FACILITATING MULTI-TURN FUNCTION CALLING FOR LLMS VIA COMPOSITIONAL INSTRUCTION TUNING

Anonymous authors
Paper under double-blind review

ABSTRACT

Large Language Models (LLMs) have exhibited significant potential in performing diverse tasks, including the ability to call functions or use external tools to enhance their performance. While current research on function calling by LLMs primarily focuses on single-turn interactions, this paper addresses the overlooked necessity for LLMs to engage in multi-turn function calling—critical for handling compositional, real-world queries that require planning with functions but not only use functions. To facilitate this, we introduce an approach, `BUTTON`, which generates synthetic compositional instruction tuning data via bottom-up instruction construction and top-down trajectory generation. In the bottom-up phase, we generate simple atomic tasks based on real-world scenarios and build compositional tasks using heuristic strategies based on atomic tasks. Corresponding functions are then developed for these compositional tasks. The top-down phase features a multi-agent environment where interactions among simulated humans, assistants, and tools are utilized to gather multi-turn function calling trajectories. This approach ensures task compositionality and allows for effective function and trajectory generation by examining atomic tasks within compositional tasks. We produce a dataset `BUTTONInstruct` comprising 8k data points and demonstrate its effectiveness through extensive experiments across various LLMs.

1 INTRODUCTION

Large Language Models (LLMs) have demonstrated remarkable capabilities across various tasks (OpenAI, 2023; Dubey et al., 2024). Beyond generating human-like text, recent studies have shown that LLMs can also call functions (i.e., use external tools) to perform specific actions or operations (Qin et al., 2023; Patil et al., 2023; Mu et al., 2024; Liu et al., 2024b). Leveraging external tools through the function calling ability has proven to be an effective way to enhance the performance of LLMs. For instance, retrieving relevant knowledge from external knowledge bases via search functions can help mitigate the problem of hallucination in LLMs (Schick et al., 2023; Gao et al., 2023; Zhao et al., 2024). Additionally, LLM-based agents can utilize function calls to interact with a wide range of existing external APIs. These functions offer standardized interfaces for engaging with diverse systems, thereby enhancing the utility and versatility of LLMs in real-world applications (Chen & Li, 2024; Wang et al., 2024a; Zeng et al., 2024).

Existing research on aligning LLMs for function calling predominantly focuses on a single-turn approach, primarily constructing instruction data to teach and evaluate them on selecting appropriate functions and providing the correct arguments (Patil et al., 2023; Liu et al., 2024b). While it is important for LLMs to learn how to understand and ***use functions***, these studies often overlook the crucial ability to ***plan with functions***. Many real-world user queries are complex and cannot be resolved in a single step. For example, “List the flight schedule from London to Edinburgh” may be a single-step task since simply retrieving exact information can complete it, while “Book me the first flight from London to Edinburgh” requires calling multiple functions sequentially: first retrieving the flight schedule and finding the first one, then booking a ticket for that flight. Real-world complex tasks are inherently compositional (Press et al., 2023; Hayati et al., 2024; Hu et al., 2024), requiring LLMs not only to invoke functions but also to decompose these tasks into manageable steps and plan the sequence of function calls. Therefore, in this study, we focus on constructing an instruction-tuning (Ouyang et al., 2022; Longpre et al., 2023) dataset where the inputs are complex compositional queries and the outputs are their decompositions into multi-turn function calls, addressing real-world scenarios of function calling for LLMs via *Compositional Instruction Tuning*.

However, acquiring such data from existing sources is unrealistic. First, selecting and identifying instructions in a compositional manner is challenging (Hayati et al., 2024; Hu et al., 2024), and finding instructions paired with their corresponding functions is even more difficult (Shen et al., 2023; Schick et al., 2023; Patil et al., 2023). Additionally, we need a "solution" in the form of labeled multi-turn function calls that align with the compositional instructions based on the given functions. All these factors make it difficult to obtain such data without extensive manual annotation. Recently, synthetic data has emerged as a promising solution to the lack of manually curated data, with data being created through advanced generative LLMs using tailored processes and simulations (Liu et al., 2024a). Compared to synthetic data in general domains (Xu et al., 2023; Lou et al., 2023; Xu et al., 2024a), data in our scenarios must consider the following challenges: 1) How to ensure the compositionality of generated instructions so that they are complex, reasonable and solvable; 2) How to ensure the compatibility of an instruction with its functions; 3) How to simulate high-quality multi-turn function calling trajectories without human supervision.

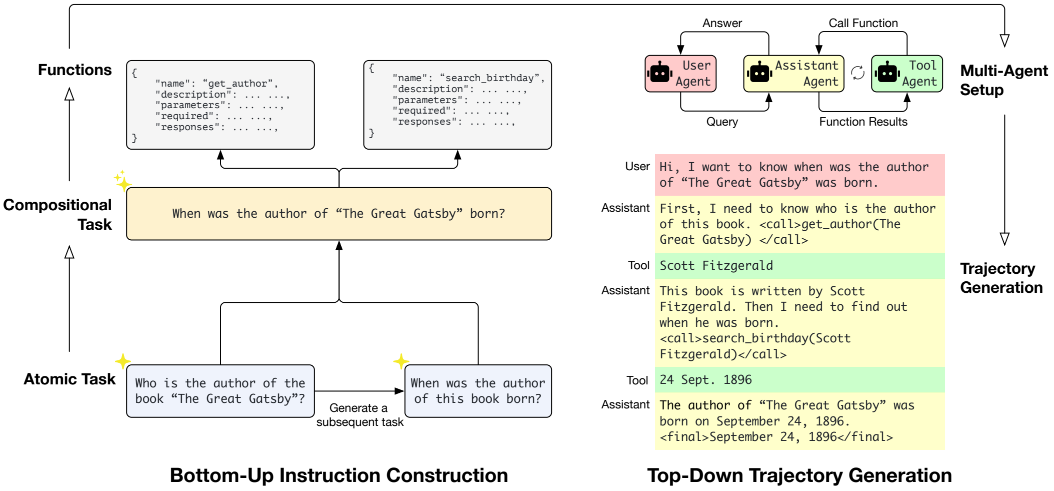
To address these challenges, we propose `BUTTON`, a "**B**ottom-**U**p **T**hen **T**op-d**O**w**N**" pipeline for generating synthetic compositional instruction tuning data to enhance the multi-turn function calling abilities of LLMs. In the "*Bottom-Up*" phase, we begin by generating atomic tasks from general real-world scenarios. These tasks are designed to be simple, clear, and executable in a single step without the need for planning. Compositional tasks are constructed based on atomic tasks using two heuristic strategies: Sequential Composition and Parallel-then-Sequential Composition. Although straightforward, these two composition strategies, combined with the entire pipeline, can generate diverse compositional instructions. Then, corresponding functions are generated based on compositional tasks with the conscious of their atomic tasks. During "*Top-Down*" phase, we set up a multi-agent environment where the human, assistant and tools are simulated by generative LLMs steered by specifically curated system prompts, where tool agents are simulated according to previous generated function definitions. The trajectory of multi-turn function calling, initiated by a user and involving interactions between an assistant and tools, is collected based on this simulated environment. Finally, the collected trajectories, along with their corresponding function definitions, are filled into a predefined prompt template to serve as instruction tuning data for LLMs. The bottom-up procedure, rather than generating complex tasks directly, ensures compositionality (challenge 1). Generating functions with an awareness of the atomic tasks within compositional tasks makes these functions more general and suitable for fine-grained sub-tasks, rather than being monolithic (challenge 2). Using multi-agents to simulate the trajectories enhances their quality, and examining the sub-tasks for compositional tasks also guides the agents toward effective decomposition and planning with functions (challenge 3). Based on `BUTTON`, we collected a compositional instruction tuning dataset called `BUTTONInstruct`, consisting of 8k high-quality data points labeled with multi-turn function call trajectories. We demonstrate that LLMs fine-tuned with `BUTTONInstruct` show improved performance on multi-turn function calling benchmarks.

2 RELATED WORK

Synthetic Data Data has always been the key driver behind the success of LLMs. Recent advancements are largely due to the availability of large-scale, diverse, and high-quality datasets for training these models (Lin et al., 2023). However, the scarcity and high costs of obtaining such datasets present substantial challenges (Xie et al., 2024; Xu et al., 2023). Recent progress in generating synthetic data has shown promising results across various domains (Liu et al., 2024a). Synthetic data holds great potential for building large-scale, high-quality datasets. Researchers have explored multiple approaches to enhance the quality, diversity, and utility of synthetic data (Wang et al., 2024c; Wei et al., 2023; Lou et al., 2023; Yang et al., 2023). Recent studies have also focused on synthetic data for complex and compositional instructions. Chain-of-Instruct (Hayati et al., 2024) proposed a pipeline for building instructions composed of subtasks, allowing LLMs to solve compositional tasks step-by-step in an explainable manner. Sequential Instruction Tuning (Hu et al., 2024) introduced a data construction pipeline for automatic instruction augmentation, where intermediate tasks are seeded from a single-task instruction. However, existing works do not focus on constructing compositional instructions for multi-turn function calling tasks, where identifying, invoking, and planning with functions are all necessary.

Function Calling Calling functions or using tools effectively has been an important factor to instruction tune LLMs (Wang et al., 2024a; Zeng et al., 2024; Shen et al., 2023; Xu et al., 2024b; Liu et al., 2024b; Patil et al., 2023), and is a crucial feature for LLMs as it enhances their ability to perform complex tasks by enabling modular and structured interactions. Traditional LLMs often generate text-based outputs based on their training data; however, many applications require more than just generating natural language. Function calling allows LLMs to invoke specific operations or calculations, facilitating a more dynamic and interactive problem-solving approach. Patil et al. (2023) collected APIs from TorchHub, TensorHub and HuggingFace and then generate synthetic user question prompts per API using Self-Instruct (Wang et al., 2023). Qin et al. (2023) collected additional API data from RapidAPI, and generate diverse instructions involving such APIs, covering different function calling scenarios. However, the descriptions for most APIs are not clear and a large number of API calls are not available with various errors, making pool solution path annotation generated by LLMs (Guo et al., 2024). Liu et al. (2024b) proposed APIGen, a pipeline for generating diverse function calling datasets by leveraging a multi-stage verification process only focus only on the single-turn function calling scenario.

3 METHOD



```
{
    "name": "get_author",
    "description": ... ...,
    "parameters": ... ...,
    "required": ... ...,
    "responses": ... ...,
}
```

```
{
    "name": "search_birthday",
    "description": ... ...,
    "parameters": ... ...,
    "required": ... ...,
    "responses": ... ...,
}
```

When was the author of “The Great Gatsby” born?

Who is the author of the book “The Great Gatsby”?

When was the author of this book born?

User: Hi, I want to know when was the author of “The Great Gatsby” was born.

Assistant: First, I need to know who is the author of this book. <call>get_author(The Great Gatsby) </call>

Tool: Scott Fitzgerald

Assistant: This book is written by Scott Fitzgerald. Then I need to find out when he was born. <call>search_birthday(Scott Fitzgerald)</call>

Tool: 24 Sept. 1896

Assistant: The author of “The Great Gatsby” was born on September 24, 1896. <final>September 24, 1896</final>

Figure 1: Overview of our bottom-up then top-down pipeline.

In this section, we introduce the details of our method for constructing compositional instruction-tuning data for multi-turn function calling tasks. This framework consists of two stages: 1) bottom-up instruction construction, and 2) top-down trajectory generation. We refer to this framework as the “Bottom-Up Then Top-dOwN” pipeline, denoted as `BUTTON`.

During the bottom-up instruction construction phase, we begin by gathering a variety of real-world scenarios. Drawing from these scenarios, we proceed to construct a series of atomic tasks, each as simple as possible and capable of being completed in one step. Compositional tasks will be evolved from such atomic tasks. Lastly, for each compositional task, we further generate functions that are likely to be called in this task. The term “bottom-up” signifies our approach of constructing comprehensive compositional tasks with their corresponding functions, starting from the foundation of simple atomic tasks, which can be shown in the left part of Figure 1.

During the top-down trajectory generation phase, we collect multi-turn function calling interaction trajectories for compositional tasks and functions that were constructed earlier. This step simulates the usage process of functions in each task, providing supervision data that guides the LLMs in learning how to call functions in multi-turn manners. The term “top-down” indicates that from a compositional task with corresponding functions, we simulate and gather the interaction trajectories that demonstrate the breakdown of complex tasks and the invocation of corresponding functions in a multi-turn manner, as depicted in the right part of Figure 1. In essence, the bottom-up instruction construction is a process of composition, while the top-down trajectory generation is a process of decomposition.

Definitions We begin by collecting real-world scenarios $\mathcal{C} = \{c_i\}$ and transforming them into atomic tasks $\mathcal{A} = \{a_i\}$. For compositional tasks requiring multiple function calls, we generate related atomic tasks from a defined atomic task a_i, forming a sub-task set $\mathcal{S}_i$. This set is used to compose a compositional task c_i, represented as $\mathcal{C} = \{(c_i, \mathcal{S}_i)\}$. Functions are then constructed based on these tasks, forming instruction tuples $\mathcal{I} = \{(c_i, \mathcal{F}_i, \mathcal{S}_i)\}$, where $\mathcal{F}_i$ are the functions for task c_i. These functions are defined by their descriptions, allowing us to simulate interactions without actual implementations. The task breakdown $\mathcal{S}_i$ is retained to enhance multi-agent interaction for trajectory generation, without being disclosed in the final data. After obtaining $\mathcal{I}$, we generate user, assistant, and tool interactions, resulting in data $\mathcal{D} = \{(\mathcal{F}_i, t_i)\}$, where t_i are the collected trajectories. These function definitions and trajectories are integrated into a prompt template for instruction-tuning data.

3.1 BOTTOM-UP INSTRUCTION CONSTRUCTION

In this section, we detail the procedures for constructing instructions using a bottom-up approach. The process begins with simple scenarios, from which we generate tasks at the atomic level. These atom tasks are then evolved to create more complex, composite tasks along with their corresponding functions.

Scenario Collection To ensure our generated tasks are grounded in everyday experiences and not meaningless, we first extract a series of real-world scenarios from existing datasets that focus on function calling for LLMs. Such scenarios can be a concise overview, like "book a flight" or "ordering meals". We then conduct a deduplication operation on the collected scenarios. This involves using sentence embeddings to calculate scenario similarities, and setting a specific threshold to filter out similar ones (Xiao et al., 2023). Furthermore, to expand our scenario collection, we also attempt to generate new scenarios from existing ones by altering their actions or subjects. Details of seed data for scenario extraction, prompts for extracting and expanding scenarios can be found in Appendix A.1.

Atomic Task Construction Based on the collected scenarios, we construct atomic tasks, each of which can be considered as a straightforward problem, query or instruction. We anticipate that these atomic tasks should be simple, clear, and don't need complex planning for human to solve. Such atomic tasks are able to serve as atomic units for constructing complex compositional tasks. In designing the prompts for transforming collected scenarios into atomic tasks, we focus on the following three aspects:

- **Reasonable**: The atomic task should be realistic, reasonable, and representative of tasks frequently encountered in the real world.
- **Self-contained**: The atomic task should be solvable based on the information it provides. It must contain sufficient details and information necessary for calling functions.
- **Function-agnostic**: During the articulation of the atomic task, we do not consider the specific functions that can be employed to solve this task. The task should not mention any specific function or solution.

Note that despite having numerous descriptions of our anticipated atomic tasks, we do not provide a strict definition of atomic tasks, nor of the following compositional tasks. We use specific prompts and the powerful instruction-following capabilities of cutting-edge LLMs to ensure that the generated data aligns with our general expectations. The carefully crafted prompt can be found in Appendix A.2.

Compositional Task Construction To enhance the capability of multi-turn function calling for LLMs, it is essential to construct compositional tasks that require multiple interactions to be resolved. Starting with the atomic tasks created in the previous step, we develop compositional tasks using two heuristic strategies: "Sequential Composition" and "Parallel-then-Sequential Composition". The principle behind sequential composition is to start with an atomic task and generate a subsequent task that needs to be solved based on the result of the first, combining them into a new compositional task. For parallel-then-sequential composition, we begin by generating a task that can be solved in parallel with the atomic task. Then, a subsequent task is generated based on the

Table 1: Examples of compositional task construction.

Sequential Composition	
Initial Atomic Task:	Who is author of the book "The Great Gatsby"?
Subsequent Task:	When was the author of this book born?
Composition Task:	When was the author of the book "The Great Gatsby" born?
Parallel-then-Sequential Composition	
Initial Atomic Task:	Give me the flight schedule from London to Edinburgh today.
Parallel Task:	Find the every hour weather forecast in Edinburgh today.
Subsequent Task:	What is the weather condition when the first flight arrives?
Composition Task:	I am in London, and I want to know the weather condition when the first flight arrives in Edinburgh today.

results of the first two tasks, and they are all composed together. Examples can be found in Table 1. Prompts for implementing these two strategies can be found in Appendix A.3. Although these two heuristic strategies seem simple, they do not compromise the diversity of the dataset collected using our method. For instance, parallel function calls are not limited to the first turn; multiple functions may be generated for a single atomic task in subsequent function generations. Details on the data diversity can be found in Sec. 3.3. To ensure the quality of the generated compositional tasks, we filter out any that are inconsistent with their original atomic tasks. The filtering criterion is as follows: since the quality of atomic tasks is more controllable, we filter compositional tasks by checking whether each one can be completed by its atomic sub-tasks. This allows us to filter out low-quality compositional tasks. The task filtering prompt can be found in Appendix A.3.

Function Generation After constructing the compositional tasks, we generate functions that are likely to be called in these tasks. This differs from most previous works, which first collect functions and then generate tasks based on these collected functions (Patil et al., 2023; Liu et al., 2024b). Our task-generation procedure is function-agnostic, which we believe allows for the construction of more realistic tasks, rather than those based solely on specific functions. Using the aforementioned methods, we have constructed a series of compositional tasks for which we know the corresponding sub-tasks (i.e., the breakdown of the complex compositional task). These task breakdowns can be used as hints for function generation. This represents the advantage of our bottom-up instruction construction method, where we can examine the decomposition of the compositional task and generate corresponding functions. During the generation of function definitions, we mainly focus on the following points:

- **Descriptive**: The name and description of the function should be illustrative to aid in distinguishing different functions. The input arguments and output returns should also be clear since we not only use these definitions to but also use them to simulate corresponding functions.
- **General**: The function should possess a level of generality that enables its use for future tasks as well. In the real world, a function is more likely to be constructed for a frequently encountered atomic task rather than a highly specific one. For instance, a function `get_weather(city)` is more likely to be utilized than `get_weather_in_london()`.
- **Consistency**: As we need to generate multi-turn function calling interaction trajectories in later steps, the input arguments and output results of these functions should maintain consistency. For example, if two functions will be called sequentially, the output of the first should either align with or constitute a part of the input for the second function, regardless of the varying parameter terminologies.

The generated function definitions include five main fields: name, description, parameters, responses, and required. The name indicates the function name, while description details its usage and capabilities. Parameters and responses cover the input and output, including the type and description of each argument. The required field lists necessary input parameters. We allow flexibility in mapping sub-tasks to functions; a sub-task may require zero, one, or multiple functions. If a sub-task involves logic, comparison, set operations, or calculations manageable by language models, no function is needed. For more details on the format and prompts, see Appendix A.4.

3.2 TOP-DOWN TRAJECTORY GENERATION

After obtaining the compositional tasks and their corresponding functions through the bottom-up instruction construction method, we create multi-turn function calling interaction trajectories. These trajectories simulate how LLMs use these functions and serve as supervision data, teaching LLMs to perform multi-turn function calls.

Multi-agent Setup How to effectively simulate the multi-turn function calling interaction process is the key to collecting high-quality interaction trajectories. In our framework, we set up a multi-agent environment in which each agent simulates a specific role during the multi-turn function calling interactions, as shown in the right part of Figure 1. We design three types of agents to simulate the interaction process: the user, the assistant, and the tool. The user agent initiates the interaction and provides the query to the assistant agent based on a specific compositional task. The assistant agent decomposes the task into sub-tasks and calls the corresponding functions to address these sub-tasks. The tool agent simulates the specific implementations of a function. It's important to note that a tool agent simulates a specific function based on its definition. We do not implement the actual functionality of the function as we merely require reasonable feedback from the tool agents to advance the interaction. Specifically, the assistant agent is aware of the available tools, compositional tasks, and the task breakdown. Since our compositional tasks are constructed in a bottom-up manner, the breakdown of these tasks naturally comprises their atomic components. For each function, we establish a tool agent based on its definitions. The behavior of the agents is steered by their system prompts, and the details of system prompts are listed in Appendix A.5.

Interaction Trajectory Collection. After setting up the multi-agent environments, given a specific compositional task and corresponding functions, we tailor prompts for each agent. The interaction trajectory begins with the user agent. The assistant agent reviews the task, decides which functions to call, and determines the function parameters. The assistant's response includes: first, observations and thoughts in free text, similar to the ReAct (Yao et al., 2023) format; second, a specified function call. This function call is parsed as an action to invoke the corresponding tool agent and obtain simulated function call results. Finally, when the assistant has the final answer to the user's question, it invokes the function that provides the final response to the user.

3.3 DATASET COLLECTION VIA BUTTON

BUTTONInstruct Based on the aforementioned pipeline, we leverage the cutting-edge LLM, GPT-4o[1], to generate data at each step of bottom-up instruction construction, progressing from simple scenarios to compositional tasks and functions, and conducting trajectory generation as agents. We ultimately collect 8,000 multi-turn function calling data points, `BUTTONInstruct`, each containing several entries, including content with roles such as 'system', 'user', 'assistant', and 'tool'. The available functions for the current user question are listed in the system prompt. More examples of finally generated data can be found in Appendix B.1.

Parallel Function Calling Furthermore, in our collected data, we consider scenarios involving parallel function calling. If multiple functions can be called independently, they can be executed in parallel. The effectiveness of this parallel calling is discussed in Section 4.3. To control the behavior of conducting parallel calling, we use different system prompts to guide whether parallel calling should be executed. Details on how to construct data for aligning LLMs with the corresponding calling behaviors can be found in Appendix B.2.

Data Diversity To demonstrate the diversity of the collected `BUTTONInstruct`, we analyzed the distribution of the total number of assistant turns (#Turn), as well as the number of function calls (#FC) throughout the entire trajectory and at each step. Figure 2 presents key statistics of our dataset. In Figure 2(a), the frequency distribution of the total number of turns shows that most data

---

[1] gpt-4o-2024-05-13 from `https://platform.openai.com/docs/models/gpt-4o`

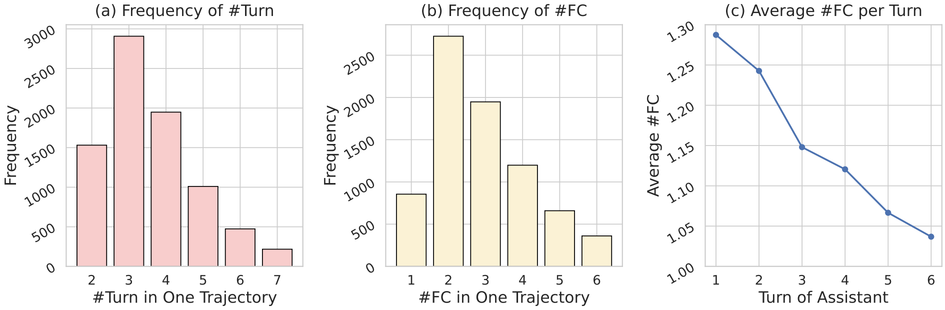


Figure 2: Statistic investigation on our collected data `BUTTONInstruct`.

points involve three or more turns of assistant responses. We plotted the distribution of the total number of function calls for each trajectory in Figure 2(b) and found that most data points contain more than two function calls. By plotting the average number of function calls per turn in Figure 2(c), we observed that every turn averages more than one function call. These findings indicate the diversity in our collected data and demonstrate that, even with simple heuristic strategies to generate compositional tasks from atomic tasks, the final collected data are diverse across different aspects. Furthermore, more details about the distribution of the functions in the `BUTTONInstruct` are provided in Appendix B.3.

4 EXPERIMENTS

To evaluate the effectiveness of our multi-turn function calling data `BUTTONInstruct` collected via our proposed `BUTTON` pipeline, we train two series of open-source LLMs of different sizes: Llama3-8B, Llama3-70B (Dubey et al., 2024), Qwen2-7B, and Qwen2-72B (Yang et al., 2024). We denote models that have been instruction-tuned using `BUTTONInstruct` with the suffix '-BUTTON'. In our experiments, we primarily focus on the following questions: 1) *Q1*: Can our proposed `BUTTON` approach enhance multi-turn function calling abilities compared to existing instruction-tuned models designed for general purposes? 2) *Q2*: Are the bottom-up and top-down procedures effective and necessary? 3) *Q3*: What is the influence of data size and parallel calling on model performance?

4.1 EXPERIMENTS SETUP

Benchmarks. We evaluate performance using two benchmarks, GTA and Tool-Query. **GTA** (Wang et al., 2024b), a benchmark for General Tool Agents, consists of 229 human-crafted queries designed to reflect real-world tasks. The queries span a total of 14 real-world deployed tools (i.e., functions) across the perception, operation, logic, and creation categories. Each query is accompanied by one or two authentic image files and the LLM is tasked with solving the queries based on the multimodal context and user queries. The tasks in this benchmark require multiple steps to solve and necessitate LLMs to reason about suitable tools and plan the solution steps. More details and examples about this benchmark can be found in Appendix B of Wang et al. (2024b). **Tool-Query** (Ma et al., 2024) is a tool-using environment in the domains of weather, movies, and academia. It consists of 60 tasks requiring complex multi-round interactions with corresponding tools. There are 18, 14, and 7 tools (i.e., functions) in the weather, movie, and academia environments respectively, which are developed by corresponding real-world APIs and databases. This benchmark not only contains annotated final answers but also intermediate subgoals, which makes it easier to evaluate the process of function calling during multi-turn interactions. Tasks are also labeled as hard or easy based on the number of subgoals, with a count of 4 in this benchmark. More details and examples of Tool-Query can be found in Appendix F.4.1 of Ma et al. (2024).

Evaluation Metrics. For each benchmark, we follow their original evaluation strategies and metrics. For **GTA**, there are two modes and nine metrics. In the Step-by-Step Mode, the model is provided with steps 1 to n from a set of human-labeled function calling chains, and it is tasked with predicting the function call in the $n + 1$ step. This demonstrates performance in a fine-grained way. In the End-to-End Mode, the model initiates its function calling process based solely on the user's question and proceeds until it arrives at the answer. This reflects the performance of the model in real-world applications. Four metrics are used during the step-by-step mode evaluation: Instruction Accuracy (*Inst.*) is the accuracy of executing without errors, which indicates that the model knows how to follow the instruction to conduct a function call; Tool-selection Accuracy (*Tool.*) and Argument Accuracy (*Arg.*) denote the accuracy of selecting tools and predicting arguments respectively; Summary Accuracy (Summ.) denotes the model's ability to summarize and derive the answer based on all previous steps. During end-to-end mode, we show the F1 scores of tool selection on perception (*P.*), operation (*O.*), logic (*L.*), and creativity (*C.*) tasks, and the final answer accuracy (*Ans.*). The final answer accuracy is only calculated solely on queries with pure text answers, excluding image generation queries. For **Tool-Query**, Grounding Accuracy (*G.A.*) is used to denote the accuracy of generating valid, executable function calls. Process Rate is used to evaluate the completion proportion of subgoals during the handling of complex user queries and the subgoals are labeled in this dataset. Furthermore, Success Rate is the accuracy of the final answer. More details of metric calculation can be found in Appendix C.1.

Baselines. We showcase the performance on cutting-edge API-based LLMs, including GPT-4o, GPT-4-Turbo, and GPT-3.5-Turbo. Furthermore, since our collected data `BUTTONInstruct` is adapted for tuning the Llama3 and Qwen2 base models, we also use their original instruction-tuned versions as baselines, including Llama3-8B-Instruct, Llama3-70B-Instruct, Qwen2-7B-Instruct, and Qwen2-72B-Instruct (Dubey et al., 2024; Yang et al., 2024).

Implementation. We conduct full-parameter supervised fine-tuning for all base models, with a maximum sequence length of 8,192. The models are trained on 4×8 NVIDIA H800 GPUs. In addition, we randomly select 100,000 general instruction tuning data from OpenHermes-2.5 (Teknium, 2023) and mix them with `BUTTONInstruct` to align the models' basic instruction-following capabilities. For implementation details, please refer to Appendix C.2.

4.2 MAIN RESULTS

As shown in Table 2 and Table 3, LLMs tuned with compositional instruction tuning data constructed by our proposed `BUTTON` method perform better than their corresponding original instructed versions. For smaller models, the improvements are significant. For example, we improved the answer accuracy of Llama3-8B from 1.4% to 30.5%. The low performance of Llama3-8B-Instruct on this metric is consistent with the findings in the original benchmark paper. Notably, the results of Llama3-80B-BUTTON and Qwen2-72B-BUTTON are comparable to GPT-4o, demonstrating the effectiveness of the data collected through our proposed data collection pipeline.

Table 2: Main results(%) on GTA. Accuracy of *Inst.*, *Tool.*, *Arg.*, and *Summ.*. F1 score of *P.*, *O.*, *L.*, and *C.*. *Ans.* is the final answer accuracy. **Bold** numbers highlight better performance between the original instruction model and our tuned versions, while <u>underlined</u> numbers denote the best performance across all models.

Model	**Step-by-Step Mode**				**End-to-End Mode**				
	Inst.	*Tool.*	*Arg.*	*Summ.*	*P.*	*O.*	*L.*	*C.*	*Ans.*
GPT-4o	90.0	70.3	<u>38.6</u>	72.9	76.4	88.2	84.8	90.0	<u>46.0</u>
GPT-4-Turbo	84.6	60.6	34.3	73.5	51.8	87.7	61.8	86.1	30.6
GPT-3.5-Turbo	64.8	33.1	22.4	66.2	60.2	48.4	69.0	95.8	18.3
Llama3-8B-Instruct	70.9	23.6	2.2	42.9	23.5	18.5	23.6	24.6	1.4
Llama3-8B-BUTTON	**90.7**	**63.4**	**32.3**	**65.6**	**84.2**	**76.5**	**73.5**	**88.9**	**30.5**
Qwen2-7B-Instruct	59.1	28.5	3.9	54.8	39.1	65.4	56.1	72.7	13.1
Qwen2-7B-BUTTON	**89.4**	**62.5**	**30.7**	**63.0**	**80.3**	**83.5**	**82.6**	**89.2**	**27.3**
Llama3-70B-Instruct	75.2	46.7	22.2	68.4	67.9	83.8	71.0	95.9	40.1
Llama3-70B-BUTTON	**<u>96.4</u>**	**<u>73.6</u>**	**38.1**	**70.5**	**84.9**	**<u>96.2</u>**	**<u>89.5</u>**	**<u>96.1</u>**	**43.5**
Qwen2-72B-Instruct	73.4	49.2	17.9	**<u>73.9</u>**	46.5	67.5	46.7	64.3	27.3
Qwen2-72B-BUTTON	**91.9**	**69.3**	**38.1**	71.5	**<u>85.0</u>**	**87.4**	**86.7**	**91.4**	**45.7**

For Tool-Query, LLMs equipped with our compositional instruction tuning data `BUTTONInstruct` demonstrate improved performance across various metrics. We observe that even though the grounding accuracy for both the original instruction models and those tuned with our dataset is quite high (near or above 95%), our models achieve better process and success rates. This suggests that the challenge lies not only in using functions correctly but also in effectively planning with them. Overall, from the main results from GTA and Tool-Query, we can conclude that `BUTTONInstruct` can align LLMs with better ability on multi-turn function calling, and `BUTTON` is effective on such tasks.

Table 3: Main results(%) on Tool-Query. *G.A.* indicate grounding accuracy. Process Rate and Success Rate are presented for *Easy*, *Hard* and *ALL* test samples. **Bold** numbers highlight better performance between the original instruction model and our tuned versions, while underlined numbers denote the best performance across all models.

Model	G.A.	Process Rate			Success Rate		
		Easy	*Hard*	*All*	*Easy*	*Hard*	*All*
GPT-4o	92.3	83.2	70.6	76.5	50.0	31.3	40.0
GPT-4-Turbo	95.4	80.7	78.9	79.8	50.0	34.4	41.7
GPT-3.5-Turbo	93.6	54.9	43.2	48.7	3.6	9.4	6.7
Llama3-8B-Instruct	96.7	55.1	42.0	48.1	10.7	0.0	5.0
Llama3-8B-BUTTON	**97.4**	**72.9**	**54.8**	**63.2**	**50.0**	**21.9**	**35.0**
Qwen2-7B-Instruct	**97.0**	66.7	46.8	56.0	32.1	**15.6**	23.3
Qwen2-7B-BUTTON	95.5	**69.5**	**59.0**	**63.9**	**42.9**	**15.6**	**28.3**
Llama3-70B-Instruct	**95.6**	80.8	61.5	70.5	42.9	21.9	31.7
Llama3-70B-BUTTON	94.0	**85.2**	**77.2**	**80.9**	**71.4**	**46.9**	**58.3**
Qwen2-72B-Instruct	95.8	83.7	72.2	77.6	50.0	34.4	41.7
Qwen2-72B-BUTTON	**98.4**	**85.5**	**77.0**	**81.0**	**71.4**	**46.9**	**58.3**

4.3 FURTHER ANALYSIS

Ablation Study To evaluate the effectiveness of the "bottom-up instruction construction" and "top-down trajectory generation" procedures in `BUTTON` respectively, we conduct an ablation study by simplifying these two procedures into single direct generation steps using one prompt with generative LLMs, instead of our curated prompts and procedures. Specifically, to simplify the bottom-up procedure, we instruct generative LLMs to directly generate a compositional complex task based on a given scenario. As a result, no sub-tasks are revealed for the subsequent function generation and trajectory generation steps. To reduce the top-down procedure, we do not set up the multi-agent environment. Instead, we use a monolithic prompt that instructs the LLMs to act as the user, assistant, and tools, generating trajectories based on previously constructed tasks with functions. The results of the ablation study on Tool-Query are shown in Figure 3. We perform a comparison using the aforementioned two ablation settings (i.e., w/o Buttom-Up and w/o Top-Down), and the default setting (i.e., w/ BUTTON) on Llama3-8B and Llama3-70B. By calculating

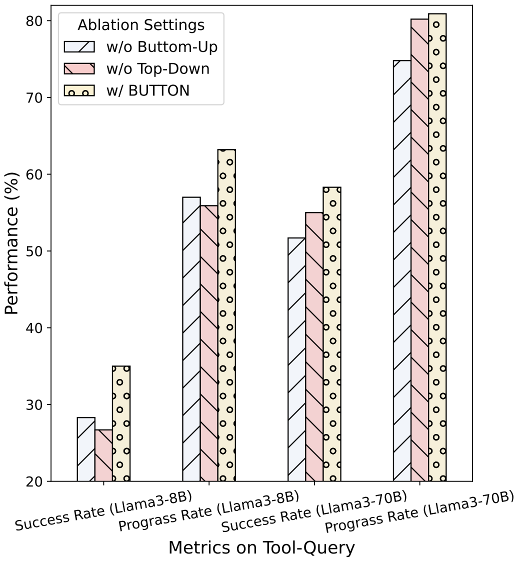


Figure 3: Comparison of performance in the ablation study.

the relative performance degradation, we found that the smaller model was influenced more, with average relative degradations on progress rate and success rate of 16.1%, and that decline for Llama3-70B is 6.4%. From the perspective of metrics, we found that the average relative success rate decline for both model sizes with both ablation settings is 15.0%, and the average relative decline for the progress rate is 7.5%. This indicates that while models tuned without `BUTTON` can execute the correct functions contributing to the progress rate, they struggle to plan effectively with these functions to arrive at the final answer, thereby impacting the success rate.

Table 4: Results(%) on Tool-Query with Llama3-8B tuned with varying data sizes.

#Data	Process Rate			Success Rate		
	Easy	*Hard*	*All*	*Easy*	*Hard*	*All*
2,000	67.5	46.9	56.5	35.7	9.4	21.7
4,000	73.1	45.8	58.5	**50.0**	12.5	30.0
6,000	**74.6**	51.5	62.3	46.4	15.6	30.0
8,000	72.9	**54.8**	**63.2**	**50.0**	**21.9**	**35.0**
AGR	13.5	32.8	18.4	2.7	5.5	3.8

Data Scaling In this section, we investigate the influence of data size on compositional instruction tuning data constructed by `BUTTON`. We vary the data size from 2,000 to 8,000 and tune Llama3-8B with the corresponding data. As shown in Table 4, we present the results on Tool-Query with varying data sizes. By calculating the average growth rate (AGR), we found that as the data size increases, the process rate and success rate increase accordingly, with AGRs of 13.5% and 2.7%, respectively. Furthermore, we found that the improvement on hard samples is greater than on easy samples, indicating that our constructed data can effectively enhance performance on multi-turn function calling as the data size increases, particularly for tasks that require more turns of function calling.

Efficiency on Parallel Calling As described in Section 3.3, we have mentioned that our tuned model can conduct parallel function calling when multiple functions can be called independently within a single turn. This capability can significantly enhance performance when operating under restricted step conditions. By turning off the parallel calling ability by changing the system prompt, we found that performance on different metrics is affected. For example, the success rate of Llama3-8B-BUTTON on Tool-Query decreases from 35.0% to 28.3%, and the progress rate decreases from 63.2% to 58.7%. This indicates the effectiveness of parallel calling and our proposed `BUTTON` method. More cases about comparisons of parallel calling can be found in Appendix C.4.

5 CONCLUSION

In this work, we address the importance of multi-turn function calling in the field of LLMs by focusing on their ability to plan with functions, rather than merely use them. We introduce `BUTTON`, a novel "bottom-up then top-down" pipeline for generating synthetic compositional instruction tuning data. This approach effectively tackles the challenges of ensuring compositionality of tasks, generating compatible function, and high-quality multi-turn function calling trajectories without human supervision via the curated prompts and procedures during the pipeline. Our methodology, which includes the generation of atomic tasks, compositional task construction, function generation, and a multi-agent simulation environment, has resulted in the creation of `BUTTONInstruct`, a dataset of 8,000 high-quality data points labeled with multi-turn function call trajectories. The effectiveness of this approach is demonstrated by the improved performance of LLMs fine-tuned with `BUTTONInstruct` on multi-turn function calling benchmarks. However, although our method has been empirically proven effective through experiments and analysis, the quality of the data currently relies on our prompts and procedures, with no additional verification steps applied. In future work, we will implement more curated data verification or filtering stages to enhance the quality of the synthetic data. Furthermore, we may focus on extending the pipeline to align LLMs with more real-world applications, including Embodied AI, where tool use, complex reasoning, and planning need to be integrated to complete more complex tasks.

REFERENCES

Wei Chen and Zhiyuan Li. Octopus v4: Graph of language models. *CoRR*, abs/2404.19296, 2024.

Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, Ahmad Al-Dahle, Aiesha Letman, Akhil Mathur, Alan Schelten, Amy Yang, Angela Fan, et al. The llama 3 herd of models. *arXiv preprint arXiv:2407.21783*, 2024.

Yunfan Gao, Yun Xiong, Xinyu Gao, Kangxiang Jia, Jinliu Pan, Yuxi Bi, Yi Dai, Jiawei Sun, Qianyu Guo, Meng Wang, and Haofen Wang. Retrieval-augmented generation for large language models: A survey. *CoRR*, abs/2312.10997, 2023.

glaiveai. glaive-function-calling-v2. `https://huggingface.co/datasets/glaiveai/glaive-function-calling-v2`, 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 *ACL (Findings)*, pp. 11143–11156. Association for Computational Linguistics, 2024.

Shirley Anugrah Hayati, Taehee Jung, Tristan Bodding-Long, Sudipta Kar, Abhinav Sethy, Joo-Kyung Kim, and Dongyeop Kang. Chain-of-instructions: Compositional instruction tuning on large language models. *CoRR*, abs/2402.11532, 2024.

Hanxu Hu, Pinzhen Chen, and Edoardo M. Ponti. Fine-tuning large language models with sequential instructions. *CoRR*, abs/2403.07794, 2024.

Zinan Lin, Sivakanth Gopi, Janardhan Kulkarni, Harsha Nori, and Sergey Yekhanin. Differentially private synthetic data via foundation model apis 1: Images. *CoRR*, abs/2305.15560, 2023.

Ruibo Liu, Jerry Wei, Fangyu Liu, Chenglei Si, Yanzhe Zhang, Jinmeng Rao, Steven Zheng, Daiyi Peng, Diyi Yang, Denny Zhou, and Andrew M. Dai. Best practices and lessons learned on synthetic data for language models. *CoRR*, abs/2404.07503, 2024a.

Zuxin Liu, Thai Hoang, Jianguo Zhang, Ming Zhu, Tian Lan, Shirley Kokane, Juntao Tan, Weiran Yao, Zhiwei Liu, Yihao Feng, et al. Apigen: Automated pipeline for generating verifiable and diverse function-calling datasets. *arXiv preprint arXiv:2406.18518*, 2024b.

Shayne Longpre, Le Hou, Tu Vu, Albert Webson, Hyung Won Chung, Yi Tay, Denny Zhou, Quoc V Le, Barret Zoph, Jason Wei, et al. The flan collection: Designing data and methods for effective instruction tuning. *arXiv preprint arXiv:2301.13688*, 2023.

Renze Lou, Kai Zhang, Jian Xie, Yuxuan Sun, Janice Ahn, Hanzi Xu, Yu Su, and Wenpeng Yin. MUFFIN: curating multi-faceted instructions for improving instruction-following. *CoRR*, abs/2312.02436, 2023.

Chang Ma, Junlei Zhang, Zhihao Zhu, Cheng Yang, Yujiu Yang, Yaohui Jin, Zhenzhong Lan, Lingpeng Kong, and Junxian He. Agentboard: An analytical evaluation board of multi-turn LLM agents. *CoRR*, abs/2401.13178, 2024.

Yao Mu, Qinglong Zhang, Mengkang Hu, Wenhai Wang, Mingyu Ding, Jun Jin, Bin Wang, Jifeng Dai, Yu Qiao, and Ping Luo. Embodiedgpt: Vision-language pre-training via embodied chain of thought. *Advances in Neural Information Processing Systems*, 36, 2024.

OpenAI. GPT-4 technical report. *CoRR*, abs/2303.08774, 2023.

Long Ouyang, Jeffrey Wu, Xu Jiang, Diogo Almeida, Carroll L. Wainwright, Pamela Mishkin, Chong Zhang, Sandhini Agarwal, Katarina Slama, Alex Ray, John Schulman, Jacob Hilton, Fraser Kelton, Luke Miller, Maddie Simens, Amanda Askell, Peter Welinder, Paul F. Christiano, Jan Leike, and Ryan Lowe. Training language models to follow instructions with human feedback. In *NeurIPS*, 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.

Ofir Press, Muru Zhang, Sewon Min, Ludwig Schmidt, Noah A. Smith, and Mike Lewis. Measuring and narrowing the compositionality gap in language models. In *EMNLP (Findings)*, pp. 5687–5711. Association for Computational Linguistics, 2023.

Yujia Qin, Shihao Liang, Yining Ye, Kunlun Zhu, Lan Yan, Yaxi Lu, Yankai Lin, Xin Cong, Xiangru Tang, Bill Qian, et al. Toolllm: Facilitating large language models to master 16000+ real-world apis. *arXiv preprint arXiv:2307.16789*, 2023.

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

Yongliang Shen, Kaitao Song, Xu Tan, Dongsheng Li, Weiming Lu, and Yueting Zhuang. Hugginggpt: Solving AI tasks with chatgpt and its friends in hugging face. In *NeurIPS*, 2023.

Teknium. Openhermes 2.5: An open dataset of synthetic data for generalist llm assistants, 2023. URL `https://huggingface.co/datasets/teknium/OpenHermes-2.5`.

Guanzhi Wang, Yuqi Xie, Yunfan Jiang, Ajay Mandlekar, Chaowei Xiao, Yuke Zhu, Linxi Fan, and Anima Anandkumar. Voyager: An open-ended embodied agent with large language models. *Trans. Mach. Learn. Res.*, 2024, 2024a.

Jize Wang, Zerun Ma, Yining Li, Songyang Zhang, Cailian Chen, Kai Chen, and Xinyi Le. GTA: A benchmark for general tool agents. *CoRR*, abs/2407.08713, 2024b.

Yifei Wang, Jizhe Zhang, and Yisen Wang. Do generated data always help contrastive learning? *CoRR*, abs/2403.12448, 2024c.

Yizhong Wang, Yeganeh Kordi, Swaroop Mishra, Alisa Liu, Noah A. Smith, Daniel Khashabi, and Hannaneh Hajishirzi. Self-instruct: Aligning language models with self-generated instructions. In *ACL (1)*, pp. 13484–13508. Association for Computational Linguistics, 2023.

Yuxiang Wei, Zhe Wang, Jiawei Liu, Yifeng Ding, and Lingming Zhang. Magicoder: Source code is all you need. *CoRR*, abs/2312.02120, 2023.

Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, and Jamie Brew. Huggingface's transformers: State-of-the-art natural language processing. *CoRR*, abs/1910.03771, 2019.

Shitao Xiao, Zheng Liu, Peitian Zhang, and Niklas Muennighoff. C-pack: Packaged resources to advance general chinese embedding, 2023.

Chulin Xie, Zinan Lin, Arturs Backurs, Sivakanth Gopi, Da Yu, Huseyin A. Inan, Harsha Nori, Haotian Jiang, Huishuai Zhang, Yin Tat Lee, Bo Li, and Sergey Yekhanin. Differentially private synthetic data via foundation model apis 2: Text. *CoRR*, abs/2403.01749, 2024.

Can Xu, Qingfeng Sun, Kai Zheng, Xiubo Geng, Pu Zhao, Jiazhan Feng, Chongyang Tao, Qingwei Lin, and Daxin Jiang. Wizardlm: Empowering large pre-trained language models to follow complex instructions. In *ICLR*. OpenReview.net, 2024a.

Canwen Xu, Daya Guo, Nan Duan, and Julian J. McAuley. Baize: An open-source chat model with parameter-efficient tuning on self-chat data. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing, EMNLP 2023, Singapore, December 6-10, 2023*, pp. 6268–6278, 2023.

Yiheng Xu, Hongjin Su, Chen Xing, Boyu Mi, Qian Liu, Weijia Shi, Binyuan Hui, Fan Zhou, Yitao Liu, Tianbao Xie, Zhoujun Cheng, Siheng Zhao, Lingpeng Kong, Bailin Wang, Caiming Xiong, and Tao Yu. Lemur: Harmonizing natural language and code for language agents. In *ICLR*. OpenReview.net, 2024b.

An Yang, Baosong Yang, Binyuan Hui, Bo Zheng, Bowen Yu, Chang Zhou, Chengpeng Li, Chengyuan Li, Dayiheng Liu, Fei Huang, et al. Qwen2 technical report. *arXiv preprint arXiv:2407.10671*, 2024.

Dongjie Yang, Ruifeng Yuan, Yuantao Fan, Yifei Yang, Zili Wang, Shusen Wang, and Hai Zhao. Refgpt: Dialogue generation of gpt, by gpt, and for GPT. In *Findings of the Association for Computational Linguistics: EMNLP 2023, Singapore, December 6-10, 2023*, pp. 2511–2535. Association for Computational Linguistics, 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 *ICLR*. OpenReview.net, 2023.

Aohan Zeng, Mingdao Liu, Rui Lu, Bowen Wang, Xiao Liu, Yuxiao Dong, and Jie Tang. Agenttuning: Enabling generalized agent abilities for llms. In *ACL (Findings)*, pp. 3053–3077. Association for Computational Linguistics, 2024.

Penghao Zhao, Hailin Zhang, Qinhan Yu, Zhengren Wang, Yunteng Geng, Fangcheng Fu, Ling Yang, Wentao Zhang, and Bin Cui. Retrieval-augmented generation for ai-generated content: A survey. *arXiv preprint arXiv:2402.19473*, 2024.

A PROMPT DETAILS

A.1 SCENARIO COLLECTION

In our work, the seed data for scenario extraction is derived from glaive-function-calling-v2 (glaiveai, 2023) and ToolLLama datasets (Qin et al., 2023).

Here are prompts for extracting and expanding scenarios. The placeholders {`conversation`} and {`scenario`} are used to fill in a conversation for extracting a scenario and a scenario for being modified, respectively.

Prompt for Extracting Scenarios

```
Please analyze the conversation below between a user and an
   assistant bot and identify the general life scenario it
   represents. Provide a concise overview of the scenario type,
   such as 'booking flights' or 'ordering meals'. Avoid
   mentioning specific details like numbers or items. Your
   response should be a description of the scenario without
   additional commentary, and should not exceed 10 words.

Conversation:
{conversation}

Concise Overview of the Scenario:
```

Prompt for Expanding Scenarios

```
Based on the provided daily scenario, creatively generate a new
   and entirely different scenario. The new scenario must meet
   the following requirements:
1. You may alter the action or subject of the original scenario.
2. The new scenario should differ substantially from the
   original.
3. Ensure the new scenario is realistic and feasible within a
   daily life context.
4. Retain the same format as the original scenario.
5. Limit your response to 10 words and present the new scenario
   in a single sentence.

Original Scenario:
{scen}
```

```
Modified Scenario:
```

A.2 ATOMIC TASK CONSTRUCTION

Here is the prompt for generating an atomic task from a scenario. The placeholder {`scenario`} will be substituted with a collected scenario when generating a specific task.

Prompt for Atomic Task Construction

```
You are training a model that can take a user’s task description
     or query, and available functions as input, and generate a
    sequence of function calls to accomplish the task. Currently,
     you are generating basic atom tasks. Given a general life
    scenario as the context, please generate a basic atom task
    that can be accomplished in one step.

Requirements of the task:
1. The task should be a reasonable real life task based on the
    given scenario, and can be accomplished in one step.
2. If you mention some information, criteria or constraints in
    the task, please give the details of these information,
    criteria or constraints. Do not assume the model has access
    to your personal information or prior knowledge, and it does
    not have chance to ask you for clarification.
3. Please give enough details and make the task description as
    specific as possible, so the model can make deterministic
    function calls with deterministic arguments. Do not include
    any ambiguous or vague information.
4. Do not mention specific tools or functions in the task
    description, and do not propose solutions, hints, or project
    outcomes.
5. Limit the task description to 30 words, and avoid using
    adjectives and ambiguous words.

Given Scenario:
{scenario}

Please give your response in one line directly, without any
    extra notation or format:
```

A.3 COMPOSITIONAL TASK CONSTRUCTION

Following two prompts are used for constructing compositional tasks from atomic tasks, including sequential composition and parallel-then-sequential composition strategies.

Prompt for Sequential Composition

```
You are training a model that can take a user’s task description
     or query, and available functions as input, and generate a
    sequence of function calls to accomplish the task. Currently,
     you are generating complex tasks for model training. Given a
     task, you need to add a subsequent task for this given task
    to make a more complex task.

The requirements for the subsequent task are as follows:
```

```
1. The subsequent task should use the output of the given task as input.
2. The subsequent can only be conducted after the given task has been completed.
3. The subsequent task and the given task can form a new compositional task, and composing them can make a more complex multi-step task.

## Examples:
### Given Task: Give me a list of all the pets.
### Subsequent Task: What is the most common kind of pet in the list?
### Composition Task: Check the most common kind of pet in the list of all the pets.

### Given Task: Who is author of the book "The Great Gatsby"?
### Subsequent Task: When was the author of this book born?
### Composition Task: When was the author of the book "The Great Gatsby" born.

### Given Task: Give me the flight schedule from London to Edinburgh today.
### Subsequent Task: Which fight has the shortest duration?
### Composition Task: Give me the flight from London to Edinburgh with the shortest duration according to the flight schedule today.

### Given Task: Retrieve the headlines of the news today from BBC.
### Subsequent Task: What is the sentiment of the news respectively?
### Composition Task: What is the sentiment of each headline in today's news from BBC?

### Given Task: Which team won the World Cup in 2018?
### Subsequent Task: What is the team's captain?
### Composition Task: Who is the captain of the team that won the World Cup in 2018.

## Here is the given task, please give your response following the above format:
### Given Task: {task}
```

Prompt for Parallel-then-Sequential Composition

```
You are training a model that can take a user's task description or query, and available functions as input, and generate a sequence of function calls to accomplish the task. Currently, you are generating complex tasks for model training. Given a task, you need to add a paralle task and a subsequent task for this given task to make a more complex task.

The requirements for the parallel task are as follows:
1. The parallel task should be related to the given task, and the input should independent of the output of the given task.
2. The parallel task can conduct at the same time as the given task, and they can be independent of each other.
```

```
3. The output of the given task and the parallel task can be used together to conduct a subsequent task.

The requierments for the subsequent task are as follows:
1. The subsequent task should use the output of the given task and generate parallel task as input.
2. The subsequent can only be conducted after the given task and the parallel task have been completed.
3. The subsequent task, the given task and the parallel task can form a new compositional task, and composing them can make a more complex multi-step task.

## Examples:
### Given Task: Give me a list of all the pets.
### Parallel Task: Find available pet food currently in the store.
### Subsequent Task: Check if the pet food is suitable for the pets in the list.
### Composition Task: Check if the pet food is suitable for the pets in the list of all the pets.

### Given Task: When was the author of the book "The Great Gatsby" born.
### Parallel Task: Find the publication date of the book "The Great Gatsby".
### Subsequent Task: When the book was published, how long had it been since the author was born?
### Composition Task: How old was the author of the book "The Great Gatsby" when the book was published?

### Given Task: Give me the flight schedule from London to Edinburgh today.
### Parallel Task: Find the every hour weather forecast in Edinburgh today.
### Subsequent Task: What is the weather condition when the first flight arrives?
### Composition Task: I am in London, and I want to know the weather condition when the first flight arrives in Edinburgh today.

### Given Task: What is the sentiment of each headline in today’s news from BBC?
### Parallel Task: Find the sentiment of each headline in today’s news from CNN.
### Subsequent Task: Which news source has more positive news today?
### Composition Task: Compare the sentiment of each headline in today’s news from BBC and CNN, and check which news source has more positive news.

### Given Task: Who is the captain of the team that won the World Cup in 2018?
### Parallel Task: Who is the coach of the team that won the World Cup in 2018?
### Subsequent Task: Are the captain and the coach from the same country?
### Composition Task: Check if the captain and the coach of the team that won the World Cup in 2018 are from the same country.

## Here is the given task, please give your response following the above format:
### Given Task: {task}
```

The following is the prompt for filtering compositional tasks, and the key idea is to verify the consistency between a compositional task and its atomic sub-tasks.

Prompt for Filtering Compositional Tasks

```
You are an expert in task decomposition. Currently, you are given a compositional task and its potential task breakdown. Please check if the sub-tasks can be used to complete the compositional task.

Compositional task:
{task}

Potential task breakdown:
{sub_tasks}

Please check if the sub-tasks can be used to complete the compositional task. You should first give your analysis and thinking, and finally give your conclusion (yes or no) enclosed in <ans>, for example, <ans>yes</ans> or <ans>no</ans>:
```

A.4 FUNCTION GENERATION

Prompt for Function Generation

```
You are training a model that can take a user's task description or query, and available functions as input, and generate a sequence of function calls to accomplish the task. Currently, you are generating the training data for this model.

Given a compositional task and its task breakdown, please generate corresponding aviliable functions that can be used to accomplish each sub-task, and finally the compositional task can be accomplished by calling these functions sequentially.

## Requirements for the functions:
1. The functions must possess a succinct, comprehensible name and description.
2. The functions should not tailored for a current task, are to be used for other future tasks as well, hence the design of APIs should be sufficiently generalized.
3. Avoid the recurrence of the task or its components in the function description and name, offering a generic perspective that can be employed across different contexts.
4. Make every function sufficiently granular and independent, avoiding the conflation of multiple tasks within a single function and avert creating monolithic APIs.
```

~~~
5. Consistency in terms of parameters and returns from each
   function is critical. For instance, if two functions are
   called sequentially, the output of the first should either
   align with or constitute a part of the input for the second
   function, irrespective of varying parameter terminologies.

## Requirements for the number of functions:
1. One sub-task may need zero, one or multiple functions to
   complete it.
2. If a sub-task is about logic, comparision, set operation or
   calculation, which can be solved by large language models,
   then no function is needed for this sub-task, just leave the
   func_list of this sub-task empty.

## Compositional task:
{task}

## Task breakdown:
{sub_task}

## Response format:
```json
[
{
    "sub_task": "a sub task from the task breakdown",
    "func_list": [
        {
            "name": "<function name>",
            "description": "<function usage description>",
            "parameters": {
                "<param1>": {
                    "type": "<can be string, number, boolean,
                       object, array, enum and anyOf>",
                    "description": "<param1 description>",
                    ... <more keys if needed>
                },
                ... <more parameters if needed>
            },
            "required": "<array of required parameters, maybe
               not all parameters above are required>"
            "responses": {
                "<res1>" {
                    "type": "<value1 type>",
                    "description": "<value1 description>"
                },
                "<res2>": {
                    "type": "<value2 type>",
                    "description": "<value2 description>"
                }
            }
        },
        {
        ... <more functions if needed>
        }
    ]
}
... <more sub tasks and corresponding functions if needed>
]
~~~

~~~~
```

## Please respond following the format above:
~~~~

A.5 MULTI-AGENT

System Prompt for User Agent

~~~~
Assume that you are a human interacting with an AI assistant.
   You need to engage in a meaningful conversation while always
   remembering to demonstrate human-like behaviour. Avoid
   inquiring if the AI assistant requires assistance, as this
   contradicts your human role. Your main objective is to
   sustain a conversation as a typical user would.

Currently, your goal is to complete a predefined task, and you
   are seeking the AI assistant for this purpose.

**Task**
{task}

During this conversation, you should take on an active role and
   explore the AI assistant's capability to solve problems \
within the **Task** using a series of function (tool) calls. You
    should adhere to the following guidelines:

1. Your task involves a complex task requiring multiple steps to
    complete. In your initial question to the AI assistant, you
   should provide a detailed explanation of the task, including
   necessary information (such as potential data) that might be
   needed to solve the problem. However, you should withhold
   specific solution steps (e.g., avoid sequential terms like "
   firstly," "secondly") and not dictate which functions (tools)
    the AI should use - that is for the AI to determine.
2. Remember, during this multi-turn dialogue, you are portraying
    the role of a human user. Your questions and responses
   should reflect this human aspect. All your outputs should
   enclose within "<human>" tag, for example, "<human> ... </
   human>".
~~~~

System Prompt for Assistant Agent

~~~~
You are simulating the role of an expert in using functions (i.e
   ., tools) to solve users' tasks. You already possess
   knowledge on how to decompose the task into subtasks and
   understand which tools to use for their resolution.

**Subtasks**
{sub_task}

**Available Functions for Subtasks**
{subtask_func}

Please use the tools provided above to answer the question posed
    by "<human>". You must try as much as possible to use these
~~~~

```
    tools, instead of directly answering the question using your
    prior knowledge.

Your response must obey the following format:
Observation: Carefully observe the user "<human>"’s question as
    well as the output of the function call (often enclosed
    within the "<func_return>" tag). Be sure to check for any
    errors in previous outputs, as they may not always be
    accurate. Enclose your observation within the "<observation>"
     tag.
Thought: After observing and combining the previously listed
    steps, give detailed and clear thoughts, reasonings, or
    reflections, and according to the plan decide the next step.
    Note: When you believe the task to be complete, you may use ’
    final_answer’ to provide a detailed summary of the results to
     give to the user. Enclose your thoughts within the "<thought
    >" tag.
Function Call: Name and arguments of the function call. The
    function name must be same as its name in above function list
    , and the arguments must obey the format required by the
    function. Enclose the function call within the "<func_call>"
    tag. If possible, you can call multiple functions in parallel
    , be sure the functions called parallelly are independent of
    each other.

Example 1 (regular function call):
<observation> User has provided two numbers - 15 and 25. </
    observation>
<thought> Based on user’s request, we need to find the greatest
    common divisor of these two numbers. We can use the function
    ’find_greatest_common_divisor’ to solve this problem. </
    thought>
<func_call>[
{
    "name": "find_greatest_common_divisor",
    "arguments": {"num1": 15, "num2": 25}
}
]</func_call>

Example 2 (parallel function call):
<observation> User wants to know the weather in two cities - New
     York and London. </observation>
<thought> We can use the function ’get_weather’ to find the
    weather in New York and London. And the call to this function
     can be done in parallel. </thought>
<func_call>[
{
    "name": "get_weather",
    "arguments": {"city": "New York"}
},
{
    "name": "get_weather",
    "arguments": {"city": "London"}
}
]</func_call>

Example 3 (call final_answer):
```

```
<observation> find_greatest_common_divisor returns the result "5". </observation>
<thought> The result returned by the function call, along with the information collected previously, is sufficient to answer the user’s question, therefore we now use ’final_answer’ to provide the user with the answer. </thought>
<function_call>[
{
    "name": "final_answer",
    "arguments": {"final_answer": "5"}
}
]</function_call>

Furthermore, when the user "<human>" raises a question, you need to provide a structured plan to solve the question (’structured’ means that the plan needs to include steps in sequential order, such as Step 1, 2, 3, etc., or logic processes that include loops and decision branches). The contents of the plan can be placed in the first round response’s <thought>, and try as much as possible to follow this plan in every subsequent function call. However, as necessary, you may also modify the relevant plans according to the result of the function call.
```

System Prompt for Tool Agent

```
You are simulating a computer system with powerful computational capabilities and a complete setup. You possess ample external prior knowledge, allowing you to run any arbitrary function and execute calls to produce results, and you never make errors. Give a following function, you should simulate the operation of a computer system program as closely as possible.

**Function**
{function}

Given a function call, you should execute the function and provide the results in JSON format. Your response should directly provide the results in JSON format, should not contain irrelevant information, and must enclose within "<func_return>" tag.

### Example of function return:
<func_call>
{
    "name": "get_weather",
    "arguments": {"city": "New York"}
}

<func_return>
{
    "temperature": "25C",
}
</func_return>
```

B DATA COLLECTION

B.1 EXAMPLE OF COLLECTED DATA

Collected Data Example 1

```
System:
You are an expert in using functions (i.e., tools) to solve users’ tasks. The functions available for you to use are detailed below:
<tool>[
    {
        "name": "get_current_timestamp",
        "description": "Fetches the current timestamp from the device.",
        "parameters": {},
        "required": []
    },
    {
        "name": "get_humidity_reading",
        "description": "Fetches the current humidity reading from a device.",
        "parameters": {
            "device_id": {
                "type": "string",
                "description": "The ID of the device."
            }
        },
        "required": [
            "device_id"
        ]
    },
    {
        "name": "log_data_to_database",
        "description": "Logs data to a server’s database.",
        "parameters": {
            "server_id": {
                "type": "string",
                "description": "The ID of the server."
            },
            "data": {
                "type": "object",
                "description": "The data to be logged.",
                "properties": {
                    "message": {
                        "type": "string",
                        "description": "The status update message."
                    },
                    "timestamp": {
                        "type": "string",
                        "description": "The current timestamp."
                    },
                    "temperature": {
                        "type": "number",
                        "description": "The current temperature reading."
                    },
                    "humidity": {
                        "type": "number",
                        "description": "The current humidity
                           reading."
                    }
                },
                "required": [
                    "message",
                    "timestamp",
                    "temperature",
                    "humidity"
                ]
            }
        },
        "required": [
            "server_id",
            "data"
        ]
    },
    {
        "name": "send_message_to_server",
        "description": "Sends a message from a device to a
           server.",
        "parameters": {
            "device_id": {
                "type": "string",
                "description": "The ID of the device sending the
                    message."
            },
            "server_id": {
                "type": "string",
                "description": "The ID of the server receiving
                   the message."
            },
            "message": {
                "type": "string",
                "description": "The message to be sent."
            }
        },
        "required": [
            "device_id",
            "server_id",
            "message"
        ]
    },
    {
        "name": "get_temperature_reading",
        "description": "Fetches the current temperature reading
           from a device.",
        "parameters": {
            "device_id": {
                "type": "string",
                "description": "The ID of the device."
            }
        },
        "required": [
            "device_id"
        ]
    }
]</tool>

In your response, you need first provide your observation and
   thought on the user's task, the current situation, and what
   you plan to do next. After your thinking, you can do
   following two things:
**Function Call**: For fountion calling, you need to provide the
    function name and its arguments. The function name must be
   same as its name in above function list, and the arguments
   must obey the format required by the function. Enclose the
   function call within the tag "<call></call>". If possible,
   you can call multiple functions in parallel, be sure the
   functions called parallelly are independent of each other.
**Final Answer**: When you believe the task is complete, you may
    use 'final_answer' to provide a detailed summary of the
   results to give to the user, enclose the final answer within
   the tag "<final></final>".

User:
Hi, I need to send a status update from DeviceA to ServerB. This
    update should include the current timestamp. Additionally, I
    want to log this status update along with the current
   temperature and humidity readings in the database on ServerB.
    Could you help me with this?

Assistant:
The user wants to send a status update from DeviceA to ServerB
   including the current timestamp, and then log this status
   along with the current temperature and humidity readings on
   ServerB's database. To achieve this task, we will follow
   these steps:
1. Send a status update message from DeviceA to ServerB
   including the device's current timestamp.
   - Fetch the current timestamp from DeviceA.
   - Send the status update message with the timestamp to
      ServerB.
2. Get the current temperature and humidity readings from
   DeviceA.
3. Log the status update message along with the temperature and
   humidity readings on ServerB's database.

We can perform steps 1 and 2 in parallel since they are
   independent of each other. Once we have the required data, we
    will proceed to step 3.
<call>[
    {
        "name": "get_current_timestamp",
        "arguments": {}
    },
    {
        "name": "get_temperature_reading",
        "arguments": {
            "device_id": "DeviceA"
        }
    },
    {
        "name": "get_humidity_reading",
        "arguments": {
            "device_id": "DeviceA"
        }
    }
]</call>

Tool:
[
    {
        "name": "get_current_timestamp",
        "arguments": {},
        "results": {
            "timestamp": "2023-10-03T14:22:00Z"
        }
    },
    {
        "name": "get_temperature_reading",
        "arguments": {
            "device_id": "DeviceA"
        },
        "results": {
            "temperature": 22.5
        }
    },
    {
        "name": "get_humidity_reading",
        "arguments": {
            "device_id": "DeviceA"
        },
        "results": {
            "humidity": 45.3
        }
    }
]

Assistant:
We have successfully fetched the current timestamp, temperature,
    and humidity readings from DeviceA. The details are as
   follows:
- Timestamp: 2023-10-03T14:22:00Z
- Temperature: 22.5C
- Humidity: 45.3% Now, we need to send a status update message
   from DeviceA to ServerB including the timestamp. After that,
   we will log the status update along with the temperature and
   humidity readings in ServerB’s database.
<call>[
    {
        "name": "send_message_to_server",
        "arguments": {
            "device_id": "DeviceA",
            "server_id": "ServerB",
            "message": "Status update at 2023-10-03T14:22:00Z"
        }
    }
]</call>

Tool:
[
    {
        "name": "send_message_to_server",
        "arguments": {
            "device_id": "DeviceA",
            "server_id": "ServerB",
            "message": "Status update at 2023-10-03T14:22:00Z"
        },
        "results": {
            "status": "Message delivered successfully"
        }
    }
]

Assistant:
The status update message was successfully delivered from
   DeviceA to ServerB. The message content was: "Status update
   at 2023-10-03T14:22:00Z". Now, we need to log this status
   update message along with the temperature and humidity
   readings in ServerB’s database. We will use the following
   data:
- Message: "Status update at 2023-10-03T14:22:00Z"
- Timestamp: 2023-10-03T14:22:00Z
- Temperature: 22.5C
- Humidity: 45.3%
<call>[
    {
        "name": "log_data_to_database",
        "arguments": {
            "server_id": "ServerB",
            "data": {
                "message": "Status update at 2023-10-03T14:22:00
                   Z",
                "timestamp": "2023-10-03T14:22:00Z",
                "temperature": 22.5,
                "humidity": 45.3
            }
        }
    }
]</call>

Tool:
[
    {
        "name": "log_data_to_database",
        "arguments": {
            "server_id": "ServerB",
            "data": {
                "message": "Status update at 2023-10-03T14:22:00
                   Z",
                "timestamp": "2023-10-03T14:22:00Z",
                "temperature": 22.5,
                "humidity": 45.3
            }
        },
        "results": {
            "log_status": "Data logged successfully on server
               ServerB"
        }
    }
]

Assistant:
The status update message along with the temperature and
   humidity readings was successfully logged in ServerB’s
   database. The task has been completed successfully. A status
   update message was sent from DeviceA to ServerB including the
    current timestamp, and the data was logged on ServerB’s
   database along with the current temperature and humidity
   readings.
<final>The status update message including the current timestamp
    was successfully sent from DeviceA to ServerB, and the data
   was logged in ServerB’s database along with the temperature
   (22.5C) and humidity (45.3%) readings.</final>
```

B.2 PARALLEL FUNCTION CALLING

We use different system prompts to guide the behavior of whether to conduct parallel calling or not. We demonstrate both the system prompt allowing parallel calling and the one prohibiting it. The only difference is the instruction at the end of `**Function Call**`. For enabling parallel calling, we use: “If possible, you can call multiple functions in parallel. Be sure the functions called in parallel are independent of each other”. For disabling parallel calling, we use: “You should call one function at a time and wait for the response before calling the next function”. These instructions help distinguish between turning parallel calling on or off. {`func_list`} is the placeholder for the function definition list in JSON format.

To align LLMs with the correct behavior regarding parallel calling, we implement a 50% probability of turning off parallel calling during trajectory generation for compositional tasks where sub-tasks can be executed in parallel. Since we generate compositional tasks from the bottom up, we inherently know the sub-tasks involved. We fill these trajectories into prompts that prohibit parallel calling. For the other 50% of compositional tasks, where sub-tasks can be executed in parallel, we use system prompts that encourage parallel calling. We also configure trajectories conducted by compositional instructions, where sub-tasks cannot be done in parallel, to use the system prompt that enables parallel calling with a probability of 50%. Finally, the constructed data with the designed prompts can effectively align LLMs to either conduct parallel calling or not, according to the corresponding system prompts. In our work, the accuracy of the parallel calling behavior is not the focus, and we plan to address it in future work.

System Prompt Enabling Parallel Calling

```
You are an expert in using functions (i.e., tools) to solve
   users’ tasks. The functions available for you to use are
   detailed below:
<tool>{func_list}</tool>

In your response, you need first provide your observation and
   thought on the user’s task, the current situation, and what
   you plan to do next. After your thinking, you can do
   following three things:
**Function Call**: For fountion calling, you need to provide the
    function name and its arguments. The function name must be
   same as its name in above function list, and the arguments
   must obey the format required by the function. Enclose the
   function call within the tag "<call></call>". If possible,
   you can call multiple functions in parallel, be sure the
   functions called in parallel are independent of each other.
```

```
**Final Answer**: When you believe the task is complete, you may
     use ’final_answer’ to provide a detailed summary of the
    results to give to the user, enclose the final answer within
    the tag "<final></final>".
```

System Prompt Disabling Parallel Calling

```
You are an expert in using functions (i.e., tools) to solve
    users’ tasks. The functions available for you to use are
    detailed below:
<tool>{func_list}</tool>

In your response, you need first provide your observation and
    thought on the user’s task, the current situation, and what
    you plan to do next. After your thinking, you can do
    following three things:
**Function Call**: For fountion calling, you need to provide the
     function name and its arguments. The function name must be
    same as its name in above function list, and the arguments
    must obey the format required by the function. Enclose the
    function call within the tag "<call></call>". You should call
     one function at a time, and wait for the response before
    calling the next function.
**Final Answer**: When you believe the task is complete, you may
     use ’final_answer’ to provide a detailed summary of the
    results to give to the user, enclose the final answer within
    the tag "<final></final>".
```

B.3 FUNCTION DISTRIBUTION

We show a sunburst chart of the distribution of generated functions in our proposed `BUTTONInstruct` in Figure 4, where the inner circle and outer circle represent the first and second words in a function name, respectively. It shows the diversity of our synthesized data, and the distribution of these functions is also consistent with our daily tasks.

C EXPERIMENTS

C.1 EVALUATION METRICS

For metric calculation for GTA and Tool-Query, we follow the methodologies outlined in their original papers with slight modifications. Specifically, during the end-to-end evaluation mode in GTA, the MathOCR functionality is implemented using the Mathpix API (https://mathpix.com/). However, since this API requires a subscription and we needed to conduct numerous pilot experiments and analyses, we did not evaluate questions on end-to-end mode that would invoke this API. The number of test samples excluding these questions is 209. For Tool-Query, we refined the metric calculation by comparing the final answer with the ground truth. The original implementation was based on exact match; however, such strategies can overlook many successful answers. For example, consider the question “Which paper has received more citations: ‘Stability and Risk Bounds of Iterative Hard Thresholding’ or ‘Compressive Wideband Spectrum Sensing and Signal Recovery With Unknown Multipath Channels’?”, models may finished with “The paper ‘Stability and Risk Bounds of Iterative Hard Thresholding’ has received more citations (5) compared to ‘Compressive Wideband Spectrum Sensing and Signal Recovery With Unknown Multipath Channels’ (2)”. However, the ground truth answer is labeled as “Stability and Risk Bounds of Iterative Hard Thresholding”, and exact match strategies may incorrectly label this answer as unsuccessful. Thus, we refined the metric strategy to check if the final answer is present in the model output. Note that all these

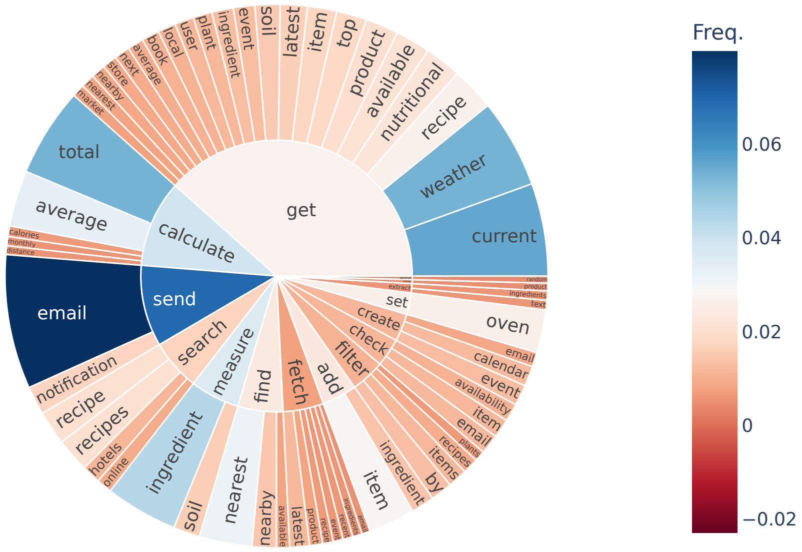


Figure 4: Distribution of the generated functions in `BUTTONInstruct`.

modifications are applied to all models, including baselines, ensuring that the comparison between baselines and models is fair.

C.2 IMPLEMENTATION

All instruction-tuning training is performed on 4×8 NVIDIA H800 GPUs, using the training framework based on HuggingFace Transformers (Wolf et al., 2019). We use the corresponding instruction format for Llama and Qwen models. To enhance training efficiency, we pack short instances into longer ones and apply flash attention. During model training, we optimize the loss only on the response content from assistant roles. We use a learning rate of 2e-5 with cosine decay and a batch size of 64 for all models. For Llama3-8B and Qwen2-7B, we train for five epochs, and for Llama3-70B and Qwen2-72B, we train for two epochs.

C.3 PROMPTS FOR ABLATION STUDY

Here is the monolithic prompt for the ‘w/o Bottom-Up Setting’ in the ablation study. The placeholders {`scen`} represents the given scenario. This prompt is used to generate compositional tasks directly, without our proposed bottom-up process.

Monolithic Task Construction Prompt for the w/o Bottom-Up Setting

```
You are training a model that can take a user’s task description
    or query, and available functions as input, and generate a
   sequence of function calls to accomplish the task. Currently,
    you are generating the training data for this model. Given a
    general life scenario as the context, please first generate
   a task.
```

```
## Requirements for each task:
1. The task should be accomplishable by calling multiple functions with multiple and no more than 7 steps (i.e., turns).
2. If you mention some information, criteria or constraints in the task, please give the details of these information, criteria or constraints. Do not assume the model has access to your personal information or prior knowledge, and it does not have chance to ask you for clarification.
3, Please give enough details and make the task description as specific as possible, so the model can make deterministic function calls with deterministic arguments. Do not include any ambiguous or vague information.
4. Do not mention specific tools or functions in the task description, and do not propose solutions, hints, or project outcomes.
5. Limit the task description to 30 words, and avoid using adjectives and ambiguous words.

## Given scenario:
{scen}

## Please respond a task directly following the requirements above in one line:
```

Here are the monolithic prompts for the 'w/o Top-Down Setting' in the ablation study. The two prompts are used for tasks with or without parallel function calling, respectively. The placeholders `{task}`, `{sub_task}`, and `{subtask_func}` represent a specific generated task, its sub-tasks, and the corresponding generated functions for the sub-tasks.

Monolithic Trajectory Generation Prompt for the w/o Top-Down Setting (Non-parallel)

```
You are labeling data for training an AI assistant that can solve a complex compositional task by using tools in a multi-turn manner.  Given a complex compositional task, its potential subtasks and the available tools (i.e., functions) to solve these subtasks, you should generate synthetic data about the trajectory of solving the task by using tools in a multi-turn manner.

**Task**
{task}

**Subtasks**
{sub_task}

**Available Functions for Sub-tasks**
{subtask_func}

During trajectory generation, you should simulate three roles:
1. human: ask questions to the assistant
2. assistant: answer the questions of human by leveraging the tools
3. tool: execute the functions and return the results to the assistant

The requirements for the human are:
```

```
The human need give the initial question to the AI assistant
   based on the given task, and should provide a detailed
   explanation of the task, including necessary information (
   such as potential data) that might be needed to solve the
   problem. However, you should withhold specific solution steps
    (e.g., avoid sequential terms like "firstly," "secondly")
   and not dictate which functions (tools) the AI should use -
   that is for the AI to determine.

The requirements for the assistant are:
1. The assistant should use the tools provided above to answer
   the question posed by human. It must try as much as possible
   to use these tools, instead of directly answering the
   question using your prior knowledge.
2. The format must obey the following format:
    a) Observation. Carefully observe the human’s question as
       well as the output of the tool call. Be sure to check for
        any errors in previous outputs, as they may not always
       be accurate. Enclose your observation within the "<
       observation>" tag.
    b) Thought. Give detailed and clear thoughts, reasoning, or
       reflections, and according to the plan decide the next
       step. Enclose your thoughts within the "<thought>" tag.
    c) Function call. Give the name and arguments of the
       function call. The function name must be same as its name
        in above function list, and the arguments must obey the
       format required by the function. The function call should
        enclosed within the "<func_call>" tag. Note: When you
       believe the task to be complete, you may use ’
       final_answer’ to provide a detailed summary of the
       results to give to the user.

The requirements for the tool are:
1. You should simulate the operation of a computer system
   program as closely as possible. Your response should directly
    provide the results in JSON format, should not contain
   irrelevant information.
2. You should also provide the response in the format of JSON
   including name, arguments and results.

### Example:
<role>Human</role>
Hi, I want to know when was the author of "The Great Gatsby" was
    born.
<role>Assistant</role>
<observation>The user has provided a book name "The Great Gatsby
   " and wants to know the author’s birthdate.</observation>
<thought>We can use the function ’get_book_author’ to find the
   author of the book and the ’get_author_info’ to find the
   birthdate of the author.</thought>
<func_call>[
{
    "name": "get_book_author",
    "arguments": {"book_name": "The Great Gatsby"}
}
]</func_call>
<role>Tool</role>
[{
    "name": "get_book_author",
    "arguments": {"book_name": "The Great Gatsby"},
    "results": {"name": "F. Scott Fitzgerald"}
}]
<role>Assistant</role>
<observation>The function ’get_book_author’ returns the author
   of the book "The Great Gatsby" is F. Scott Fitzgerald.</
   observation>
<thought>Now we can use the function ’get_author_info’ to find
   the birthdate of the author.</thought>
<func_call>[
{
    "name": "get_author_info",
    "arguments": {{"name": "F. Scott Fitzgerald"}}
}
]</func_call>
<role>Tool</role>
[{
    "name": "get_author_info",
    "arguments": {"name": "F. Scott Fitzgerald"}
    "results": {"birthdate": "September 24, 1896"}
}]
<role>Assistant</role>
<observation>The function ’get_author_info’ returns the
   birthdate of the author "F. Scott Fitzgerald" is September
   24, 1896.</observation>
<thought>The result returned by the function call, along with
   the information collected previously, is sufficient to answer
    the user’s question, therefore we now use ’final_answer’ to
   provide the user with the answer.</thought>
<func_call>[
{
    "name": "final_answer",
    "arguments": {"final_answer": "F. Scott Fitzgerald was born
       on September 24, 1896."}
}
]</func_call>

You need only generate the trajectory in the above format,
   without any other explanation or comments.
```

Monolithic Trajectory Generation Prompt for the w/o Top-Down Setting (Parallel)

```
You are labeling data for training an AI assistant that can
   solve a complex compositional task by using tools in a multi-
   turn manner. Given a complex compositional task, its
   potential subtasks and the available tools (i.e., functions)
   to solve these subtasks, you should generate synthetic data
   about the trajectory of solving the task by using tools in a
   multi-turn manner.

**Task**
{task}

**Subtasks**
{sub_task}
```

```
**Available Functions for Subtasks**
{subtask_func}

During trajectory generation, you should simulate three roles:
1. human: ask questions to the assistant
2. assistant: answer the questions of human by leveraging the
   tools
3. tool: execute the functions and return the results to the
   assistant

The requirements for the human are:
The human need give the initial question to the AI assistant
   based on the given task, and should provide a detailed
   explanation of the task, including necessary information (
   such as potential data) that might be needed to solve the
   problem. However, you should withhold specific solution steps
    (e.g., avoid sequential terms like "firstly," "secondly")
   and not dictate which functions (tools) the AI should use -
   that is for the AI to determine.

The requirements for the assistant are:
1. The assistant should use the tools provided above to answer
   the question posed by human. It must try as much as possible
   to use these tools, instead of directly answering the
   question using your prior knowledge.
2. The format must obey the following format:
    - a) Observation. Carefully observe the human’s question as
       well as the output of the tool call. Be sure to check for
        any errors in previous outputs, as they may not always
       be accurate. Enclose your observation within the "<
       observation>" tag.
    - b) Thought. Give detailed and clear thoughts, reasonings,
       or reflections, and according to the plan decide the next
        step. Enclose your thoughts within the "<thought>" tag.
    - c) Function call. Give the name and arguments of the
       function call. The function name must be same as its name
        in above function list, and the arguments must obey the
       format required by the function. The function call should
        enclosed within the "<func_call>" tag. If possible, you
       can call multiple functions in parallel, be sure the
       functions called parallelly are independent of each other
       . Note: When you believe the task to be complete, you may
        use ’final_answer’ to provide a detailed summary of the
       results to give to the user.

The requirements for the tool are:
1. You should simulate the operation of a computer system
   program as closely as possible. Your response should directly
    provide the results in JSON format, should not contain
   irrelevant information.
2. You should also provide the response in the format of JSON
   including name, arguments and results.

### Example 1:
<role>Human</role>
Hi, I want to know when was the author of "The Great Gatsby" was
    born.
<role>Assistant</role>
```

```
<observation>The user has provided a book name "The Great Gatsby
   " and wants to know the author’s birthdate.</observation>
<thought>We can use the function ’get_book_author’ to find the
   author of the book and the ’get_author_info’ to find the
   birthdate of the author.</thought>
<func_call>[
{
    "name": "get_book_author",
    "arguments": {"book_name": "The Great Gatsby"}
}
]</func_call>
<role>Tool</role>
[{
    "name": "get_book_author",
    "arguments": {"book_name": "The Great Gatsby"},
    "results": {"name": "F. Scott Fitzgerald"}
}]
<role>Assistant</role>
<observation>The function ’get_book_author’ returns the author
   of the book "The Great Gatsby" is F. Scott Fitzgerald.</
   observation>
<thought>Now we can use the function ’get_author_info’ to find
   the birthdate of the author.</thought>
<func_call>[
{
    "name": "get_author_info",
    "arguments": {"name": "F. Scott Fitzgerald"}
}
]</func_call>
<role>Tool</role>
[{
    "name": "get_author_info",
    "arguments": {"name": "F. Scott Fitzgerald"}
    "results": {"birthdate": "September 24, 1896"}
}]
<role>Assistant</role>
<observation>The function ’get_author_info’ returns the
   birthdate of the author "F. Scott Fitzgerald" is September
   24, 1896.</observation>
<thought>The result returned by the function call, along with
   the information collected previously, \
is sufficient to answer the user’s question, therefore we now
   use ’final_answer’ to provide the user with the answer.</
   thought>
<func_call>[
{
    "name": "final_answer",
    "arguments": {{"final_answer": "F. Scott Fitzgerald was born
         on September 24, 1896."}}
}
]</func_call>

### Example 2:
<role>Human</role>
What is the age when the author of "The Great Gatsby" published
   the book.
<role>Assistant</role>
```

```
<observation>The user mention the book "The Great Gatsby" and
   wants to know the how old the author was when he published
   the book.</observation>
<thought>We can use the function ’get_book_author’ to find the
   author of the book and the ’get_book_publish_date’ to find
   the publish date of the book, such two function can be used
   in parallel.</thought>
<func_call>[
{
    "name": "get_book_author",
    "arguments": {"book_name": "The Great Gatsby"}
},
{
    "name": "get_book_publish_date",
    "arguments": {"book_name": "The Great Gatsby"}
}
]</func_call>
<role>Tool</role>
[{
    "name": "get_book_author",
    "arguments": {"book_name": "The Great Gatsby"},
    "results": {"name": "F. Scott Fitzgerald"}
},
{
    "name": "get_book_publish_date",
    "arguments": {"book_name": "The Great Gatsby"},
    "results": {"publish_date": "April 10, 1925"}
}]
<role>Assistant</role>
<observation>The function ’get_book_author’ returns the author
   of the book "The Great Gatsby" is F. Scott Fitzgerald, and
   the function ’get_book_publish_date’ returns the publish date
    of the book "The Great Gatsby" is April 10, 1925.</
   observation>
<thought>To determine the age of the author when the book was
   published, we need to calculate the difference between the
   publish date and the author’s birthdate, so we need to use
   the function ’get_author_info’ to get the birthdate of the
   author.</thought>
<func_call>[
{
    "name": "get_author_info",
    "arguments": {"name": "F. Scott Fitzgerald"}
}
]</func_call>
<role>Tool</role>
[{
    "name": "get_author_info",
    "arguments": {"name": "F. Scott Fitzgerald"},
    "results": {"birthdate": "September 24, 1896"}
}]
<role>Assistant</role>
<observation>The function ’get_author_info’ returns the
   birthdate of the author "F. Scott Fitzgerald" is September
   24, 1896.</observation>
<thought>Previously, we have got the publish date of the book "
   The Great Gatsby" is April 10, 1925, so we can infer that the
```

```
    author was 28 years old when he published the book.</thought
   >
<func_call>[
{
    "name": "final_answer",
    "arguments": {"final_answer": "F. Scott Fitzgerald was 28
       years old when he published "The Great Gatsby"."}
}
]</func_call>


You need only generate the trajectory in the above format,
   without any other explanation or comments.
```

C.4 CASES ON PARALLEL CALLING

We present two cases of conducting Llama3-70B-BUTTON on Tool-Query. In both cases, the functions `authorEdgeCheck` and `paperNodeCheck` are called in parallel where appropriate. This parallel calling effectively reduces the number of turns during the multi-turn function calling procedure. For example, in case 2, with parallel calling, the language model only requires 6 steps (including providing the final answer) to complete the task. Without parallel calling, 2 of these steps would expand to 4 steps each, resulting in a total of 12 steps.

Parallel Calling Case 1

```
User: Who has the most collaborations with Lazhar Labiod in the
   DBLP citation network?

Assistant: To answer this question, we need to follow these
   steps:
1. Load the AuthorNet.
2. List the first-order neighbors (collaborators) of Lazhar
   Labiod.
3. Determine which collaborator has the most collaborations with
    Lazhar Labiod.

Let’s start by loading the AuthorNet.
<call>[
    {
        "name": "loadAuthorNet",
        "arguments": {}
    }
]</call>

Tool: AuthorNet is loaded.

Assistant: AuthorNet is loaded successfully. Next, we need to
   list the first-order neighbors (collaborators) of Lazhar
   Labiod.
<call>[
    {
        "name": "neighbourCheck",
        "arguments": {
            "graph": "AuthorNet",
            "node": "Lazhar Labiod"
        }
    }
]</call>

Tool: ['Mohamed Nadif', 'Chakib Fettal']

Assistant: The collaborators of Lazhar Labiod are Mohamed Nadif
   and Chakib Fettal. Now, we need to determine which of these
   collaborators has the most collaborations with Lazhar Labiod.
    We can do this by checking the number of co-authored papers
   between Lazhar Labiod and each of his collaborators.
<call>[
    {
        "name": "authorEdgeCheck",
        "arguments": {
            "node1": "Lazhar Labiod",
            "node2": "Mohamed Nadif"
        }
    },
    {
        "name": "authorEdgeCheck",
        "arguments": {
            "node1": "Lazhar Labiod",
            "node2": "Chakib Fettal"
        }
    }
]</call>

Tool: [{'collaborative_papers': ['TensorClus: A python library
   for tensor (Co)-clustering', 'Efficient Graph Convolution for
    Joint Node Representation Learning and Clustering']}", "{'
   collaborative_papers': ['Efficient Graph Convolution for
   Joint Node Representation Learning and Clustering']}]

Assistant: Lazhar Labiod has co-authored 2 papers with Mohamed
   Nadif and 1 paper with Chakib Fettal. Based on the number of
   co-authored papers, Mohamed Nadif has the most collaborations
    with Lazhar Labiod. Now, I will provide the final answer to
   the user.
<final>Mohamed Nadif has the most collaborations with Lazhar
   Labiod, with a total of 2 co-authored papers.</final>
```

Parallel Calling Case 2

```
User: How many citations do papers co-authored by Florian
   Kirchbuchner and Fadi Boutros have in the DBLP citation
   network? Please give me a numerical value as an answer.

Assistant: To answer this question, we need to follow these
   steps:
1. Load the AuthorNet.
2. Check the collaboration relationship between Florian
   Kirchbuchner and Fadi Boutros.
3. Count the total number of citations of the papers they co-
   authored.

Let's start by loading the AuthorNet.
<call>[
    {
        "name": "loadAuthorNet",
        "arguments": {}
    }
]</call>

Tool: AuthorNet is loaded.

Assistant: AuthorNet is loaded successfully. Next, we need to
   check the collaboration relationship between Florian
   Kirchbuchner and Fadi Boutros to get the list of papers they
   co-authored.
<call>[
    {
        "name": "authorEdgeCheck",
        "arguments": {
            "node1": "Florian Kirchbuchner",
            "node2": "Fadi Boutros"
        }
    }
]</call>

Tool: {'collaborative_papers': ['PocketNet: Extreme Lightweight
   Face Recognition Network Using Neural Architecture Search and
    Multistep Knowledge Distillation', 'ElasticFace: Elastic
   Margin Loss for Deep Face Recognition.', 'Template-Driven
   Knowledge Distillation for Compact and Accurate Periocular
   Biometrics Deep-Learning Models', 'Self-restrained triplet
   loss for accurate masked face recognition']}

Assistant: The papers co-authored by Florian Kirchbuchner and
   Fadi Boutros are:
1. PocketNet: Extreme Lightweight Face Recognition Network Using
    Neural Architecture Search and Multistep Knowledge
   Distillation
2. ElasticFace: Elastic Margin Loss for Deep Face Recognition.
3. Template-Driven Knowledge Distillation for Compact and
   Accurate Periocular Biometrics Deep-Learning Models
4. Self-restrained triplet loss for accurate masked face
   recognition

We need to find the total number of citations for these papers.
   To find the total number of citations for these papers, we
   will check the citation count for each paper individually and
    then sum them up.
<call>[
    {
        "name": "paperNodeCheck",
        "arguments": {
            "node": "PocketNet: Extreme Lightweight Face
                Recognition Network Using Neural Architecture
                Search and Multistep Knowledge Distillation"
        }
    },
    {
        "name": "paperNodeCheck",
        "arguments": {
            "node": "ElasticFace: Elastic Margin Loss for Deep
                Face Recognition."
        }
    },
    {
        "name": "paperNodeCheck",
        "arguments": {
            "node": "Template-Driven Knowledge Distillation for
               Compact and Accurate Periocular Biometrics Deep-
               Learning Models"
        }
    },
    {
        "name": "paperNodeCheck",
        "arguments": {
            "node": "Self-restrained triplet loss for accurate
               masked face recognition"
        }
    }
]</call>

Tool: ['Please load the PaperNet first.', 'Please load the
   PaperNet first.', 'Please load the PaperNet first.', 'Please
   load the PaperNet first.']

Assistant: The system requires PaperNet to be loaded before
   checking the details of individual papers. We need to load
   PaperNet first before proceeding to check the citation counts
    of the papers.
<call>[
    {
        "name": "loadPaperNet",
        "arguments": {}
    }
]</call>

Tool: PaperNet is loaded.

Assistant: PaperNet is loaded successfully. Now that PaperNet is
    loaded, we can proceed to check the citation counts for each
    of the papers co-authored by Florian Kirchbuchner and Fadi
   Boutros.
<call>[
    {
        "name": "paperNodeCheck",
        "arguments": {
            "node": "PocketNet: Extreme Lightweight Face
               Recognition Network Using Neural Architecture
               Search and Multistep Knowledge Distillation"
        }
    },
    {
        "name": "paperNodeCheck",
        "arguments": {
            "node": "ElasticFace: Elastic Margin Loss for Deep
               Face Recognition."
        }
    },
    {
        "name": "paperNodeCheck",
        "arguments": {
            "node": "Template-Driven Knowledge Distillation for
                Compact and Accurate Periocular Biometrics Deep-
                Learning Models"
        }
    },
    {
        "name": "paperNodeCheck",
        "arguments": {
            "node": "Self-restrained triplet loss for accurate
                masked face recognition"
        }
    }
]</call>

Tool: {’authors’: [’Fadi Boutros’, ’Naser Damer’, ’Florian
   Kirchbuchner’, ’Arjan Kuijper’], ’year’: 2022, ’venue’: ’IEEE
    ACCESS’, ’n_citation’: 0, ’keywords’: [’Computer
   architecture’, ’Microprocessors’, ’Training’, ’Task analysis
   ’, ’Network architecture’, ’Computational modeling’, ’
   Architecture’, ’Computer vision’, ’deep learning’, ’face
   recognition’], ’doc_type’: ’Journal’}", "{’authors’: [’Fadi
   Boutros’, ’Naser Damer’, ’Florian Kirchbuchner’, ’Arjan
   Kuijper’], ’year’: 2022, ’venue’: ’IEEE Conference on
   Computer Vision and Pattern Recognition’, ’n_citation’: 43, ’
   keywords’: [], ’doc_type’: ’Conference’}", "{’authors’: [’
   Fadi Boutros’, ’Naser Damer’, ’Florian Kirchbuchner’, ’Arjan
   Kuijper’], ’year’: 2022, ’venue’: ’SENSORS’, ’n_citation’: 0,
    ’keywords’: [’biometrics’, ’knowledge distillation’, ’
   periocular verification’], ’doc_type’: ’Journal’}", "{’
   authors’: [’Fadi Boutros’, ’Naser Damer’, ’Florian
   Kirchbuchner’, ’Arjan Kuijper’], ’year’: 2022, ’venue’: ’
   Pattern Recognition’, ’n_citation’: 8, ’keywords’: [’COVID
   -19’, ’Biometric recognition’, ’Identity verification’, ’
   Masked face recognition’], ’doc_type’: ’Journal’}

Assistant: The citation counts for the papers co-authored by
   Florian Kirchbuchner and Fadi Boutros are as follows:
1. PocketNet: Extreme Lightweight Face Recognition Network Using
    Neural Architecture Search and Multistep Knowledge
   Distillation - 0 citations
2. ElasticFace: Elastic Margin Loss for Deep Face Recognition. -
    43 citations
3. Template-Driven Knowledge Distillation for Compact and
   Accurate Periocular Biometrics Deep-Learning Models - 0
   citations
4. Self-restrained triplet loss for accurate masked face
   recognition - 8 citations

The total number of citations is the sum of these counts. The
   total number of citations for the papers co-authored by
   Florian Kirchbuchner and Fadi Boutros is \(0 + 43 + 0 + 8 =
   51\). I will now provide the final answer.
<final>The total number of citations for the papers co-authored
   by Florian Kirchbuchner and Fadi Boutros is 51.</final>
```