4:	Split task instructions $Q$ into observed set $Q^o$ and held-out set $Q^h$ .
5:	Sample API trajectories $\mathcal{A} \sim \mathcal{M}_t^o(\cdot   Q^o)$ .
6:	for trajectory A in $\mathcal{A}$ do
7:	Execute A in $\mathcal{E}$ to acquire data to update $\mathcal{M}^p$ to $\hat{\mathcal{M}}^p$ .
8:	Collect performance gain $S(A)$ of $\hat{\mathcal{M}}^p$ on $Q^h$ , and API cost $C(A)$ .
9:	Add $(T, A, S, C)$ to $\mathcal{B}$ .
10:	end for
11:	end for
12:	Optimize $\mathcal{M}_t^o$ to $\mathcal{M}_{t+1}^o$ using reinforcement learning on $\mathcal{B}$ .
13:	end for
14:	return $\mathcal{M}_N^o$ .

API Name	Parameter	Return	Description	Cost
Information Retrieval	Query	Document	Sparse and Dense Retrieval	Low
Demonstration Generation	Topic	Instruction-Response Pair	Synthesis with the Policy	Medium
Question Answering	Question	Question-Answer Pair	Annotated by Stronger LLM	High

Table 1: Implementation details of our data collecting APIs.

## 4 EXPERIMENTAL SETUP

#### 4.1 APIs

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225 We design three distinct data-collecting APIs to facilitate the *acquisition*, *utilization*, and *enhance*-226 ment of knowledge. The first API is Information Retrieval, which employs both sparse and 227 dense retrieval to retrieve relevant documents from external knowledge databases such as Wikipedia, 228 thereby supporting knowledge acquisition, analogous to the pre-training stage of LLMs. The second 229 API is Demonstration Generation, which utilizes the policy model to generate appropriate 230 exemplar instruction-response pairs, tailored to various knowledge application scenarios, reminis-231 cent of the alignment stages of LLMs. The last API is Question Answering, which resorts 232 to the wisdom of human experts, mimicking how humans learn from each other.<sup>1</sup>. It provides to-233 the-point answers to questions proposed by the optimizer model. Notably, this framework is not restrictive and can accommodate additional APIs as needed. In each API trajectory, these APIs 234 are invoked sequentially, e.g., api\_name\_1 (api\_param\_1) . . . api\_name\_n (api\_param\_n). 235 Subsequently, the corresponding API calls are executed to formalize the training dataset. We then 236 combine the training datasets from different API calls to update the policy model. For tasks where 237 the model possesses the required capabilities, a "none" option is incorporated. We present the API 238 implementation details in Table 1. 239

To avoid excessive API calls, e.g., asking questions that the policy model already knows the answer to, we take into account the API cost in our implementation. The cost associated with each API varies according to their practical complexities and computational overhead. Concretely, we assign relative costs as follows: Information Retrieval is at one since retrieval is fast and cheap, Demonstration Generation at two given generation is slow and resource-intensive, and Question Answering at three as it requires a more powerful model or manual efforts. Further implementation details of APIs are provided in Appendix A.

247 4.2 DATASET

248 To train and evaluate the optimizer model, it is essential to collect a diverse set of "target tasks" 249 for which we aim to optimize the performance of the policy model. For this purpose, we adopt the 250 general instruction-following dataset Llama-3-Magpie-Air-3M-v0.1 (Xu et al., 2024). Each instruc-251 tion in this dataset is associated with several labels such as task category, intent, and difficulty. The 252 instructions and labels are generated by Llama-3-8B-Instruct (Dubey et al., 2024). Subsequently, we 253 group the instructions with identical labels into different clusters, with each cluster representing a distinct "target task". We discard tasks with fewer than five instructions. The resulting dataset com-254 prises 10,239 distinct tasks, which we partition into 8,739 tasks for training, 500 tasks for validating, 255 and 1,000 tasks for testing. In the train and valid splits, we allocate three observed instructions per 256 task for trajectory generation and reserve two held-out instructions for performance measurement. 257 This approach ensures that the optimizer learns to improve performance at *task level* rather than *in*-258 stance level, as over-fitting on the observed instructions may not necessarily translate performance 259 gains on the held-out instructions. For the test split, to enhance the robustness of evaluation, we aug-260 ment the initial five instructions per task to 100 using Self-Instruct (Wang et al., 2023), with three 261 instructions as observed and 97 as held-out. More details of our dataset are shown in Appendix B. 262

**263 4.3** EVALUATION METHODS

In-house Evaluation We employ both the RM and GPT-4 (Achiam et al., 2023) to compare responses generated by the original and updated policy models on held-out instructions across our test tasks. We report the average win, tie, and lose rate across all tasks. For RM evaluation, we sample five API trajectories and compute the average RM score among them, ensuring statistical robustness. For GPT-4 judgment, we employ a head-to-head comparison using the pairwise evaluation prompt

<sup>&</sup>lt;sup>1</sup>For efficiency and reproducibility, we employ a stronger LLM as a proxy for human supervision in practice.

proposed by Zheng et al. (2024). We try two different response orders to prevent order sensitivity. To save token usage, we only sample one trajectory and test on two held-out instructions per task.

273 **Generalizing to Public Benchmarks** We additionally utilize three well-established benchmarks 274 for further evaluating the generalizability of the trained optimizer models, including AlpacaEval 2.0 275 (Dubois et al., 2024), Arena-Hard (Li et al., 2024), and MT-Bench (Zheng et al., 2024). AlpacaEval 2.0 includes 805 instructions for daily chat scenarios while Arena-Hard contains 500 more chal-276 lenging real-world questions. MT-Bench consists of 80 multi-turn dialogues spanning eight distinct 277 domains<sup>2</sup>. Since the original version of MT-Bench contains incorrect reference responses, we fol-278 low previous works (Adler et al., 2024; Wan et al., 2024) to use the updated version for evaluation. 279 The proposed approach aims to optimize the performance on specific target tasks. However, these 280 benchmarks (AlpacaEval 2.0, Arena-Hard, and MT-Bench) cover a wide range of distinct tasks, 281 which can be too broad to be considered as a single target task. To conduct meaningful experiments, 282 we make the following adaptations. First, we cluster the original instructions based on task cate-283 gory and difficulty, utilizing the approach in Xu et al. (2024). This process yields 38, 34, and 21 284 "target tasks" for AlpacaEval 2.0, Arena-Hard, and MT-Bench, respectively. Then, we employ the 285 Self-Instruct approach to generate three new instructions for each task and use them as the observed 286 instructions for that task. We only assess model performance on the original instructions provided 287 in these benchmarks. Following conventions (Meng et al., 2024; Adler et al., 2024), we conduct a standard evaluation using GPT-4 judgment. We adhere to the default setups and report the win 288 rate of the updated policy models against the GPT-4 baseline for each benchmark. Additionally, 289 we conduct a supplementary evaluation using RM as judgment and report the average adjusted win 290 rate, calculated as win rate  $+0.5 \times$  tie rate. For both RM and GPT-4 judgments, we also report the 291 weighted averages of these benchmarks based on their number of samples. Further details of the 292 evaluation process can be found in Appendix D. 293

#### 94 4.4 TRAINING DETAILS

We employ Qwen-2-7B-Instruct (Yang et al., 2024a) and Gemma-2-9B-Instruct (Riviere et al., 2024) as our policy models<sup>3</sup>. The optimizer model is initialized using the corresponding policy model.

During each iteration of ADS, the optimizer model generates five API trajectories per target task, 298 based on the observed instructions. To further enhance the diversity of the trajectories, we incorpo-299 rate three additional default trajectories, each corresponding to a specific API type. These trajecto-300 ries are executed in the data-collecting environments to construct a comprehensive training dataset. 301 Next, the policy model is updated through either in-context learning or fine-tuning using this training 302 data. Considering the frequent policy model updating for each target task, we use in-context learn-303 ing to maintain computational efficiency while preserving performance, since extensive research has 304 demonstrated that in-context learning can achieve comparable effectiveness to fine-tuning (Mosbach 305 et al., 2023; Agarwal et al.). We then determine the reward signal of each API call trajectory by 306 evaluating the performance gains of the updated policy model on the held-out instructions. We use 307 FsfairX-Llama-3-RM-v0.1 (Xiong et al., 2024) as the RM for evaluation. Finally, we iteratively 308 update the optimizer model by direct preference optimization (DPO) (Rafailov et al., 2024) on the chosen and rejected trajectories with the highest and lowest rewards. To ensure training stability, we 309 perform warm-up rejection sampling (RS) (Bai et al., 2022a) on the chosen trajectories exhibiting 310 the highest rewards before iterative DPO for optimizer model training. In Section 6.1, we further 311 illustrate the comparison between DPO and RS, as well as investigate the impact of the default API 312 trajectories. The iterative training process of the optimizer model is presented as follows: 313

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- Prompting:  $\mathcal{M}^{o}$  is initialized from  $\mathcal{M}^{p}$  without fine-tuning, then direct prompting.
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- RS Iteration 0:  $\mathcal{M}_0^o$  is initialized from  $\mathcal{M}^o$ , then warm-up RS on chosen API trajectories.
- DPO Iteration 1, 2, 3:  $\mathcal{M}_1^o$ ,  $\mathcal{M}_2^o$ ,  $\mathcal{M}_3^o$  are initialized from  $\mathcal{M}_0^o$ ,  $\mathcal{M}_1^o$ ,  $\mathcal{M}_2^o$ , then DPO on chosen and rejected API trajectories.

To enhance the optimizer model's capacity for reward improvements while minimizing API costs, we introduce a novel cost-control approach, which draws inspiration from the length-control strategy

<sup>&</sup>lt;sup>2</sup>Given that our dataset focuses on single-turn tasks, we evaluate the 1st turn performance for consistency.

<sup>&</sup>lt;sup>3</sup>Since our training data are generated by Llama-3-8B-Instruct, we exclude it from our choices of policy models to avoid any potential biases.

324 Updated (Left) Wins Tie Original (Right) Wins 325 DPO Iter 3 vs. Original 4.511.2 14.9 40.1 14.3 84.3 4.113.3 45.7 46.0 39.1 82.6 326 DPO Iter 2 9.4 13.9 16.9 4.015.8 47.1 15.2 76.7 37.6 80.2 37.8 327 45.6 vs. Original 328 DPO Iter 1 63.5 20.4 16.1 35.2 47.1 17.8 <mark>4.516.6</mark> 39.2 47.5 13.3 78.9 vs. Original RS Iter 0 37.4 41.7 20.9 26.4 52.2 21.5 70.9 6.6 22.5 45.6 14.7 330 39.8 vs. Original 331 Prompting vs. Original 23.4 22.1 60.8 17.1 18.4 36.7 39.9 7.7 25.3 48.4 332 (b) Qwen-2-7B-Instruct GPT-4 Judge. (d) Gemma-2-9B-Instruct GPT-4 Judge. (a) Owen-2-7B-Instruct (c) Gemma-2-9B-Instruct RM Judge. 333 RM Judge

Figure 2: Comparisons between responses generated by the updated and original policy models 335 across in-house test tasks with both RM and GPT-4 judgments. The updated policy models are 336 developed on training data collected by different iterations of optimizer models.

338 employed in LLM alignment (Wu et al., 2024). Our approach posits that among trajectories with 339 comparable rewards, those associated with lower costs are more valuable for optimization and thus 340 deserve higher reinforcement feedback. Specifically, we introduce a cost tier parameter  $\tau \in [0, 1]$ 341 to control the trade-off between rewards and costs. Trajectories within the top-tier rewards ranging 342  $[(1-\tau)R_{\text{max}} + \tau R_{\text{min}}, R_{\text{max}}]$  are considered to have similar performance. From this subset, we select 343 the trajectory with the lowest cost as the chosen trajectory. Conversely, for the reject trajectory, we select the one with the highest cost within  $[R_{\min}, (1 - \tau)R_{\min} + \tau R_{\max}]$ . To maintain an optimal 344 balance between reward and cost, we empirically determine the cost tier parameter at 0.1. We further 345 conduct experiments to illustrate the effectiveness of the proposed cost-control approach in Section 346 6.2. More information on training details can be found in Appendix C. 347

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#### 5 MAIN RESULTS

351 5.1 IN-HOUSE EVALUATION

352 Figure 2 illustrates the evaluation results on target tasks across in-house test split. We compare the 353 responses generated by the updated and original policy models, displaying the task win, tie, and lose 354 rates with both RM and GPT-4 judgments. 355

356 ADS presents significant superiority across 1,000 in-house test tasks. We can first observe 357 that the prompting method yields slight performance gains. For instance, the updated policy model 358 achieves a win rate of 36.7% compared to the original policy model's 23.4% in RM judgment, 359 and 22.1% to 17.1% in GPT-4 judgment for Qwen-2-7B-Instruct. Following the iterative training 360 process, the final model exhibits a remarkable enhancement, with a win rate of 84.3% versus 11.2% 361 in RM evaluation and 46.0% versus 14.9% in GPT-4 evaluation. These substantial performance 362 improvements can be attributed to the valuable training data discovered by the optimizer model in 363 ADS, which enhances the knowledge and capabilities required to accomplish these test tasks.

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- Iterative ADS boosts consistent performance improvements. During the initial iteration of DPO training, our optimizer model exhibits rapid adaptation to high-reward API trajectories. Con-366 sequently, the updated policy model achieves substantial improvements in win rates: from 37.4% to 367 63.5% according to RM judgment, and from 26.4% to 35.2% as evaluated by GPT-4 for Owen-2-368 7B-Instruct. As the number of training iterations increases, the updated policy model consistently 369 demonstrates improved win rates. Given that the training tasks remain constant across different iter-370 ations, we posit that the consistent performance gains are from the automatic weakness identification 371 and refinement during the iterative training process, thus progressively increasing the probabilities 372 of generating optimal API trajectories for self-improvement. 373
- 374 5.2 PUBLIC BENCHMARKS
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- 376 In Table 2, we present the evaluation results on three public benchmarks, including AlpacaEval 2.0, 377 Arena-Hard, and MT-Bench. We compare the responses generated by the policy model and the GPT-4 baseline model and show the win rates with both RM and GPT-4 judgments.

Madala		RM Ju	dgment			GPT-4 Ju	ıdgment	
Widdels	AE	AH	MT	Avg.	AE	AH	MT	Avg.
Qwen-2-7B-Instruct $(\mathcal{M}^p)$	31.7	56.1	66.9	42.6	24.0	25.6	55.9	26.4
Prompting $(\mathcal{M}^o \to \mathcal{M}^p)$	33.2	57.0	68.1	43.8	24.9	26.7	52.5	27.2
RS Iteration 0 ( $\mathcal{M}_0^o \to \mathcal{M}^p$ )	32.4	56.7	68.1	43.2	24.2	26.7	53.8	26.8
DPO Iteration 1 ( $\mathcal{M}_1^o \to \mathcal{M}^p$ )	34.9	57.9	66.9	45.0	28.6	28.0	53.8	29.8
DPO Iteration 2 ( $\mathcal{M}_2^o \to \mathcal{M}^p$ )	<u>36.5</u>	<u>60.6</u>	<u>69.4</u>	<u>47.1</u>	<u>30.6</u>	28.8	<u>57.7</u>	<u>31.5</u>
DPO Iteration 3 $(\mathcal{M}_3^{\overline{o}} \to \mathcal{M}^p)$	38.8	61.1	71.9	48.8	31.9	30.1	59.4	32.8
$\Delta$ to Qwen-2-7B-Instruct	(+22.3%)	(+8.9%)	(+7.5%)	(+14.6%)	(+32.9%)	(+17.7%)	(+6.2%)	(+24.3%)
Gemma-2-9B-Instruct $(\mathcal{M}^p)$	28.6	70.0	71.3	46.0	34.8	37.5	55.0	36.9
Prompting $(\mathcal{M}^o \to \mathcal{M}^p)$	28.0	59.2	70.0	41.7	33.8	30.0	56.3	33.7
RS Iteration $0 (\mathcal{M}_0^o \to \mathcal{M}^p)$	30.5	65.6	71.3	45.5	35.3	34.8	51.3	36.0
DPO Iteration 1 ( $\mathcal{M}_1^o \to \mathcal{M}^p$ )	30.4	48.4	66.9	39.0	<u>36.7</u>	22.4	54.4	32.6
DPO Iteration 2 $(\mathcal{M}_2^o \to \mathcal{M}^p)$	33.0	67.9	70.6	47.8	36.2	35.2	57.5	37.1
DPO Iteration 3 ( $\mathcal{M}_3^o \to \mathcal{M}^p$ )	<u>32.8</u>	65.7	69.4	<u>46.8</u>	37.0	<u>37.4</u>	<u>56.9</u>	38.3
$\Delta$ to Gemma-2-9B-Instruct	(+14.5%)	(-6.1%)	(-2.6%)	(+1.6%)	(+6.3%)	(-0.2%)	(+3.4%)	(+3.7%)
Llama-3.1-70B-Instruct	53.0	76.7	83.8	63.3	39.5	57.0	75.0	47.9
Qwen-2-72B-Instruct	38.9	66.8	73.1	50.9	35.1	48.3	66.9	41.7
Gemma-2-27B-Instruct	33.6	80.2	75.0	52.8	37.0	49.9	60.6	43.0

Table 2: Comparisons between responses generated by the updated policy models and the baseline GPT-4 on AlpacaEval 2.0 (AE), Arena-Hard (AH), and MT-Bench (MT) with both reward model (RM) and GPT-4 judgment. Percentages indicate the relative improvements/decreases observed in the final iteration of the updated policy model when compared to the original policy model.



Figure 3: Fine-grained evaluation of different updated policy models and the original Qwen-2-7B-Instruct across various task categories (left) and difficulties (right) in AlpacaEval 2.0.

**ADS demonstrates generalized capabilities on public benchmarks.** For the target tasks from public benchmarks, our approach exhibits generalized improvements. Overall, the updated policy model of Qwen-2-7B-Instruct shows significant relative gains across all benchmarks, with an av-erage enhancement of +14.6% and +24.3% in RM and GPT-4 judgment, respectively. Notably, in AlpacaEval 2.0, the improvements are even more pronounced, e.g., +22.3% in RM evaluation and +32.9% in GPT-4 evaluation. These findings reveal that our optimizer model, despite being trained on limited target tasks, demonstrates the capacity to find valuable training data for practical tasks, effectively addressing the challenges for real-world task optimization.

**ADS enhances policy model to rival that of more powerful LLMs.** We show that with the help of training data collected from our optimizer model, smaller and weaker policy models can achieve comparable results to those of larger and stronger LLMs. Specifically, in the RM evaluation within AlpacaEval 2.0, Qwen-2-7B-Instruct with ADS achieves a win rate of 38.8%, which is almost equivalent to the performance of the substantially larger Qwen-2-72B-Instruct. Similarly, in the GPT-4 evaluation, Gemma-2-9B-Instruct with ADS, achieves a win rate of 37.0%, matching the performance of larger Gemma-2-27B-Instruct. 

**ADS typically enhances knowledge-intensive and reasoning-related tasks.** We conduct a fine-grained evaluation across distinct task categories in AlpacaEval 2.0. The results of Qwen-2-7B-



Figure 4: Ablation study results of Qwen-2-7B-Instruct across in-house test tasks with RM judgment (left) and public benchmarks with GPT-4 judgment (right), where "w/o DPO" refers to the replacement of direct preference optimization with rejection sampling algorithm, while "w/o Default" denotes the exclusion of default API trajectories for optimizer model training.

448 Instruct are illustrated in Figure 3 (left). We find that compared to the original baseline, ADS 449 improves the performance in most of the categories, especially for those that require substantial 450 general or specific knowledge and advanced reasoning abilities, such as information-seeking, role-451 playing, reasoning, and planning. However, in categories like editing, creative writing, and coding 452 & debugging, our approach only has slight improvements or maintains comparable to the baseline. 453 This limited enhancement can be potentially attributed to the inherent nature of these tasks, which primarily involve format and style rewriting, as well as fragment modifications, presenting inherent 454 455 challenges for optimization through in-context learning from acquired training data.

ADS particularly improves in complex and challenging tasks. In Figure 3 (right), we further
 demonstrate the performance across tasks with various levels of difficulty. The results reveal that
 ADS yields more substantial improvements as task complexity increases. Specifically, the relative
 performance enhancement increases from +14.2% for very easy tasks to a remarkable +76.5% for
 tasks categorized as very hard. These results further demonstrate the potential of ADS for continuous self-improving, typically in complex tasks that lack expert supervision.

## 463 6 ABLATION AND ANALYSIS

#### 464 465 6.1 Ablation Studies

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In this section, we delve into the key components in our practical implementation of ADS, focusing
on the training algorithm and the construction of API trajectories. We first investigate and compare
the performance of the optimizer model when trained iteratively using rejection sampling and direct
preference optimization. Subsequently, we analyze the influence of adding default API trajectories
into the optimizer model's training process. The evaluation results across in-house test tasks with
RM judgment and public benchmarks with GPT-4 judgment are shown in Figure 4.

472 **DPO enhances discrimination between chosen and rejected trajectories.** We can observe that 473 compared to rejection sampling, the implementation of direct preference optimization substantially 474 improves the optimizer model's capacity to differentiate between chosen and rejected API trajectories, which is illustrated by a significant increase in the average win rate from 49.1% to 84.3% 475 across in-house test tasks. Similarly, in public benchmarks, the win rate improved from 28.6% to 476 32.8%. This enhanced discriminative capability facilitates more effective weakness identification 477 and decision-making processes of our optimizer model, ultimately leading to high-reward API tra-478 jectory exploration and optimal training data acquiring for deficiency enhancement. 479

Incorporating default API trajectories enhances trajectory diversity. In addition to the five
 trajectories sampled by the optimizer during its training process, we incorporate three default trajectories, each corresponding to a distinct data-collecting API in our implementation. Table 4 in
 Appendix C illustrates an example of both default and generated trajectories. The inclusion of these
 default API trajectories alongside the self-generated candidates results in a more diverse set of trajectories for optimizer model training, facilitating improved average win rates across all iterations, both in in-house test tasks and public benchmarks.

# 486 6.2 ANALYSIS RESULTS

488 We further make an in-depth analysis to investigate the factors contributing to the efficacy 489 of ADS, focusing on two key aspects: the ad-490 vantages of self-explored training data and the 491 implementation of the cost-control mechanism. 492 To evaluate the impact of self-explored training 493 data, we compare the API trajectories generated 494 by our optimizer model against those curated 495 using a baseline strategy. This baseline ap-496 proach utilizes the Question Answering 497 API for each observed instruction in the tar-498 get task to construct the corresponding API 499 trajectory. Subsequently, we employ the col-500 lected data for policy model optimization in both cases. Regarding the cost-control mecha-501 nism, we compare our method with an alterna-502 tive approach that prioritizes reward maximiza-



Figure 5: Effectiveness of self-explored training data and cost-control mechanism in maximizing win rate while minimizing API cost.

tion without considering API costs. Figure 5 illustrates these analytical results, encompassing both in-house test tasks using RM judgment (left) and public benchmarks with GPT-4 judgment (right).

Self-explored data presents more suitable for LLMs training. Despite employing the most so phisticated and expensive Question Answering API for training data construction, the approach without self-explored training data achieves a relatively lower win rate, e.g., 81.9% versus
 84.3% across in-house test tasks, while incurring higher API costs, e.g., 9,000 versus 8,219, compared to our approach. The optimizer model in ADS is designed to automatically identify and address the potential capability gaps in specified tasks based on the developed self-knowledge. Consequently, our approach provides a more tailored and targeted performance improvement.

513 **Cost-control mechanism reduces the API cost while improving performance.** To maximize the 514 potential for self-improvement while maintaining appropriate resource allocation, we implement 515 a cost-control mechanism that optimizes the trade-off between minimizing costs and maximizing 516 performance during the training process of the optimizer model, as detailed in Section 4.4. In comparison to the approach that focuses solely on maximizing performance without considering 517 costs, our method not only achieves a lower cost as expected but also demonstrates an improved win 518 rate. The performance improvements can be attributed to the increased trajectory diversity compared 519 to the reward maximization approach. This observation indicates that our approach enables the 520 development of a robust and cost-effective system for data acquisition, ultimately contributing to 521 improved overall performance and reduced computational overhead.

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## 7 CONCLUSION & LIMITATIONS

In this study, we explored enabling LLMs to autonomously acquire optimal training data for self-526 improvement with minimal human intervention. We proposed a novel framework, ACTIVE DATA 527 SEARCH (ADS), which utilizes LLMs themselves as an optimizer to strategically invoke appro-528 priate APIs, facilitating the discovery of tailored training datasets from external environments for 529 self-training. To ensure efficient data-collecting decisions, we introduced an iterative refinement 530 algorithm for the optimizer, guided by reinforcement feedback signals aiming to maximize task per-531 formance while minimizing computation costs. Through a series of experiments on 1,000 in-house test tasks and three public benchmarks, we demonstrated the effectiveness and generalizability of 532 ADS. Notably, ADS exhibited the capacity to enhance the performance of smaller and weaker lan-533 guage models to be comparable with larger and stronger LLMs on AlpacaEval 2.0. This automated 534 process of data discovery and self-training presents opportunities to reduce the reliance on human 535 expertise in LLM development, providing a new direction for future research in this domain. 536

The current implantation is a proof-of-concept with several limitations. First, the optimizer and policy models are separate. Unifying them is an interesting avenue for future work. Second, the APIs included currently are far from covering all existing data techniques. Third, we did not consider multi-turn optimization of the policy models in the framework.

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#### 756 DETAILS OF APIS А 757

758 In this section, we first present the prompt for API trajectory generation of the optimizer 759 model in Figure 6, then show the detailed implementation of our data collecting APIs, in-760 cluding (1) Information Retrieval, which facilitates efficient knowledge acquisition; (2) 761 Demonstration Generation, which enables various knowledge utilization scenarios; and (3) Question Answering, which serves to enhance and refine the acquired knowledge. 762

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764	Prompt for API Trajectory Generation
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766	# Task Overview
767	Your goal is to analyze input prompts, identify knowledge gaps, and strategically use
768	provided APIs to enhance your knowledge and capabilities.
769	# Described ADIs
770	# PIOVIDED APIS
771	1 "information retrieval(query: string)". Retrieves relevant documents for a given search
772	query. Use for factual knowledge gaps.
773	2. "example_instantiation(topic: string)": Generates practical instances based on a given
774	topic. Use for applying knowledge to concrete situations.
775	3. "question_answering(question: string)": Provides answers to a given question. Use for
776	deeper understanding of knowledge.
777	
778	# Constraints and Guidelines
779	1. Focus on common and general knowledge and capabilities requirements across all the
780	input prompts.
781	2. Use API cans only to address competence gaps when necessary, not to directly solve the
782	3 If you need to make API calls formatted as < ani calls > < ani > ani name 1(ani naram 1)
783	<pre>//api&gt;<api>api name 2(api param 2) </api></pre>
784	4. If you do not need to make API calls, formated as <api_calls>none</api_calls>
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786	# Input:
787	{observed_instructions}

Figure 6: Prompt for API trajectory generation of the optimizer model. {observed\_instructions} is the placeholder for the observed instructions in the target task.

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**Information Retrieval** For our retrieval corpus, we utilize the Wikipedia (en) from December 20th, 2022<sup>4</sup>, encompassing approximately 8.59 million paragraphs. Our retrieval process employs a two-stage approach. Initially, we implement sparse retrieval using the BM25<sup>5</sup> algorithm to identify the top 1,000 most relevant documents for a given search query. Subsequently, we refine this selection through dense retrieval, leveraging the BGE-Large-EN-v1.5 (Xiao et al., 2023) embedding model to obtain the most appropriate document from the previously identified candidates.

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**Demonstration Generation** To obtain knowledge utilization examples, we employ an approach 800 that relies solely on the policy model itself without incorporating external tools. Specifically, we 801 leverage the policy model to synthesize demonstrations by generating instructions and correspond-802 ing responses based on a given knowledge topic. The prompt used for demonstration generation is 803 shown in Figure 7. 804

**Question Answering** To enhance the comprehension of acquired knowledge, we employ Llama-3.1-70B-Instruct (Dubey et al., 2024) as a replacement for human experts to generate comprehensive responses to complex questions. The prompt used for question answering is illustrated in Figure 8.

<sup>4</sup>https://huggingface.co/datasets/Cohere/wikipedia-22-12 <sup>5</sup>https://github.com/xhluca/bm25s

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## Prompt for Demonstration Generation

Generate an Instruction and the corresponding comprehensive Response related to the Topic.

Topic: {topic}

Figure 7: Prompt for Demonstration Generation. {topic} is the placeholder for the knowledge topic.

#### Prompt for Question Answering

Provide a detailed Answer to the given Question.

Question: {question}

Figure 8: Prompt for question answering. {question} is the placeholder for the given question.

## **B** DETAILS OF DATASET

We group instructions into clusters based on three key attributes: category, intent, and difficulty. The category attribute represents the broad task type, encompassing areas such as creative writing, reasoning, and coding. The intent attribute indicates the primary objectives within the instructions, including getting helpful tips, identifying logical fallacy, develop software extensions. The difficulty attribute quantifies the complexity of following the instructions, ranging from very easy to very hard.

835 To improve the robustness of evaluation re-836 sults, we augment the size of the held-out set 837 for each target task in the test split. Specifi-838 cally, we leverage five existing instructions as 839 seed examples, and prompt GPT-4 to generate 840 new instructions that are significantly different 841 from these initial examples but belong to the 842 same task (Wang et al., 2023). To maintain 843 distinctiveness, we employ a filtering mecha-844 nism whereby any generated instructions with

Statistics	Train	Valid	Test
# Task	8,739	500	1,000
# Category	12	12	12
# Intent	4,982	371	902
# Difficulty	5	5	5
# Obs. Inst. Per Task	3	3	3
# Held. Inst. Per Task	2	2	97

Table 3: Statistics of train, valid, and test splits.

a Rouge-L similarity score exceeding 0.7 when compared to the original instructions are eliminated.
The prompt for instruction augmentation is illustrated in Figure 9. The statistics of our train, valid, and test splits are shown in Table 3.

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## C DETAILS OF TRAINING PROCESS

For policy model updating, we employ ICL on the collected training dataset for each target task,
including retrieved documents, instantialized instruction-response pairs, and answers to complex
questions, as the supplementary information to address the given held-out instruction. The prompt
for ICL of the policy model is shown in Figure 10.

855 For optimizer model updating, We train the optimizer model with a batch size of 128 and a maximum 856 sequence length of 2048. The training is conducted on a single node with 8x80GB Nvidia A100 857 GPUs for one epoch per iteration. We perform RS for a single iteration and DPO for three iterations. 858 The models are optimized using the AdamW (Loshchilov & Hutter, 2019) optimizer with  $\beta_1 = 0.9$ and  $\beta_2 = 0.999$ . We use a weight decay of 0.0 and gradient clipping of 1.0. A cosine learning rate 859 schedule is employed, with a warmup ratio of 0.1 and a maximum learning rate of 2e-5 for RS and 860 5e-7 for DPO. The  $\beta$  parameter in DPO is set to 0.01. Our training framework is developed based 861 on the HuggingFace Transformers (Wolf et al., 2020) and TRL (Werra et al., 2020). We show an 862 example of default and generated API trajectories in Table 4. 863



Figure 9: Prompt for task-specific instructions augmentation. {task} is the placeholder for the given task. {seed\_instruction\_i} is the placeholder for i-th seed instruction.

#### Prompt for ICL

{collected\_data}

Your task is to read the above text to answer the following question.

1. Note that the above information is only visible to you, don't indicate that you have read above text in your answer. For example, don't say "according to the information provided above".

2. Do not solely rely on the provided information. You know much more than the provided information. Use it as a hint to write an comprehensive, informative, elaborate, and helpful answer.

{held\_out\_instruction}

Figure 10: Prompt for ICL of the policy model. {collected\_data} is the placeholder for the training dataset derived from the optimizer model. {held\_out\_instruction} is the placeholder for the held-out instruction in the target task.

Example o	of Default and Generated API Trajectories
Observed	Instructions.
Explain the Describe the Analyze the	e implications of the Einstein-Podolsky-Rosen paradox on quantum entanglement. he mathematical formulation of the wave function collapse in the Copenhagen interpr te potential applications of quantum tunneling in developing next-generation transistor
Generated	I API Trajectory:
# Analysis	of Requirements
After analy	uring the input prompts. I have identified the required background knowledge and br
bilities as f	follows:
1. Advance	ed knowledge of quantum physics
2. Ability	to explain complex scientific concepts
3. Underst	anding of quantum mechanics principles
4. Familiai	ity with practical applications of quantum theory
# Compete	ence Assessment
I have kno	wledge gaps in quantum mechanics principles and capability gaps in explaining com
tinc conce	pts. Therefore, Theed to make API calls for this set of prompts.
# API Call	S
<api_calls< td=""><td>&gt;</td></api_calls<>	>
<api>ret</api>	instances("Quantum theory application")
<api>ask</api>	question("How to describe and analysis complex scientific concepts?")
<td>\$&gt;</td>	\$>
Default A	PI Trajectory:
# Analysis	of Requirements
After analy	vzing the input prompts. I have identified the required background knowledge and br
bilities.	in the second
# Compete	ence Assessment
I have kno	wledge gaps and canability gaps. Therefore, I need to make API calls for this set of n
- nuve kilo	meese sure expressing super mererore, r need to make mir teams for any set of p
# API Call	8
<or -11<="" td=""><td>x</td></or>	x
<api_calls< td=""><td>&gt; auestion("Explain the implications of the Finstein-Podolsky-Rosen paradox on quar</td></api_calls<>	> auestion("Explain the implications of the Finstein-Podolsky-Rosen paradox on quar
glement.")	Applies of the Emission Foundation of the Emission Foundation of quality of the Construction of the Emission of the Em
-api>ask	question("Describe the mathematical formulation of the wave function collapse in
hagen inter	repretation.")
<ap1>ask.</ap1>	question (Analyze the potential applications of quantum tunneling in develo transistors ")
<td>S&gt;</td>	S>
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Table 4. A	In example of default and generated API trajectories for a set of observed in

#### **DETAILS OF EVALUATION SETUPS** D

We first show the detailed implementation of our in-house evaluation and public benchmarks in Table 5. Then, we provide the corresponding task statistics of AlpacaEval 2.0, Arena-Hard, and MT-Bench in Table 6 and Table 7 by category and difficulty, respectively.

Benchmark	# Task	# Ins.	Baseline Model	RM Judgment	GPT-4 Judgment
In-house Test Split	1,000	97,000	Original Policy Model	FsfairX-Llama-3-RM-v0.1	GPT-4-1106-Preview
AlpacaEval 2.0	38	805	GPT-4-1106-Preview	FsfairX-Llama-3-RM-v0.1	GPT-4-1106-Preview
Arena-Hard	34	500	GPT-4-0314	FsfairX-Llama-3-RM-v0.1	GPT-4-1106-Preview
MT-Bench	21	80	GPT-4-0314	FsfairX-Llama-3-RM-v0.1	GPT-4-0125-Preview

Table 5: Implementation details of evaluation on in-house test tasks and public benchmarks.

Catagony	AlpacaEval 2.0		Arena-Hard		MT-Bench	
Category	Number	Percentage	Number	Percentage	Number	Percentage
Advice Seeking	79	9.8%	12	2.4%	4	5.0%
Brainstorming	25	3.1%	5	1.0%	1	1.3%
Coding & Debugging	42	5.2%	204	40.8%	7	8.8%
Creative Writing	54	6.7%	6	1.2%	5	6.3%
Data Analysis	7	0.9%	66	13.2%	3	3.8%
Editing	73	9.1%	19	3.8%	5	6.3%
Information Seeking	381	47.3%	63	12.6%	21	26.3%
Math	40	5.0%	56	11.2%	17	21.3%
Planning	61	7.6%	45	9.0%	3	3.8%
Reasoning	27	3.4%	17	3.4%	11	13.8%
Role Playing	14	1.7%	4	0.8%	3	3.8%

Table 6: The task category statistics of AlpacaEval 2.0, Arena-Hard, and MT-Bench.

D:66 14	Alpac	aEval 2.0	Aren	a-Hard	MT-Bench	
Difficulty	Number	Percentage	Number	Percentage	Number	Percentage
Very Easy	27	3.4%	0	0.0%	1	1.3%
Easy	491	61.0%	81	16.2%	25	31.3%
Medium	256	31.8%	339	67.8%	52	65.0%
Hard	25	3.1%	79	15.8%	2	2.5%
Very Hard	6	0.7%	1	0.2%	0	0.0%

Table 7: The task difficulty statistics of AlpacaEval 2.0, Arena-Hard, and MT-Bench.

#### COMPARISON BETWEEN ADS AND DATA CONSTRUCTION BASELINES E

1016 In this section, we expand our experimental evaluation by comparing the proposed ADS framework 1017 with several baseline methods for training data construction. These methods include: (1) Prompt-1018 ing, which constructs API trajectories through optimizer model prompting without fine-tuning; (2) 1019 Retrieval Augmentation, which employs both sparse and dense retrieval to identify relevant doc-1020 uments based on target task instructions, similar to the Information Retrieval API; (3) 1021 Self-Instruct, which utilizes the policy model to generate new instruction-response pairs for the target task, functioning analogously to the Demonstration Generation API; (4) Rule-based 1022 QA, which leverages an stronger LLM to answer each instruction in the target task, comparable to 1023 the Question Answering API. The empirical results presented in Table 8 indicate that ADS, 1024 incorporating all three APIs, significantly outperforms these baseline methods across both in-house 1025 test tasks and public benchmarks, and maintaining its simplification without human intervention.

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9	9	9	
1	0	0	0
1	0	0	1
1	0	0	2
1	0	0	3
1	0	0	4
1	0	0	5
1	0	0	6
1	0	0	7
1	0	0	8
1	0	0	9
1	0	1	0
1	0	1	1
1	0	1	2
1	0	1	3

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026	Methods	Qwen-2-7B-Instruct		Gemma-2-9B-Instruct	
027		In-house Test Tasks	Public Benchmarks	In-house Test Tasks	Public Benchmarks
028	Prompting	36.7	27.2	67.0	33.7
129	Retrieval Augmentation	24.2	26.8	46.4	32.6
0_00	Self-Instruct	55.8	31.6	76.9	35.1
030	Rule-based QA	81.9	32.0	79.7	36.0
031	ADS	84.3	32.8	82.6	38.3

Table 8: Comparison between ADS and training data construction baseline methods.

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# INFLUENCE OF THE INSTRUCTION-FOLLOWING DATASET

1037 Since we adopt the instructions from Llama-3-Magpie-Air-3M-v0.1 (Xu et al., 2024) as the task 1038 instructions in our optimizer training process, we conduct a controlled experiment to ensure a fair 1039 comparison. Specifically, we fine-tune our base models using this dataset and evaluate their per-1040 formance on public benchmarks before and after fine-tuning. As shown in Table 9, the fine-tuning 1041 process leads to a notable degradation in model performance. This decline can be attributed to the 1042 fact that our base models (Qwen-2-7B-instruct and Gemma-2-9-Instruct) have already undergone 1043 extensive fine-tuning with high-quality training data, whereas the Llama-3-Magpie-Air-3M-v0.1 1044 dataset may contain relatively lower-quality data. These empirical findings substantiate that the per-1045 formance improvements observed in our experiments stem from the effectiveness of the proposed ADS, rather than from the instruction-following dataset. 1046

#### 1047 Owen-2-7B-Instruct Gemma-2-9B-Instruct 1048 Methods AlpacaEval 2.0 Arena-Hard MT-Bench AlpacaEval 2.0 Arena-Hard MT-Bench Average Average 1049 Base Model 24.0 25.6 55.9 26.4 34.8 37.5 55.0 36.9 Base Model w/ Magpie 11.9 11.7 43.1 13.6 14.8 12.0 44.9 15.5 1050

Table 9: Comparison between the base models before and after fine-tuning on the instruction-following dataset, where "w/ Magpie" denotes the base models after fine-tuning.

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