PLAY2PROMPT: ZERO-SHOT TOOL INSTRUCTION OPTIMIZATION FOR LLM AGENTS VIA TOOL PLAY

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ABSTRACT

Large language models (LLMs) are increasingly integrated with external tools to complete user requests. Many real-world applications require LLMs to use specialized tools in a zero-shot setting. To achieve this, current methods primarily rely on prompting LLMs with tool-specific information, yet tool documentation is often underspecified or noisy, limiting effectiveness. Manual improvements are inefficient and impractical, as they require domain expertise to rewrite documentation and test on carefully curated held-out datasets to evaluate performance gains. Automatic prompt engineering techniques are not applicable either, because they require labeled examples, which is unavailable in the zero-shot setting. In this work, we introduce PLAY2PROMPT, an automated framework that iteratively refines tool documentation and generates usage examples. PLAY2PROMPT enables LLMs to explore tool input-output behaviors, allowing us to effectively search the space of possible tool descriptions and examples. The generated examples not only guide LLM inference but also serve as validation data to ensure more effective tool use. Extensive experiments on real-world tasks demonstrate significant improvements in zero-shot tool performance across both open- and closed-source models.

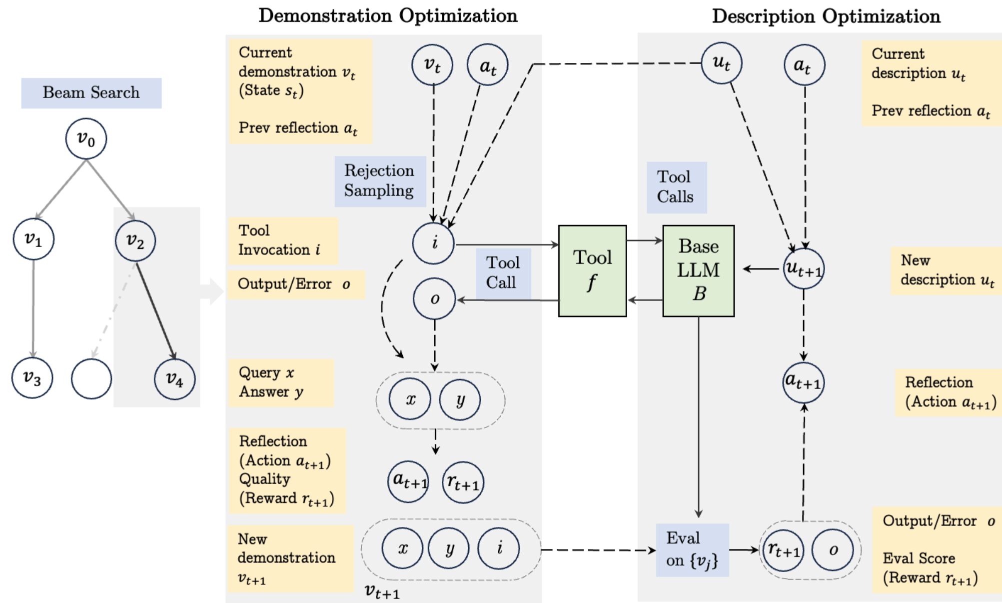
1 INTRODUCTION

Recently, there has been growing research interest in enhancing large language models (LLMs) by integrating external tools with specialized capabilities. This augmentation allows for automatic planning and execution of tool usage, thereby enabling LLMs to solve complex tasks with greater accuracy and produce responses that are more aligned with human preferences (Mialon et al., 2023; Qin et al., 2024a). For instance, open-source models have been fine-tuned on manually curated or synthetically generated function-calling data to improve performance in specific reasoning and question-answering tasks (Schick et al., 2023; Yang et al., 2023). Additionally, both open-source base models and closed-source black-box models are being trained to invoke a limited set of built-in tools, such as mathematical calculators or search engines. However, while these tools address general use cases, they often prove insufficient for real-world complicated tasks that require domain-specific functionalities. Therefore, it is essential to develop methods that enable these tool-use frameworks to dynamically learn how to use user-defined tools.

Training models to specialize in new tools necessitates extensive fine-tuning data and significant computational resources, rendering this approach impractical for large-scale applications. A more viable alternative involves augmenting the set of built-in tools by supplementing user-defined tools at inference time in a zero- or few-shot manner via prompting (Lu et al., 2023; Shen et al., 2023). This method capitalizes on the zero-shot tool-calling capabilities of current LLMs, which have been tuned with tool-use instructions to facilitate this plug-and-play functionality.

One typical such paradigm is ReAct (Yao et al., 2023), wherein the model plans and selects appropriate tools to accomplish the given task, interleaving reasoning steps with tool retrieval, tool call predictions, and executions. In the ReAct paradigm, the success of learning to use new tools, particularly in zero-shot scenarios, hinges on *comprehensive tool documentation and demonstrations* (Hsieh et al., 2023; Patil et al., 2023). Such documentation generally consists of tool descriptions, parameter specifications, output formats, and other related meta-information, which provides critical information for equipping the LLM with necessary information to utilize the tools correctly.

Figure 1: The PLAY2PROMPT framework: Beam search iteratively searches demonstrations, incorporating tool play into the exploration and self-reflection process (Left). After demonstrations are optimized, beam search is once again applied to optimize descriptions by evaluating on the demonstrations as test set, and incorporating tool use outputs/errors (Right).



However, in numerous practical cases, users fail to provide adequate documentation or exemplar demonstrations to the model, nor do they invest in crafting improved documentation tailored for LLM utilization. This lack of information can lead to failures in tool usage, such as syntax errors in both zero-shot and fine-tuned models (Zhang et al., 2023a), hallucinations due to lack of proper tool documentation (Hsieh et al., 2023), and diminished performance resulting from insufficient demonstrations (Xu et al., 2023). Manually enhancing tool documentation and creating example demonstrations is laborious and inefficient, which is further compounded by the need for labeled testing data for each tool to assess effectiveness. When attempting to scale up to larger API databases or online code repositories, these challenges become even more pronounced.

While automatic prompt engineering techniques have been shown to outperform manual optimization (Wang et al., 2024), they prove inapplicable in this context due to their reliance on labeled examples for testing—resources that are inherently unavailable in zero-shot settings (Wu et al., 2024). Existing methods for revising tool documentation typically involve directly prompting LLMs to optimize tool descriptions (Yuan et al., 2024), lacking the capacity to evaluate whether the rewritten documentation enhances the LLM's tool use performance, instead depending heavily on meticulously crafted meta-prompts and oracle example demonstrations supplied within the meta-prompts.

To address these challenges and facilitate general zero-shot tool utilization, we introduce PLAY2PROMPT, an automated framework, which iteratively refines tool documentation and generates example tool usage demonstrations, as illustrated in figure 1. PLAY2PROMPT does not rely on any external tool use examples. Instead, drawing inspiration from human trial-and-error methodologies, it prompts an LLM agent to "play" with the new tools to explore their functionalities and usage, based on which the tool use examples and refined tool descriptions are generated.

During each generation process, PLAY2PROMPT executes multiple trial-and-error iterations, leveraging both successful and erroneous tool-use instances to guide the search trajectory. We employ self-reflection (Madaan et al., 2023; Pryzant et al., 2023; Shinn et al., 2023) to generate error feedback, thereby directing the search algorithm towards progressively improved outputs. Crucially, we iteratively refine not only the tool descriptions but also generate example demonstrations. The generated examples function as a validation set, enabling LLMs to interact with and evaluate tool usage, which subsequently guides the further enhancement of tool descriptions. Throughout this iterative process, PLAY2PROMPT systematically expands the search space in a tree structure, prioritizing paths with higher self-reflection or evaluation scores. PLAY2PROMPT operates entirely in a zero-shot manner and is inherently task-agnostic, making it a practical and scalable solution for enhancing LLM tool utilization without necessitating additional labeled data or manual intervention.

We demonstrate the effectiveness of PLAY2PROMPT by applying it to real-world scenarios. On the StableToolBench benchmark (Guo et al., 2024), our approach consistently surpasses baseline methods for both open-source LLaMA models (Dubey et al., 2024) and closed-source OpenAI GPT models (Achiam et al., 2023). Extensive experiments and analyses further underscore the efficacy of our approach.

Our contributions can be summarized as follows:

- We introduce PLAY2PROMPT, a novel automated framework that iteratively refines tool documentation and generates usage examples, empowering LLMs to utilize tools more effectively in zero-shot settings without the need for labeled data.
- PLAY2PROMPT integrates a search-based trial-and-error process augmented with self-reflection, enabling LLMs to interact with tools, explore their functionalities, and iteratively refine both tool descriptions and demonstrations, thereby significantly enhancing performance.
- PLAY2PROMPT is entirely zero-shot, inherently scalable, and task-agnostic, making it broadly applicable across a wide range of tools and domains, and practical for enhancing LLM tool use at scale without additional manual effort.

2 METHODOLOGY

Tool documentation typically includes tool descriptions, parameter specifications, output formats, and other related meta-information. In our framework, we define a tool as $f = (u, I, g)$, where u denotes the tool description, I represents tool-related meta-information (such as parameter specifications and other relevant details), and g is the corresponding executable function call. Example tool usage demonstrations often vary from simple question-answer pairs to comprehensive reasoning chains. We focus on demonstrations that illustrate when and how the tool can be used; thus, we define an example demonstration as $v = (x, y, i)$, comprising a question x, an answer y, and a tool invocation i that specifies the tool call parameters. When utilizing tools during inference in the ReAct paradigm, LLMs typically interleave reasoning steps with tool invocation and execution in a chain-of-thought manner. Given an input user query x, a base LLM $\mathcal{B}$, a set of available tools $F = \{f_j\}_{j=1}^{K}$, and a set of example demonstrations $V_F = \{v_j\}_{j=1}^{M}$ for the tools F, we denote the entire ReAct chain as $\mathcal{B}(x; F; V_F)$.

Problem Formulation Consider a set of testing samples $D_{\text{test}} = \{x_j, y_j, F_j\}_{j=1}^{N}$. The evaluation of the tool-using ability of the base model $\mathcal{B}$ is given by $\mathbb{E}_{D_{\text{test}}}[\texttt{Score}(\mathcal{B}(x_j; F_j; V_{F_j}), y_j)]$, where $\texttt{Score}$ is a scoring function assessing the alignment between the model's output and the ground truth y_j. The primary objective is to maximize this evaluation score by improving tool descriptions and generating effective example demonstrations. In a zero-shot scenario, we lack access to labeled testing samples and the specific tool sets F_j for each test sample, rendering direct optimization of the objective infeasible. Therefore, we require a proxy testing set D_{proxy} and a corresponding tool set F_{proxy}. If a small validation set is available, as in automatic prompt optimization settings, it can serve as the proxy testing set and tool set. In our setting, we assume access to a new tool $t \in \cup_j F_j$ and treat each incoming tool f independently by setting $F_{\text{proxy}} = \{f\}$. Assuming a fixed number of demonstrations M, the optimization objective for the tool description u and example demonstrations $\{v_j\}_{j=1}^{M}$ becomes $u^*, \{v_j^*\}_{j=1}^{M} = \arg\max_{u \in \mathcal{U}, v_j \in \mathcal{V}} \texttt{Score}\big(\mathcal{B}(x, \{(u, I, g)\}, \{v_j\}_{j=1}^{M}), y\big)$, where $\mathcal{U}$ and $\mathcal{V}$ represent the sample spaces for tool descriptions and example demonstrations, respectively. Given the vastness of these spaces, it is essential to design an algorithm that can search through them efficiently and effectively. To this end, we propose a framework that iteratively generates the demonstrations V_F, assigns $D_{\text{proxy}} = \{x_j, y_j, F\}\ \forall (x_j, y_j, i_j) \in V_F$, and refines the descriptions u. In the following sections, we introduce PLAY2PROMPT and detail its two optimization tasks.

2.1 PLAY2PROMPT

The primary goal of PLAY2PROMPT is to integrate knowledge gained from tool interactions into tool usage descriptions and example demonstrations while ensuring an efficient exploration of the large search space. Inspired by automatic prompt optimization methodologies (Wang et al., 2024), we devise the optimization process as a search framework where each state s represents an iteration of the variable being optimized—either a demonstration ($s = v$) or a tool description ($s = u$). Each action a corresponds to a modification applied to the current state.

To navigate the search space toward higher-quality regions, we generate actions based on inputs and outputs obtained from tool interactions. Feedback from tool executions—including successful outputs and usage errors—guides further revisions, ensuring that the updated state helps the base model $\mathcal{B}$ avoid previous mistakes. This iterative refinement process is influenced by prior work on self-reflection capabilities in LLMs (Shinn et al., 2023; Pryzant et al., 2023).

Specifically, given a state s_t, an action a_t is generated by sampling from an optimization model $\mathcal{M}$, conditioned on the input-output information obtained from tool interactions. Applying the action a_t to the state s_t—also performed via sampling from $\mathcal{M}$—yields the next state s_{t+1}. A scoring function evaluates the quality of each state, assigning a score r_t that reflects the effectiveness of the current tool description or demonstration. This formulation allows for the integration of search algorithms to efficiently traverse the search space. In our work, we employ beam search to identify high-scoring states, treating each state as a node in a tree and exploring branches for potential improvements. The sampling strategies for generating s_{t+1} and a_{t+1}, as well as the reward definitions, differ between the two optimization tasks. These details are elaborated in sections 2.2 and 2.3.

The two optimization tasks are inherently interdependent: refining tool descriptions requires evaluation examples to calculate a score r, while generating high-quality example demonstrations depends on detailed and accurate tool descriptions. By iteratively alternating between generating demonstrations and refining descriptions, each step informs the other: improved demonstrations highlight areas where the tool description may be lacking, while refined descriptions enable the generation of more accurate and effective demonstrations. This synergy allows PLAY2PROMPT to progressively enhance both components, ultimately improving the base model's tool-using capabilities.

2.2 TOOL EXAMPLE DEMONSTRATION OPTIMIZATION

The objective of this task is to generate example tool usage demonstrations for a given tool f, utilizing its initial tool description u, meta-information I, and function g, with the assistance of an optimization model $\mathcal{M}$. Directly sampling query-answer pairs $(x_{t+1}, y_{t+1}) \sim p_{\mathcal{M}}(x, y \mid x_t, y_t, u, I)$ poses significant challenges, because generating high-quality queries is difficult given only potentially incomplete or noisy tool descriptions and parameter information, especially without any other query-answer demonstrations in zero-shot settings. Additionally, constraining the scope of the generated query to only the specific tool is challenging; generated queries might require the use of other tools, thus expanding the search space beyond manageable limits.

To overcome these issues, we adopt an alternative approach by first sampling the tool invocation i and then generate the corresponding query x and answer y. This method leverages the fact that the search space for tool input parameters is considerably smaller and more constrained, especially when informed by the parameter specifications in I. By sampling a tool invocation i first, we can execute it using the function g to obtain the output $o = g(i)$. This step not only validates the tool call but also provides concrete input-output examples of the tool's functionality. Generating the query x conditioned on a valid tool call i and its output o benefits from this additional information, resulting in more relevant and focused demonstrations. The optimization model $\mathcal{M}$ thus gains substantial insight from interacting with the tool, effectively narrowing the search space.

Our sampling strategy consists of two stages. In the first stage, we perform rejection sampling of the tool invocation. We sample a candidate tool invocation $i \sim p_{\mathcal{M}}(\cdot)$ using the optimization model $\mathcal{M}$, execute the tool function to obtain $o = g(i)$, and verify whether o is a valid output given the meta-information I and description u with $\mathcal{M}$. If the invocation is invalid, we reject it and repeat the sampling process until a valid tool invocation is obtained.

In the second stage, once a valid tool invocation i is secured, we proceed to generate the corresponding user query x and answer y. We sample the query $x \sim p_{\mathcal{M}}(\cdot|i)$ and then the answer $y \sim p_{\mathcal{M}}(\cdot|x, i)$. To refine these samples and enhance their quality, we perform a rollout of N_{refine} steps, with self-reflection acting as the policy guiding the refinement process. During each rollout step, the model evaluates the alignment of the query, answer, and tool output, and generates self-

Algorithm 1 DEMONSTRATIONSTATETRANSITION

Input: $s_t = v_t = (x_t, y_t, i_t)$: demonstration, u: description, a_t: reflection
Output: $s_{t+1} = v_{t+1} = (x_{t+1}, y_{t+1}, i_{t+1})$: demonstration, r_{t+1}: score, a_{t+1}: reflection

$c \leftarrow$ false
while $\neg c$ **do** ▷ Rejection Sampling of tool invocation i
  $i_{t+1} \sim p_{\mathcal{M}}(i|i_t, c, u, I, a_t, m_1)$ ▷ Sample candidate tool invocation, incorporating reflection a_t
  $o_{t+1} \leftarrow g(i_{t+1})$ ▷ Execute tool function
  $c \sim p_{\mathcal{M}}(c|i_{t+1}, o_{t+1}, u, I, m_2)$ ▷ Verify validity of tool call
end while
for $n \leftarrow 1$ to N_{refine} **do** ▷ Rollout for with self-reflection policy
  $x_{t+1} \sim p_{\mathcal{M}}(x|i_{t+1}, o_{t+1}, u, I, m_3)$ ▷ Sample user query x
  $y_{t+1} \sim p_{\mathcal{M}}(y|i_{t+1}, o_{t+1}, x_{t+1}, u, I, m_4)$ ▷ Sample corresponding answer y
  $r_{t+1} \sim p_{\mathcal{M}}(r|y_{t+1}, i_{t+1}, o_{t+1}, x_{t+1}, u, I, m_5)$ ▷ Evaluate demonstration quality
  $a_{t+1} \sim p_{\mathcal{M}}(a|r_{t+1}, y_{t+1}, i_{t+1}, o_{t+1}, x_{t+1}, u, I, m_6)$ ▷ Generate self-reflection action
end for

reflection actions to iteratively improve them. For scoring, we compute a reward r_{t+1} by querying the model $\mathcal{M}$, conditioned on the sampled i, x, and y. This score reflects the quality and coherence of the demonstration. Finally, we generate a self-reflection action a_{t+1} to guide further optimization. The detailed procedure is outlined in Algorithm 1, where each m_i is a meta-prompt.

2.3 TOOL DESCRIPTION OPTIMIZATION

Optimizing tool descriptions requires a strategy that effectively incorporates feedback from the base model's tool usage, particularly when errors occur. During a state transition, we sample a new tool description $u_{t+1} \sim p_{\mathcal{M}}(u|u_t)$ using the optimization model $\mathcal{M}$. To evaluate the effectiveness of this new description, we utilize the previously generated example demonstrations $V = \{(x_j, y_j, i_j)\}_{j=1}^{M}$. We calculate the score r_{t+1} by testing the base model $\mathcal{B}$ in the ReAct framework on the demonstration set V using u_{t+1}, the new tool description: $r_{t+1} = \mathbb{E}_j[\texttt{Score}(\mathcal{B}(x_j, \{(u_{t+1}, I, g)\}, \{\}), y_j)]$.

A critical aspect of this optimization task is incorporating tool-use information derived from the base model's interactions with the tool. When the base model $\mathcal{B}$ uses the tool incorrectly—resulting in errors such as invalid parameter usage, incorrect function calls, or misinterpretation of the tool's purpose—the errors provide valuable feedback. These errors, along with the tool outputs, are collected during the ReAct chains. We condition the generation of the self-reflection action a_{t+1} on this collected information.

By analyzing the errors encountered, the optimization model $\mathcal{M}$ can identify deficiencies or ambiguities in the current tool description u_{t+1} that may have contributed to the incorrect usage. The self-reflection action a_{t+1} then suggests specific modifications to the tool description aimed at mitigating these issues. For instance, if the base model frequently misuses a parameter due to unclear specifications, the self-reflection process may recommend clarifying that parameter's description or providing examples of correct usage. Similarly, if the base model misunderstands the overall functionality of the tool, the reflection may suggest rephrasing the tool description to be more explicit. By iteratively refining the tool description in response to observed errors, we enhance the base model's ability to use the tool correctly in future interactions, reducing the likelihood of repeated mistakes. This iterative refinement process not only improves the clarity and usefulness of the tool description but also contributes to more effective and efficient tool usage by the base model. The detailed procedure for tool description optimization is presented in Algorithm 2.

3 EXPERIMENTS

3.1 EXPERIMENTAL SETUP

Task To assess the effectiveness of tool instruction optimization in real-world applications, we evaluate on StableToolBench (Guo et al., 2024), a benchmark containing diverse user requests across

Algorithm 2 DESCRIPTIONSTATETRANSITION

Input: $s_t = u_t$: description, $V = \{(x_j, y_j, i_j)\}_{j=1}^{M}$: demonstration set, a_t: reflection

Output: : $s_{t+1} = u_{t+1}$: description, r_{t+1}: score, a_{t+1}: reflection

1: $u_{t+1} \sim p_{\mathcal{M}}(u|u_t, a_t, I, m_7)$ ▷ Sample description u_{t+1} from $\mathcal{M}$, applying reflection a_t

2: $o_j, e_j \leftarrow \mathcal{B}(x_j, \{(u_{t+1}, I, g)\}, \{\})\ \forall j$ ▷ Gather I/O & errors e_j from running $\mathcal{B}$ on demo set V with u_{t+1}

3: $r_{t+1} \leftarrow \mathbb{E}_j[\texttt{Score}(o_j, y_j)]$ ▷ Evaluation score on V

4: $a_{t+1} \sim p_{\mathcal{M}}(a|u_{t+1}, r_{t+1}, I, \{x_j, o_j, e_j\}, m_8)$ ▷ Self-reflection action

a large set of publicly available REST APIs from the RapidAPI Hub. StableToolBench improves upon the commonly used ToolBench (Qin et al., 2024b) by addressing the instability of RapidAPIs in the original version. If API access is unavailable, the benchmark employs a fallback system that uses caching and an API simulator. StableToolBench includes 16,464 APIs spanning 49 categories. Our experiments cover all six subsets of the benchmark, which include single-tool (I1) and multi-tool (I2-same category and I3-different category) test cases. In this context, an API service represents a tool that contains multiple sub-tools, with each sub-tool corresponding to f in our definition. Thus, I1 test queries often require multiple sub-tool calls within a tool, making them not strictly ”single-tool.” Although the original subsets evaluate different types of generalizability based on tool overlap with training data, our zero-shot setting does not rely on any training data, rendering these differences less significant.

Inference and Evaluation We adhere to the inference setting used in the original benchmark, where a set of tools is provided for the base LLM $\mathcal{B}$ to select from to answer user queries. ReAct serves as our baseline performance method, for which we run on the testing data using the ReAct prompts provided in dataset, with the original tool descriptions and no example demonstrations, as we operate in zero-shot setting. For PLAY2PROMPT, we run ReAct again but with the optimized descriptions and demonstrations. To test different base models $\mathcal{B}$, we evaluate with Meta LLaMA models and OpenAI GPT models, both of which are trained with tool use instructions and have zero-shot tool-calling capabilities. Specifically, we tested `llama-3-8b-instruct` and `llama-3-70b-instruct` for LLaMA, while `gpt-3.5-turbo-1106` was used for GPT experiments. Since ReAct outputs are free-form, an evaluation LLM determines whether a response adequately answers a user query. Following the original benchmark's evaluation pipeline, we reuse the provided prompts and employ solvable pass rate as our evaluation metric, which measures the percentage of queries deemed solvable by the evaluation LLM. We use `llama-3.1-70b-instruct` as the evaluation LLM, as previous work (Guo et al., 2024) reported potential evaluation instabilities with weaker models, which we do not observe with this evaluation LLM. Additional details on inference and evaluation are provided in appendix A.

Optimization Details For PLAY2PROMPT, we follow the proposed algorithms, first running beam search to optimize example demonstrations. N_{refine} is set to 5 for the demonstration optimization procedure. We set a depth limit of 5, beam width of 3 and conduct 3 explorations per node. The top 3 examples are generated and selected for each tool, which are then passed to the description optimization phase. Beam search is again applied with the same settings to select the best tool description. `llama-3-8b-instruct` is used for $\mathcal{M}$.

3.2 RESULTS AND ANALYSES

Main Results on StableToolbench The top and bottom rows for each base model in table 1 show the solvable pass rates of running ReAct with demonstrations and descriptions generated by PLAY2PROMPT, compared to the baseline of ReAct with original descriptions and no demonstrations. Across all 6 subsets, we see that PLAY2PROMPT outperforms on all base models, observing 3-6% absolute gains (6-9% relative gains) on average across all base models. For the smaller model LLaMA-3-8B, gains mainly come from I1-Cat, I1-Tool, and I3-Inst subsets, while the larger GPT-3.5 and LLaMA-3-70B models maintain consistent gains across all subsets. It is noteworthy that LLaMA-3-70B achieves the highest performance out of all 3 models, for both baseline ReAct and PLAY2PROMPT, and especially performs well on I3-Inst, the most challenging subset, where the other models struggle with the most. PLAY2PROMPT essentially boosts performance of models up

Table 1: Results on StableToolBench. Scores indicate the solvable pass rate.

Base Model	Method	I1-Inst	I1-Cat	I1-Tool	I2-Inst	I2-Cat	I3-Inst	Avg
LLaMA-3-8B	ReAct	59.2	60.8	55.8	58.1	56.7	47.7	56.4
	PLAY2PROMPT - Desc	59.9	**65.9**	57.7	58.0	56.7	50.8	58.1
	PLAY2PROMPT - Demo	57.9	65.5	58.5	58.0	56.7	**59.4**	59.3
	PLAY2PROMPT	**60.0**	65.6	**61.0**	**59.0**	**57.8**	53.4	**59.5**
LLaMA-3-70B	ReAct	70.3	75.9	66.1	70.6	76.4	76.5	72.7
	PLAY2PROMPT - Desc	71.1	78.0	66.5	76.1	78.2	79.2	74.9
	PLAY2PROMPT - Demo	**73.6**	78.5	71.8	76.3	**83.1**	76.3	76.6
	PLAY2PROMPT	**73.6**	**79.4**	**72.5**	**76.7**	80.9	**80.3**	**77.2**
GPT-3.5	ReAct	57.4	67.8	65.1	61.2	62.9	53.0	61.2
	PLAY2PROMPT - Desc	60.1	67.5	66.0	61.9	**67.9**	55.7	63.2
	PLAY2PROMPT - Demo	**62.2**	70.2	70.3	**64.6**	65.4	56.6	64.9
	PLAY2PROMPT	62.0	**70.7**	**71.7**	**64.6**	**67.9**	**64.7**	**66.9**

to the baseline performance of models that are much larger. This underscores the effectiveness of PLAY2PROMPT, operating entirely without supervision with only access to the newly given tool itself.

Effects of Demonstrations vs Descriptions To study the effectiveness of PLAY2PROMPT, we break down how much the newly optimized demonstrations contribute to the performance gains compared to the optimized descriptions. We keep our optimization procedure the same, but during inference we add two other settings: one where we use optimized demonstrations along with original descriptions, and one where we do not use demonstrations but update the descriptions with optimized ones. The results can be found labeled as PLAY2PROMPT-Desc and PLAY2PROMPT-Demo for each model in table 1. Compared against each other, we observe that the optimized example demonstrations generally contribute more to performance than optimized descriptions do. However, we still observe several subsets where one does well while the other remains close to the baseline. This varies across different base models, and we do not observe a pattern of when to choose one over another. On the other hand, using both together consistently obtains the best performance, especially for the larger models, giving us higher assurance of performance gains. This suggest that information from the optimized descriptions and demonstrations may complement each other in assisting LLMs' tool use, validating our iterative approach.

Ablation on Search Strategies To investigate the effect of search effectiveness in PLAY2PROMPT, we conduct an ablation study by comparing beam search to alternative search strategies. Specifically, we compare to Monte Carlo (MC) search with different depths, using the same transition and action strategy as in PLAY2PROMPT and only replace beam search with MC. MC in this context would be a single step of sampling a state and an action. In this ablation, we run MC with depth of 1 and 5. Additionally, we aim to quantify the effect of having N_{refine} rollout steps with the self-reflection policy when sampling query-answer pairs, and compare against a strategy of not rolling out. We run the experiments on I3-Inst, which is generally the hardest subset due to the inclusion of tools across categories. The results are presented in table 2, where MC is shown to perform worse than beam search (PLAY2PROMPT), as it does not explore the search space well enough to reach better states. Rollout refinement helps, as does increasing the depth of search due to information gained from tool play and self-reflection actions.

Analysis on Single-Tool Queries and Incomplete Descriptions We attempt to gain more insight into how the optimized demonstrations and descriptions enhance base model's tool use by focusing on certain user queries of interest. One such set contains queries that use only a single sub-tool, as it most closely matches to our optimization scenario, where we denote as the I1-Sub subset. Another interesting set are instances where a query's corresponding tool set contains at least one tool that lacks tool description, i.e., only has meta-information in the form of tool names and parameter structures. We denote this set as NoDesc. Evaluation results on these two subsets are shown in table 3. PLAY2PROMPT greatly enhances the performance of LLaMA-3-8B on both I1-Sub and NoDesc, and almost reaches the performance of the 70B model on I1-Sub. However, the 70B model

Table 2: Ablation on search strategies, ran on I3-Inst. LLaMA-3-8B is used for $\mathcal{B}$ in this experiment. MC denotes Monte Carlo search.

Search strategy	**I3-Inst**
MC (depth$= 1$)	48.1
MC (depth$= 5$)	49.9
MC (depth$= 5$) & $N_{\text{refine}} = 5$	51.9
Beam search (PLAY2PROMPT)	53.4

Table 3: Solvable pass rate on instances only using a single subtool (I1-Sub) and instances whose toolset includes at least one tool without a tool description (NoDesc). Demo indicates performance evaluated on the generated demonstration set.

Base Model	**Method**	**I1-Sub**		**NoDesc**	
		demo	test	demo	test
LLaMA-3-8B	ReAct	85.0	59.7	85.0	57.5
	ReAct+PLAY2PROMPT	93.6	72.4	98.5	72.9
LLaMA-3-70B	ReAct	92.8	74.9	93.9	86.9
	ReAct+PLAY2PROMPT	100.0	75.7	99.6	87.5

sees way less gains, even when performance on the demonstration set improves. This suggests that 1) there is still quite a generalization gap between optimized demonstrations and the testing distribution, suggesting room for improvement; and 2) meta-information conveys a certain degree of information that may be easily picked up by larger models compared to smaller models. The information gained through tool play for these tools are still very helpful for the smaller model, which essentially bridges that information gap with PLAY2PROMPT.

Optimization Model $\mathcal{M}$ We further explore the effects of using a stronger optimization model $\mathcal{M}$, as they not only may generalize better, but also provide better self-reflection capabilities to enable better search. Due to computational constraints, we explore using LLaMA-3-70B in place of LLaMA-3-8B on the subset I3-Inst, and report results in table 4. We observe a fairly large improvement, essentially doubling the performance gain on this small subset, which suggest potential overall performance gains.

Table 4: Different $\mathcal{M}$ on I3-Inst. LLaMA-3-70B is used as $\mathcal{B}$ in this experiment.

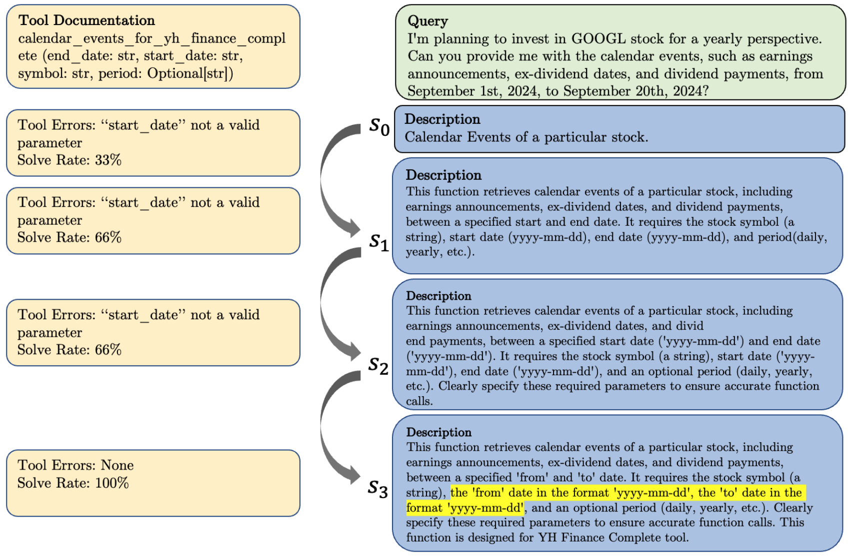
Method	$\mathcal{M}$	**I3-Inst**
ReAct	-	76.5
ReAct+PLAY2PROMPT	LM-3-8B	80.3
ReAct+PLAY2PROMPT	LM-3-70B	85.8

Qualitative Analysis To illustrate how PLAY2PROMPT leverages tool play errors to optimize demonstrations and descriptions, we show a qualitative example in figure 2, where the tool documentation is outdated, specifying `start_date` and `end_date` instead of `from` and `to`, in addition to setting them to be required parameters when in fact they are optional. We show one query out of the three we generate for the demonstration set. In this case, PLAY2PROMPT in the early states is confused by contradictory information from the tool error and the documentation, but adds more detailed information and solves some of the queries that did not require the start and end dates. It ultimately starts exploring and ends up finding the correct parameter names, leading to superior performance. An additional example of a more typical improvement by PLAY2PROMPT is shown in appendix B.

4 RELATED WORK

LLMs for Tool Use Recent years have witnessed significant advances in employing large language models (LLMs) as agents to master tool use for solving complex tasks (Mialon et al., 2023; Qin et al., 2024a), thereby enhancing LLMs' capabilities in areas such as multi-modal understanding (Gupta & Kembhavi, 2023; Surís et al., 2023; Wu et al., 2023), programming tools (Gao et al., 2023; Paranjape et al., 2023; Team et al., 2023; Zhang et al., 2023b; Cai et al., 2024), and other domain-specific functionalities. The conventional strategy involves training base models with tool-use data (Thoppilan et al., 2022; Dubey et al., 2024) or fine-tuning LLMs (Patil et al., 2023; Schick et al., 2023; Yang et al., 2023) to learn to use tools, which works well on specific tasks with a small fixed number of tools. Specifically, Parisi et al. (2022) explored tool play in a self-training context, aiming to automatically fine-tune a language model on a small number of tools. However, these approaches require continual learning as new tools are added, making the training process not scalable. Hao et al. (2023) addressed this by training tool embeddings that can be augmented onto fixed

Figure 2: An example of PLAY2PROMPT facing incorrect documentation. The beam search trajectory with the highest evaluation solve rate on the demonstration set is shown. At each state transition, a new description is explored based on error feedback.



LLMs for plug-and-play usage; however, they still require labeled data to obtain the embeddings. Alternatively, LLMs can access tools via handcrafted meta-prompts or by being trained with tool-use instructions, and then supplied the tools during inference through prompts (Lu et al., 2023; Shen et al., 2023; Song et al., 2023; Qin et al., 2024b; Zhuang et al., 2024). With the increasing number of applications and tools in which LLMs are utilized, enhancing LLMs' tool-use capabilities for novel tools remains an important problem, which we explore and improve upon with PLAY2PROMPT.

Tool Use Instructions and Optimization Tool documentation and example demonstrations are crucial components in prompting LLMs for effective tool use, as demonstrated by various studies. Hsieh et al. (2023) reported that documentation is more important than demonstrations for some tasks, and that LLMs often hallucinate tools when lacking proper documentation. Xu et al. (2023) investigated the effects of in-context example demonstrations on tool use techniques, observing diminished performance when such examples were omitted. To automate the generation of tool-use instances, Shen et al. (2024) proposed sampling tool calls from a graph of tool relations and back-instructing to construct queries, which relies on the availability of external tool graphs. In an effort to improve tool documentation, Yuan et al. (2024) utilized direct prompting to summarize and rewrite tool descriptions, but their approach relies on related documentation examples and lacks the ability to systematically search and optimize. While automatic prompt tuning methods (Pryzant et al., 2023; Wang et al., 2024) have been developed to adapt LLMs to domain-specific tasks by rewriting prompts, they typically depend on held-out testing sets to measure optimization quality, making them unsuitable for zero-shot tool instruction rewriting (Wu et al., 2024). These challenges highlight the necessity for approaches that can automatically optimize tool instructions and demonstrations without requiring labeled data or manual effort, which PLAY2PROMPT addresses by leveraging interactions with the tool itself.

5 CONCLUSION

We present PLAY2PROMPT, an automated framework that iteratively refines tool documentation and generates example tool usage demonstrations, enhancing the ability of large language models to utilize tools effectively in zero-shot settings. By employing a search-based trial-and-error approach with self-reflection, PLAY2PROMPT enables models to interact with tools, explore their functionalities, and improve both tool descriptions and demonstrations without the need for labeled data or extensive manual effort. This approach addresses the limitations of existing methods that rely on handcrafted prompts or labeled data, offering a scalable and task-agnostic solution applicable to a wide range of tools and domains. Our experiments on StableToolBench demonstrated significant improvements over baseline methods for both open-source and closed-source models. By systematically enhancing the tool-use capabilities of LLMs, this work contributes to the development of AI agents that can autonomously adapt to new tools and challenges, extending their utility in real-world applications.

Limitations and Future Work

In this work, we generate proxy testing sets based only on a single given tool and do not cover multi-tool use. Scaling from single-tool scenarios to multiple tools can likely enhance LLM's tool use effectiveness. Additionally, for example demonstrations, we use rejection sampling to generate tool invocations first, which do not work for functions whose parameter space is too large, for instance parameters that take long ID string inputs or authentication tokens that require calls to other tools beforehand. Exploring multi-tool dependencies could potentially resolve this issue and improve tool play. In our work we focus on tool descriptions and demonstrations only, relegating other information as meta-information, which could be potential next steps to explore.

References

Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. Gpt-4 technical report. *arXiv preprint arXiv:2303.08774*, 2023.

Tianle Cai, Xuezhi Wang, Tengyu Ma, Xinyun Chen, and Denny Zhou. Large language models as tool makers. In *The Twelfth International Conference on Learning Representations*, 2024. URL https://openreview.net/forum?id=qV83K9d5WB.

Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, Ahmad Al-Dahle, Aiesha Letman, Akhil Mathur, Alan Schelten, Amy Yang, Angela Fan, Anirudh Goyal, Anthony Hartshorn, Aobo Yang, Archi Mitra, Archie Sravankumar, Artem Korenev, Arthur Hinsvark, Arun Rao, Aston Zhang, Aurelien Rodriguez, Austen Gregerson, Ava Spataru, Baptiste Rozière, Bethany Biron, Binh Tang, Bobbie Chern, Charlotte Caucheteux, Chaya Nayak, Chloe Bi, Chris Marra, Chris McConnell, Christian Keller, Christophe Touret, Chunyang Wu, Corinne Wong, Cristian Cantón Ferrer, Cyrus Nikolaidis, Damien Allonsius, Daniel Song, Danielle Pintz, Danny Livshits, David Esiobu, Dhruv Choudhary, Dhruv Mahajan, Diego Garcia-Olano, Diego Perino, Dieuwke Hupkes, Egor Lakomkin, Ehab A. AlBadawy, Elina Lobanova, Emily Dinan, Eric Michael Smith, Filip Radenovic, Frank Zhang, Gabriele Synnaeve, Gabrielle Lee, Georgia Lewis Anderson, Graeme Nail, Grégoire Mialon, Guanglong Pang, Guillem Cucurell, Hailey Nguyen, Hannah Korevaar, Hu Xu, Hugo Touvron, Iliyan Zarov, Imanol Arrieta Ibarra, Isabel M. Kloumann, Ishan Misra, Ivan Evtimov, Jade Copet, Jaewon Lee, Jan Laurens Geffert, Jana Vranes, Jason Park, Jay Mahadeokar, Jeet Shah, Jelmer van der Linde, Jennifer Billock, Jenny Hong, Jenya Lee, Jeremy Fu, Jianfeng Chi, Jianyu Huang, Jiawen Liu, Jie Wang, Jiecao Yu, Joanna Bitton, Joe Spisak, Jongsoo Park, Joseph Rocca, Joshua Johnstun, Joshua Saxe, Ju-Qing Jia, Kalyan Vasuden Alwala, K. Upasani, Kate Plawiak, Keqian Li, Ken-591 neth Heafield, Kevin Stone, Khalid El-Arini, Krithika Iyer, Kshitiz Malik, Kuenley Chiu, Kunal Bhalla, Lauren Rantala-Yeary, Laurens van der Maaten, Lawrence Chen, Liang Tan, Liz Jenkins, Louis Martin, Lovish Madaan, Lubo Malo, Lukas Blecher, Lukas Landzaat, Luke de Oliveira, Madeline C. Muzzi, Mahesh Babu Pasupuleti, Mannat Singh, Manohar Paluri, Marcin Kardas, Mathew Oldham, Mathieu Rita, Maya Pavlova, Melissa Hall Melanie Kambadur, Mike Lewis, Min Si, Mitesh Kumar Singh, Mona Hassan, Naman Goyal, Narjes Torabi, Nikolay Bashlykov, Nikolay Bogoychev, Niladri S. Chatterji, Olivier Duchenne, Onur cCelebi, Patrick Alrassy, Pengchuan Zhang, Pengwei Li, Petar Vasić, Peter Weng, Prajjwal Bhargava, Pratik Dubal, Praveen Krishnan, Punit Singh Koura, Puxin Xu, Qing He, Qingxiao Dong, Ragavan Srinivasan, Raj Ganapathy, Ramon Calderer, Ricardo Silveira Cabral, Robert Stojnic, Roberta Raileanu, Rohit Girdhar, Rohit Patel, Romain Sauvestre, Ronnie Polidoro, Roshan Sumbaly, Ross Taylor, Ruan Silva, Rui Hou, Rui Wang, Saghar Hosseini, Sahana Chennabasappa, Sanjay Singh, Sean Bell, Seohyun Sonia Kim, Sergey Edunov, Shaoliang Nie, Sharan Narang, Sharath Chandra Raparthy, Sheng Shen, Shengye Wan, Shruti Bhosale, Shun Zhang, Simon Vandenhende, Soumya Batra, Spencer Whitman, Sten Sootla, Stephane Collot, Suchin Gururangan, Sydney Borodinsky, Tamar Herman, Tara Fowler, Tarek Sheasha, Thomas Georgiou, Thomas Scialom, Tobias Speckbacher, Todor Mihaylov, Tong Xiao, Ujjwal Karn, Vedanuj Goswami, Vibhor Gupta, Vignesh Ramanathan, Viktor Kerkez, Vincent Gonguet, Virginie Do, Vish Vogeti, Vladan Petrovic, Weiwei Chu, Wenhan Xiong, Wenyin Fu, Whitney Meers, Xavier Martinet, Xiaodong Wang, Xiaoqing Ellen Tan, Xinfeng Xie, Xuchao Jia, Xuewei Wang, Yaelle Goldschlag, Yashesh Gaur, Yasmine Babaei, Yiqian Wen, Yiwen Song, Yuchen Zhang, Yue Li, Yuning Mao, Zacharie Delpierre Coudert, Zhengxu Yan, Zhengxing Chen, Zoe Papakipos, Aaditya K. Singh, Aaron Grattafiori, Abha Jain, Adam Kelsey, Adam Shajnfeld, Adi Gangidi, Adolfo Victoria, Ahuva Goldstand, Ajay Menon, Ajay Sharma, Alex Boesenberg, Alex Vaughan, Alexei Baevski, Allie Feinstein, Amanda Kallet, Amit Sangani, Anam Yunus, Andrei Lupu, Andres Alvarado, Andrew Caples, Andrew Gu, Andrew Ho, Andrew Poulton, Andrew Ryan, Ankit Ramchandani, Annie Franco, Aparajita Saraf, Arkabandhu Chowdhury, Ashley Gabriel, Ashwin Bharambe, Assaf Eisenman, Azadeh Yazdan, Beau James, Ben Maurer, Ben Leonhardi, Bernie Huang, Beth Loyd, Beto De Paola, Bhargavi Paranjape, Bing Liu, Bo Wu, Boyu Ni, Braden Hancock, Bram Wasti, Brandon Spence, Brani Stojkovic, Brian Gamido, Britt Montalvo, Carl Parker, Carly Burton, Catalina Mejia, Changhan Wang, Changkyu Kim, Chao Zhou, Chester Hu, Ching-Hsiang Chu, Chris Cai, Chris Tindal, Christoph Feichtenhofer, Damon Civin, Dana Beaty, Daniel Kreymer, Shang-Wen Li, Danny Wyatt, David Adkins, David Xu, Davide Testuggine, Delia David, Devi Parikh, Diana Liskovich, Didem Foss, Dingkang Wang, Duc Le, Dustin Holland, Edward Dowling, Eissa Jamil, Elaine Montgomery, Eleonora Presani, Emily Hahn, Emily Wood, Erik Brinkman, Esteban Arcaute, Evan Dunbar, Evan Smothers, Fei Sun, Felix Kreuk, Feng Tian, Firat Ozgenel, Francesco Caggioni, Francisco Guzm'an, Frank J. Kanayet, Frank Seide, Gabriela Medina Florez, Gabriella Schwarz, Gada Badeer, Georgia Swee, Gil Halpern, Govind Thattai, Grant Herman, Grigory G. Sizov, Guangyi Zhang, Guna Lakshminarayanan, Hamid Shojanazeri, Han Zou, Hannah Wang, Han Zha, Haroun Habeeb, Harrison Rudolph, Helen Suk, Henry Aspegren, Hunter Goldman, Igor Molybog, Igor Tufanov, Irina-Elena Veliche, Itai Gat, Jake Weissman, James Geboski, James Kohli, Japhet Asher, Jean-Baptiste Gaya, Jeff Marcus, Jeff Tang, Jennifer Chan, Jenny Zhen, Jeremy Reizenstein, Jeremy Teboul, Jessica Zhong, Jian Jin, Jingyi Yang, Joe Cummings, Jon Carvill, Jon Shepard, Jonathan McPhie, Jonathan Torres, Josh Ginsburg, Junjie Wang, Kaixing(Kai) Wu, U KamHou, Karan Saxena, Karthik Prasad, Kartikay Khandelwal, Katayoun Zand, Kathy Matosich, Kaushik Veeraraghavan, Kelly Michelena, Keqian Li, Kun Huang, Kunal Chawla, Kushal Lakhotia, Kyle Huang, Lailin Chen, Lakshya Garg, A Lavender, Leandro Silva, Lee Bell, Lei Zhang, Liangpeng Guo, Licheng Yu, Liron Moshkovich, Luca Wehrstedt, Madian Khabsa, Manav Avalani, Manish Bhatt, Maria Tsimpoukelli, Martynas Mankus, Matan Hasson, Matthew Lennie, Matthias Reso, Maxim Groshev, Maxim Naumov, Maya Lathi, Meghan Keneally, Michael L. Seltzer, Michal Valko, Michelle Restrepo, Mihir Patel, Mik Vyatskov, Mikayel Samvelyan, Mike Clark, Mike Macey, Mike Wang, Miquel Jubert Hermoso, Mo Metanat, Mohammad Rastegari, Munish Bansal, Nandhini Santhanam, Natascha Parks, Natasha White, Navyata Bawa, Nayan Singhal, Nick Egebo, Nicolas Usunier, Nikolay Pavlovich Laptev, Ning Dong, Ning Zhang, Norman Cheng, Oleg Chernoguz, Olivia Hart, Omkar Salpekar, Ozlem Kalinli, Parkin Kent, Parth Parekh, Paul Saab, Pavan Balaji, Pedro Rittner, Philip Bontrager, Pierre Roux, Piotr Dollár, Polina Zvyagina, Prashant Ratanchandani, Pritish Yuvraj, Qian Liang, Rachad Alao, Rachel Rodriguez, Rafi Ayub, Raghotham Murthy, Raghu Nayani, Rahul Mitra, Raymond Li, Rebekkah Hogan, Robin Battey, Rocky Wang, Rohan Maheswari, Russ Howes, Ruty Rinott, Sai Jayesh Bondu, Samyak Datta, Sara Chugh, Sara Hunt, Sargun Dhillon, Sasha Sidorov, Satadru Pan, Saurabh Verma, Seiji Yamamoto, Sharadh Ramaswamy, Shaun Lindsay, Sheng Feng, Shenghao Lin, Shengxin Cindy Zha, Shiva Shankar, Shuqiang Zhang, Sinong Wang, Sneha Agarwal, Soji Sajuyigbe, Soumith Chintala, Stephanie Max, Stephen Chen, Steve Kehoe, Steve Satterfield, Sudarshan Govindaprasad, Sumit Gupta, Sung-Bae Cho, Sunny Virk, Suraj Subramanian, Sy Choudhury, Sydney Goldman, Tal Remez, Tamar Glaser, Tamara Best, Thilo Kohler, Thomas Robinson, Tianhe Li, Tianjun Zhang, Tim Matthews, Timothy Chou, Tzook Shaked, Varun Vontimitta, Victoria Ajayi, Victoria Montanez, Vijai Mohan, Vinay Satish Kumar, Vishal Mangla, Vlad Ionescu, Vlad Andrei Poenaru, Vlad T. Mihailescu, Vladimir Ivanov, Wei Li, Wenchen Wang, Wenwen Jiang, Wes Bouaziz, Will Constable, Xia Tang, Xiaofang Wang, Xiaojian Wu, Xiaolan Wang, Xide Xia, Xilun Wu, Xinbo Gao, Yanjun Chen, Ye Hu, Ye Jia, Ye Qi, Yenda Li, Yilin Zhang, Ying Zhang, Yossi Adi, Youngjin Nam, Yu Wang, Yuchen Hao, Yundi Qian, Yuzi He, Zach Rait, Zachary DeVito, Zef Rosnbrick, Zhaoduo Wen, Zhenyu

Yang, and Zhiwei Zhao. The llama 3 herd of models. *ArXiv*, abs/2407.21783, 2024. URL https://api.semanticscholar.org/CorpusID:271571434.

Luyu Gao, Aman Madaan, Shuyan Zhou, Uri Alon, Pengfei Liu, Yiming Yang, Jamie Callan, and Graham Neubig. Pal: Program-aided language models. In *International Conference on Machine Learning*, pp. 10764–10799. PMLR, 2023.

Zhicheng Guo, Sijie Cheng, Hao Wang, Shihao Liang, Yujia Qin, Peng Li, Zhiyuan Liu, Maosong Sun, and Yang Liu. StableToolBench: Towards stable large-scale benchmarking on tool learning of large language models. In Lun-Wei Ku, Andre Martins, and Vivek Srikumar (eds.), *Findings of the Association for Computational Linguistics ACL 2024*, pp. 11143–11156, Bangkok, Thailand and virtual meeting, August 2024. Association for Computational Linguistics. doi: 10.18653/v1/2024.findings-acl.664. URL https://aclanthology.org/2024.findings-acl.664.

Tanmay Gupta and Aniruddha Kembhavi. Visual programming: Compositional visual reasoning without training. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 14953–14962, 2023.

Shibo Hao, Tianyang Liu, Zhen Wang, and Zhiting Hu. Toolkengpt: Augmenting frozen language models with massive tools via tool embeddings. *Advances in neural information processing systems*, 36, 2023.

Cheng-Yu Hsieh, Si-An Chen, Chun-Liang Li, Yasuhisa Fujii, Alexander Ratner, Chen-Yu Lee, Ranjay Krishna, and Tomas Pfister. Tool documentation enables zero-shot tool-usage with large language models. *arXiv preprint arXiv:2308.00675*, 2023.

Pan Lu, Baolin Peng, Hao Cheng, Michel Galley, Kai-Wei Chang, Ying Nian Wu, Song-Chun Zhu, and Jianfeng Gao. Chameleon: Plug-and-play compositional reasoning with large language models. *arXiv preprint arXiv:2304.09842*, 2023.

Aman Madaan, Niket Tandon, Prakhar Gupta, Skyler Hallinan, Luyu Gao, Sarah Wiegreffe, Uri Alon, Nouha Dziri, Shrimai Prabhumoye, Yiming Yang, et al. Self-refine: iterative refinement with self-feedback. In *Proceedings of the 37th International Conference on Neural Information Processing Systems*, pp. 46534–46594, 2023.

Grégoire Mialon, Roberto Dessi, Maria Lomeli, Christoforos Nalmpantis, Ramakanth Pasunuru, Roberta Raileanu, Baptiste Roziere, Timo Schick, Jane Dwivedi-Yu, Asli Celikyilmaz, Edouard Grave, Yann LeCun, and Thomas Scialom. Augmented language models: a survey. *Transactions on Machine Learning Research*, 2023. ISSN 2835-8856. URL https://openreview.net/forum?id=jh7wH2AzKK. Survey Certification.

Bhargavi Paranjape, Scott Lundberg, Sameer Singh, Hannaneh Hajishirzi, Luke Zettlemoyer, and Marco Tulio Ribeiro. Art: Automatic multi-step reasoning and tool-use for large language models. *arXiv preprint arXiv:2303.09014*, 2023.

Aaron Parisi, Yao Zhao, and Noah Fiedel. Talm: Tool augmented language models. *arXiv preprint arXiv:2205.12255*, 2022.

Shishir G Patil, Tianjun Zhang, Xin Wang, and Joseph E Gonzalez. Gorilla: Large language model connected with massive apis. *arXiv preprint arXiv:2305.15334*, 2023.

Reid Pryzant, Dan Iter, Jerry Li, Yin Lee, Chenguang Zhu, and Michael Zeng. Automatic prompt optimization with "gradient descent" and beam search. In Houda Bouamor, Juan Pino, and Kalika Bali (eds.), *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pp. 7957–7968, Singapore, December 2023. Association for Computational Linguistics. doi: 10.18653/v1/2023.emnlp-main.494. URL https://aclanthology.org/2023.emnlp-main.494.

Yujia Qin, Shengding Hu, Yankai Lin, Weize Chen, Ning Ding, Ganqu Cui, Zheni Zeng, Yufei Huang, Chaojun Xiao, Chi Han, Yi Ren Fung, Yusheng Su, Huadong Wang, Cheng Qian, Runchu Tian, Kunlun Zhu, Shihao Liang, Xingyu Shen, Bokai Xu, Zhen Zhang, Yining Ye, Bowen Li, Ziwei Tang, Jing Yi, Yuzhang Zhu, Zhenning Dai, Lan Yan, Xin Cong, Yaxi Lu, Weilin Zhao, Yuxiang Huang, Junxi Yan, Xu Han, Xian Sun, Dahai Li, Jason Phang, Cheng Yang, Tongshuang Wu, Heng Ji, Zhiyuan Liu, and Maosong Sun. Tool learning with foundation models, 2024a. URL https://arxiv.org/abs/2304.08354.

Yujia Qin, Shihao Liang, Yining Ye, Kunlun Zhu, Lan Yan, Yaxi Lu, Yankai Lin, Xin Cong, Xiangru Tang, Bill Qian, Sihan Zhao, Lauren Hong, Runchu Tian, Ruobing Xie, Jie Zhou, Mark Gerstein, dahai li, Zhiyuan Liu, and Maosong Sun. ToolLLM: Facilitating large language models to master 16000+ real-world APIs. In *The Twelfth International Conference on Learning Representations*, 2024b. URL https://openreview.net/forum?id=dHng2O0Jjr.

Timo Schick, Jane Dwivedi-Yu, Roberto Dessì, Roberta Raileanu, Maria Lomeli, Luke Zettlemoyer, Nicola Cancedda, and Thomas Scialom. Toolformer: Language models can teach themselves to use tools. *arXiv preprint arXiv:2302.04761*, 2023.

Yongliang Shen, Kaitao Song, Xu Tan, Dongsheng Li, Weiming Lu, and Yueting Zhuang. Hugginggpt: Solving ai tasks with chatgpt and its friends in huggingface. *arXiv preprint arXiv:2303.17580*, 2023.

Yongliang Shen, Kaitao Song, Xu Tan, Wenqi Zhang, Kan Ren, Siyu Yuan, Weiming Lu, Dongsheng Li, and Yueting Zhuang. Taskbench: Benchmarking large language models for task automation. In *ICLR 2024 Workshop on Large Language Model (LLM) Agents*, 2024. URL https://openreview.net/forum?id=ZUbraGNpAq.

Noah Shinn, Federico Cassano, Ashwin Gopinath, Karthik R Narasimhan, and Shunyu Yao. Reflexion: language agents with verbal reinforcement learning. In *Thirty-seventh Conference on Neural Information Processing Systems*, 2023. URL https://openreview.net/forum?id=vAElhFcKW6.

Yifan Song, Weimin Xiong, Dawei Zhu, Cheng Li, Ke Wang, Ye Tian, and Sujian Li. Restgpt: Connecting large language models with real-world applications via restful apis. *arXiv preprint arXiv:2306.06624*, 2023.

Dídac Surís, Sachit Menon, and Carl Vondrick. Vipergpt: Visual inference via python execution for reasoning. *arXiv preprint arXiv:2303.08128*, 2023.

Gemini Team, Rohan Anil, Sebastian Borgeaud, Yonghui Wu, Jean-Baptiste Alayrac, Jiahui Yu, Radu Soricut, Johan Schalkwyk, Andrew M Dai, Anja Hauth, et al. Gemini: a family of highly capable multimodal models. *arXiv preprint arXiv:2312.11805*, 2023.

Romal Thoppilan, Daniel De Freitas, Jamie Hall, Noam Shazeer, Apoorv Kulshreshtha, Heng-Tze Cheng, Alicia Jin, Taylor Bos, Leslie Baker, Yu Du, et al. Lamda: Language models for dialog applications. *arXiv preprint arXiv:2201.08239*, 2022.

Xinyuan Wang, Chenxi Li, Zhen Wang, Fan Bai, Haotian Luo, Jiayou Zhang, Nebojsa Jojic, Eric Xing, and Zhiting Hu. Promptagent: Strategic planning with language models enables expert-level prompt optimization. In *The Twelfth International Conference on Learning Representations*, 2024. URL https://openreview.net/forum?id=22pyNMuIoa.

Chenfei Wu, Shengming Yin, Weizhen Qi, Xiaodong Wang, Zecheng Tang, and Nan Duan. Visual chatgpt: Talking, drawing and editing with visual foundation models. *arXiv preprint arXiv:2303.04671*, 2023.

Shirley Wu, Shiyu Zhao, Qian Huang, Kexin Huang, Michihiro Yasunaga, Kaidi Cao, Vassilis N Ioannidis, Karthik Subbian, Jure Leskovec, and James Zou. Avatar: Optimizing llm agents for tool-assisted knowledge retrieval. *arXiv preprint arXiv:2406.11200*, 2024.

Qiantong Xu, Fenglu Hong, Bo Li, Changran Hu, Zhengyu Chen, and Jian Zhang. On the tool manipulation capability of open-source large language models. *arXiv preprint arXiv:2305.16504*, 2023.

Rui Yang, Lin Song, Yanwei Li, Sijie Zhao, Yixiao Ge, Xiu Li, and Ying Shan. Gpt4tools: Teaching large language model to use tools via self-instruction. *Advances in Neural Information Processing Systems*, 36, 2023.

Shunyu Yao, Jeffrey Zhao, Dian Yu, Nan Du, Izhak Shafran, Karthik R Narasimhan, and Yuan Cao. React: Synergizing reasoning and acting in language models. In *The Eleventh International Conference on Learning Representations*, 2023. URL https://openreview.net/forum?id=WE_vluYUL-X.

Siyu Yuan, Kaitao Song, Jiangjie Chen, Xu Tan, Yongliang Shen, Ren Kan, Dongsheng Li, and Deqing Yang. Easytool: Enhancing llm-based agents with concise tool instruction. *arXiv preprint arXiv:2401.06201*, 2024.

Kexun Zhang, Hongqiao Chen, Lei Li, and William Wang. Syntax error-free and generalizable tool use for llms via finite-state decoding. *arXiv preprint arXiv:2310.07075*, 2023a.

Tianhua Zhang, Jiaxin Ge, Hongyin Luo, Yung-Sung Chuang, Mingye Gao, Yuan Gong, Xixin Wu, Yoon Kim, Helen Meng, and James Glass. Natural language embedded programs for hybrid language symbolic reasoning, 2023b.

Yuchen Zhuang, Xiang Chen, Tong Yu, Saayan Mitra, Victor Bursztyn, Ryan A. Rossi, Somdeb Sarkhel, and Chao Zhang. Toolchain*: Efficient action space navigation in large language models with a* search. In *The Twelfth International Conference on Learning Representations*, 2024. URL https://openreview.net/forum?id=B6pQxqUcT8.

A INFERENCE AND EVALUATION DETAILS FOR STABLETOOLBENCH

For GPT models, we keep the exact same setting as used in the original benchmark, except for requiring it to return an action from the provided toolset by supplying a flag to the OpenAI API. For LLaMA models, we adapt the ReAct prompts into its format but keep everything else fixed as much as possible. To provide fairer comparison, since LLaMA models do not have built in ways to restrict its tool calling to the provided tool set as GPT models can, we re-sample outputs for a certain amount of times if a tool hallucination falls outside of the tool set. This may also be quite easily done by constraining output tokens with certain syntax or grammar.

During inference, for PLAY2PROMPT we set the number of example demonstrations to 1, sampling temperature to 0.2 for LLaMA models.

B MORE QUALITATIVE EXAMPLES

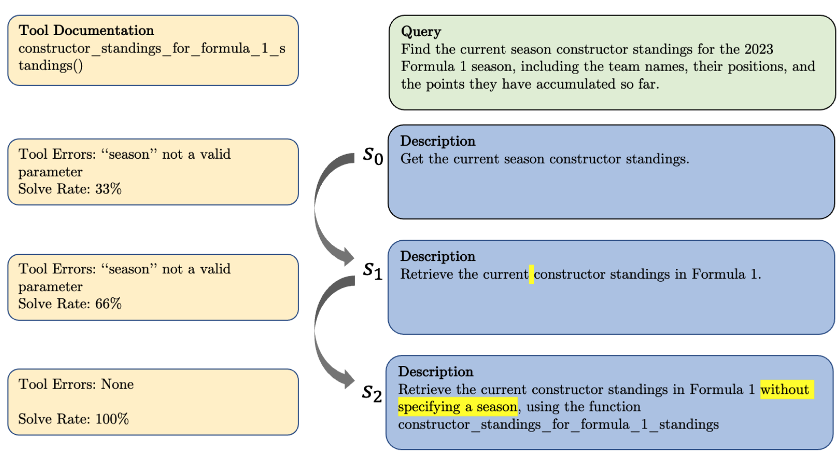


Figure 3: A typical example of PLAY2PROMPT assisting LLMs in correcting errors in generating parameter values. The base LLM gets confused by the query specifying the year, which PLAY2PROMPT first attempts to remove "year" from the description, and further explicitly prompts the base LLM to not use the parameter. The base LLM in this instance is LLaMA-3-8B.