# TOWARDS RELIABLE BENCHMARKING: A CONTAMINATION FREE, CONTROLLABLE EVALUATION FRAMEWORK FOR MULTI-STEP LLM FUNCTION CALLING

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#### **ABSTRACT**

As language models gain access to external tools through structured function calls, they become increasingly more capable of solving complex, multi-step tasks. However, existing benchmarks for tool-augmented language models (TaLMs) provide insufficient control over factors such as the number of functions accessible, task complexity, and input size, and remain vulnerable to data contamination. We present FuncBenchGen, a unified, contamination-free framework that evaluates TaLMs by generating synthetic multi-step tool-use tasks to stress-test TaLMs. The key idea is to cast tool use as traversal over a hidden function-dependency DAG where nodes are function calls and an edge between nodes represents one function consuming the output of another. Given a set of external function schemas, initial variable values, and a target variable, models must compose the correct call sequence to compute the target variable. FuncBenchGen allows users to precisely control task difficulty (e.g., graph size, dependency depth, and distractor functions) while avoiding pretraining/test-time leakage.

We apply our FuncBenchGen framework to evaluate seven open and closed LLMs on tool use tasks of varying difficulty. Reasoning-optimized models consistently outperform general-purpose models with GPT-5 significantly outperforming other available models. Performance declines sharply as dependency depth increases. Furthermore, connected distractors—irrelevant functions sharing type-compatible variables with relevant functions—prove especially difficult to handle.

We find that strong models often make syntactically valid function calls but propagate incorrect or stale argument values across steps, revealing brittle state tracking by LLMs in multi-turn tool use. Motivated by this observation, we introduce a simple mitigation strategy that explicitly restates prior variable values to the agent at each step. Surprisingly, this lightweight change yields substantial gains across models. e.g., yielding an improvement in success rate from 62.5% to 81.3% for GPT-5, without modifying the underlying architectures or training.

# 1 Introduction

Large Language Models (LLMs) equipped with external tools ("tool use") have become central to complex real-world applications, as they enable interaction with external environments and access to up-to-date information (Luo et al., 2025). A growing body of work investigates different facets of this capability, including the ability to handle large collections of callable APIs (Kwak et al., 2025), multi-step function calling (Zhong et al., 2025; Song et al., 2025), long-horizon tool use (Kate et al., 2025), and broader evaluations of tool-use skills (Li et al., 2023; Patil et al., 2025; Sun et al., 2024).

Despite recent advances, progress in this field is impeded by two key issues. First, while prior studies have curated realistic API sets and constructed tasks to assess function-calling abilities (Li et al., 2023; Qin et al., 2024), these benchmarks often exhibit limited function-set diversity due to high curation cost, and they are vulnerable to data contamination from pretraining overlap and test-time web search (Han et al., 2025), as benchmark question—answer pairs may be publicly accessible. Second, existing benchmarks provide little fine-grained control over task difficulty, e.g., the number of required functions, the function dependency depth, and the presence of *irrelevant* functions with

Table 1: Comparison of previously proposed function-calling testbeds with FuncBenchGen. Func. indicates function.

	Contamination-	Task Complexity (Controllability)				
	Free	Required Func. Size	Dependency Depth	Irrelevant Func. Type		
API-Bank (Li et al., 2023)	X	X	Х	Х		
BFCLv4 (Patil et al., 2025)	X	✓	X	X		
ToolBench (Qin et al., 2024)	X	✓	X	X		
ComplexFuncBench (Zhong et al., 2025)	X	X	X	X		
LongFuncEval (Kate et al., 2025)	X	✓	X	X		
FuncBenchGen (ours)	/	/	✓	/		

variables that are type-compatible with required functions. While some benchmarks (Patil et al., 2025; Qin et al., 2024; Kate et al., 2025) allow limited control over certain aspects of task complexity, such as the number of required functions, they lack comprehensive control across the function dependency depth and the presence/type-compatibility of irrelevant functions. These limitations reduce the generality of empirical findings and prevent us from understanding which factors most significantly impact model performance. We summarize the existing benchmarks and compare them with our proposed framework in Table 1.

In this paper, we aim to isolate and analyze the core capabilities and failure types of tool-augmented LLMs (TaLMs) in multi-step function calling scenarios. To this end, we propose FuncBenchGen, a framework for automated generation of contamination-free function calling tasks with controllable difficulty to enable systematic evaluation and analysis of TaLMs, as illustrated in Figure 1. The key idea is to represent function dependencies as a directed acyclic graph (DAG) and frame multi-step function calling as a graph traversal problem. Given a set of input variables with known values, a target variable, and a set of external function schemas, the task requires an agent to determine the value of the target variable by executing an appropriate sequence of external function calls.

Our key contributions are as follows:

- We introduce **FuncBenchGen**, a novel evaluation framework for tool-augmented language models (TaLMs). The framework automatically generates contamination-free function-calling tasks with controllable difficulty, specified by parameters such as the number of required function calls, the number and types of input/output variables, and the number and connectivity of irrelevant functions.
- Using FuncBenchGen, we conduct extensive experiments with seven state-of-the-art open and closed LLMs. Our analysis yields several important findings: reasoning-optimized models consistently outperform general-purpose ones, yet even GPT-5 struggles with longer function call sequences. For example, it achieves only a 15% success rate when 20 function calls are required. We also observed that external functions that are *irrelevant* to solving the problem, but that are "connected" to the solution DAG (i.e., that share type-compatible variables with functions involved in the solution) severely degrade performance for all LLM models. Moreover, the task success is strongly influenced by graph structure, with shallower and more sequential dependency chains being easier to solve; and although most models invoke functions with correct syntax, they frequently fail to propagate argument values across calls.
- Finally, identifying key failure types in models function calling capability, we propose a simple augmentation mitigation strategy that restates variable values from prior calls, which significantly improves success rates across models—for example, yielding an improvement in success rate from 62.5% to 81.3% for GPT-5.

We will release our framework as open-source upon acceptance to facilitate future research.

# 2 RELATED WORK

**Multi-step Reasoning in LLMs** Recent LLMs demonstrate impressive multi-step reasoning capabilities across various domains, including mathematical problem solving (Davoodi et al., 2025), multi-document reasoning (Maekawa et al., 2025), and commonsense reasoning (Yu et al., 2025).

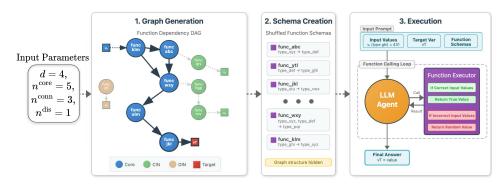


Figure 1: Overview of FuncBenchGen.  $d, n^{\text{core}}, n^{\text{conn}}$ , and  $n^{\text{dis}}$  indicate the dependency depth and the numbers of core nodes, connected irrelevant nodes (CINs), and disconnected irrelevant nodes (DINs), respectively.

Despite these advances, the robustness of their multi-step reasoning capabilities remains unclear when models are required to interact with external tools.

**Function Calling in LLMs** Models such as ToolLLM (Qin et al., 2024), Gorilla (Patil et al., 2024), and ToolACE (Liu et al., 2025a) highlight the importance of equipping LLMs with access to vast API collections to tackle real-world use cases. Tool-Planner (Liu et al., 2025b) and ToolDial (Shim et al., 2025) further extend these capabilities by incorporating planning and multi-turn dialogue for more sophisticated tool-use by using LLMs' multi-step reasoning capabilities. Meanwhile, LongFuncEval (Kate et al., 2025) and ComplexFuncBench (Zhong et al., 2025) focus on evaluating LLMs' ability to handle long-context and multi-step function calling scenarios. Despite these advances, the evaluation datasets used often lack generality and controllability, limiting their utility for systematic analysis.

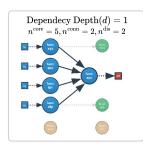
Contamination and Robustness in Evaluation Robustness and contamination issues in benchmark construction pose significant challenges. Datasets such as (Mirzadeh et al., 2025; Shojaee et al., 2025) have addressed the limitations of LLM reasoning evaluation due to dataset contamination or task leakage, e.g., when the LLM training set includes a specific tool or task included in the test set. Han et al. (2025) have shown data contamination can happen during web search tool-use. Though these studies emphasize the importance of creating bias-free and contamination-free tasks, they do not specifically address the challenges in multi-step function calling scenarios. In contrast, our work seeks to bridge this gap by offering a principled, automated framework for function set and task generation, supporting controlled stress-testing and robust analysis of TaLM capabilities.

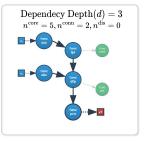
## 3 THE EVALUATION FRAMEWORK FOR FUNCTION CALLING IN LLMS

We introduce FuncBenchGen, a benchmark generation framework designed to evaluate the multistep function calling capabilities of LLMs. FuncBenchGen automatically creates synthetic, contamination-free function sets and tasks with controllable difficulty, enabling systematic analysis of the factors that affect model performance without the confounding influence of data bias or leakage. We formalize multi-step function calling as a graph traversal problem defined over a directed acyclic graph (DAG) of function dependencies. Importantly, LLMs are given only the list of generated functions and input variables, rather than the dependency graph itself, requiring them to infer the correct call sequence. The framework overview is illustrated in Figure 1.

# 3.1 TASK DEFINITION: MULTI-STEP FUNCTION CALLING

Given a set of functions  $\mathcal{F}=\{f_1,f_2,\ldots,f_n\}$ , where each function  $f_i$  takes a set of input variables  $\mathcal{V}_i^{in}$  and produces a single output variable  $v^{\text{out}}$ , along with a set of input variables  $\mathcal{V}_{input}=\{v_1,v_2,\ldots,v_k\}$  with known values and a target variable  $v_T$ , the LLM agent is tasked to determine the value of  $v_T$  by iteratively executing a sequence of function calls. For each execution step, the LLM agent can call any number of functions from  $\mathcal{F}$  and then the system returns





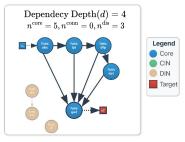


Figure 2: Examples of the different kinds of graphs that can be generated with 5 core nodes. CIN indicates connected irrelevant nodes and DIN indicates disconnected irrelevant nodes.  $n^{\text{core}}$  is the number of core nodes,  $n^{\text{conn}}$  is the number of CINs, and  $n^{\text{dis}}$  is the number of DINs.

function outputs based on the input values specified by the LLM agent. The process ends when no further calls are made, at which point the agent's final output is parsed to obtain the answer.

#### 3.2 BENCHMARK GENERATION PROCESS

FuncBenchGen is designed based on two core principles to address limitations of existing benchmarks, as discussed in Section 1: 1) **Contamination-Free**: The framework generates synthetic function sets and tasks at evaluation time, ensuring that no pretraining or test-time leakage can occur. 2) **Controllable Task Complexity**: The framework allows us to precisely control multiple dimensions of task complexity by taking as inputs the number of functions, the function dependency depth, and the amounts and type of irrelevant functions. This enables systematic analysis of how different complexity factors affect model performance by isolating each factor.

To ensure contamination-free evaluation, FuncBenchGen generates synthetic function sets and tasks at evaluation time. Also, to control task complexity, we represent function dependencies as a directed acyclic graph (DAG), where nodes represent functions and edges represent the dependencies between functions, and formulate multi-step function calling as a graph traversal problem. This idea allows us to precisely control multiple dimensions of task complexity by manipulating the underlying graph structure. Formally, a function dependency graph  $G = (\mathcal{F}, \mathcal{E})$  is a DAG where each node  $f_i \in \mathcal{F}$  represents a function with input variables  $\mathcal{V}_i^{in}$  and output variable  $v_i^{out}$  and each directed edge  $(f_i, f_j) \in \mathcal{E}$  indicates that function  $f_j$  can consume the output from function  $f_i$ . To generate the function dependency graph G, the framework takes as inputs the number  $n^{core}$  of functions that will be required to solve the task, the dependency depth d, and the number of irrelevant distractor functions that are connected to the solution DAG  $(n^{conn})$  and the number of irrelevant distractor functions that are disconnected from the DAG  $(n^{dis})$ . Recall that we define function f to be connected to the solution DAG if and only if there exists a dependency edge between f and at least one function in the solution DAG. We call the connected irrelevant nodes/functions CIN nodes and the disconnected irrelevant nodes/functions DIN nodes for brevity.

The benchmark generation process consists of two main steps: 1) **Graph Structure Generation**: Given parameters specifying the desired graph characteristics that meet the target task difficulty, the framework constructs a DAG that satisfies these constraints including the number of required functions, the dependency depth, and the presence and type of irrelevant external functions. 2) **Function Schema Creation**: Each node in the dependency graph is converted into a function schema with a randomly generated name. This on-the-fly generation ensures contamination-free evaluation.

**Graph Structure Generation** The framework takes a two-stage approach: 1) core node creation and 2) irrelevant node addition. First, we create a node sequence of length d to ensure that the generated graph contains a valid path from input variables to the target variable with the required number of function calls. Then, we iteratively add the remaining  $n^{\rm core} - (d+1)$  core nodes by randomly adding new parent nodes to the existing core nodes, while ensuring acyclicity and dependency depth. Second, we add irrelevant nodes according to the specified connection type. For connected irrelevant nodes (CINs), we randomly select nodes from the existing core nodes and add the irrelevant nodes as their children. For disconnected irrelevant nodes (DINs), we create isolated nodes and then add

at most  $\lfloor n^{\rm dis}/2 \rfloor$  edges between them while ensuring acyclicity, to simulate the possible function dependency between irrelevant nodes.

**Function Schema Creation** For the model input, each node in the dependency graph is converted into a function schema with: (1) Function name: A randomly generated identifier (e.g., func\_yep). (2) Input parameters: Variables with randomly assigned type and subtype annotations. (3) Output variable: A single variable that can serve as input to dependent functions. And, (4) Description: Natural language explanation of the function's purpose.

Functions are linked through semantic type and sub-type matching rather than variable names, serving as a lightweight proxy for the semantic reasoning that connects functions in real-world scenarios. In practice, if a function's input type and sub-type matches another's output type and sub-type, the two are connected. See A.2 for details.

#### 3.3 REAL-WORLD APPLICABILITY

Many real-world function calling scenarios can be mapped directly to DAG structures. For example, a user may ask an LLM agent to find a sightseeing tour near their hotel tomorrow and reserve a taxi for them an hour after the tour ends (example from ComplexFuncBench (Zhong et al., 2025)). Here, an agent must: 1) find the hotel's location, 2) use the location to find nearby tours, 3) filter nearby tours by date and availability, and 4) reserve a taxi at the correct time and place. This workflow naturally forms a dependency graph where each function depends on specific outputs from previous calls—tours cannot be searched for without the hotel's location, a tour cannot be selected without the tour search results, etc. Our framework abstracts this complexity into a controllable evaluation setting while preserving the essential challenge: models must infer these dependencies from function signatures alone, just as they would when interacting with unfamiliar APIs in deployment.

#### 3.4 IMPLEMENTATION DETAILS

Each variable in the system is assigned a three digit random integer value. Functions implement deterministic logic: they return the correct output value only when provided with the exact expected input values, which the agent must discover by calling the parent functions of that node. They return random incorrect outputs when given invalid inputs, simulating realistic API behavior where invalid parameters lead to silent failures or unhelpful responses. For the sake of simplicity, we set the number of output variables for each function to one.

We implement an interaction protocol between the LLM agent and the function execution environment. At each step, the model can make multiple function calls, then receive their outputs, and continue until it makes no further calls. An example of the model input is shown in Appendix A.3.

# 4 EXPERIMENTS

We apply our FuncBenchGen framework to conduct extensive experiments to explore the following research questions: (RQ1) How do LLMs perform in function calling tasks as the size of the core function set varies? (RQ2) How do irrelevant functions affect model performance? (RQ3) How does the function dependency depth impact performance? (RQ4) How do larger function sets and thinking budgets affect performance of the best performing models? (RQ5) What are common failure types in function calling tasks and how can they be mitigated?

#### 4.1 SETUP

To investigate our research questions, we test LLMs under various controlled conditions varying graph size, number of irrelevant functions, and the depth of required function call sequences. For graph size, we vary the number of core nodes in  $\{5, 10, 20\}$ . We set the number of added irrelevant nodes to  $\{0, 10, 20, 40\}$ . For each irrelevant node setting, we test three different connection types: 1) **Connected**: all irrelevant nodes are connected to the core nodes in the dependency DAG, 2) **Disconnected**: all irrelevant nodes are disconnected from the core nodes, and 3) **Half & half**: half of the irrelevant nodes are connected to the core nodes and the other half are disconnected. We also

Table 2: Success rates and average number of function calls (ACs) made by models. Results are aggregated across all test configurations: number of irrelevant functions  $\{0,5,10,20\}$ , irrelevant node connectivity type {Connected, Disconnected, Half-and-Half}, and graph dependency depth  $\{1,...n^{\rm core}-1\}$ , with 5 random trials per configuration. ACs (Succ.) and (Fail.) denote the ACs for successful and failed trials, respectively. "–" indicates that there are no successful trials.

# core nodes	5			10			20		
	Success Rate	ACs (Succ.)	ACs (Fail.)	Success Rate	ACs (Succ.)	ACs (Fail.)	Success Rate	ACs (Succ.)	ACs (Fail.)
GPT-5	72.5%	5.4	7.6	38.2%	11.5	13.0	15.0%	22.0	23.7
GPT-5-mini	16.0%	5.0	7.9	7.6%	10.0	14.2	4.2%	20.0	23.4
Gemini-2.5-Pro	46.5%	5.5	6.3	14.4%	10.6	13.2	6.0%	22.6	24.4
Gemini-2.5-Flash	31.5%	5.1	1.1	13.8%	10.3	1.3	7.2%	20.0	1.3
Qwen3	11.0%	5.4	6.1	8.2%	11.2	11.1	3.8%	24.1	19.3
GPT-4.1	12.0%	5.2	4.1	2.2%	10.3	7.1	0.2%	21.0	12.0
GPT-4.1-mini	11.0%	5.2	5.0	0.0%	_	9.0	0.0%	_	18.9

vary the dependency depth between 1 and  $n^{\rm core}-1$  for graphs with 5 and 10 core nodes. For graphs with 20 core nodes or more, we set the dependency depth for every 10% increment starting from 1, i.e.,  $1, 3, \ldots, 17, 19$  for 20 core nodes. To obtain reliable results, we generate 5 different graphs for each setting of core nodes, irrelevant nodes, and dependency depth and report the average results.

**Models** We evaluate various LLMs with reasoning-optimized and general-purpose capabilities. Reasoning models include both closed and open models: GPT-5, GPT-5-mini, Gemini-2.5-Pro, Gemini-2.5-Flash, Qwen3-235B22A (Qwen3 for short). General models include GPT-4.1 and GPT-4.1-mini. The model details are summarized in Appendix A.1. We set the thinking budgets of all the reasoning models to their default, e.g., medium for GPT-5, and set the temperature and top-p parameters to 0.0 and 1.0, respectively, for all our experiments.<sup>1</sup>

**Evaluation Metrics** We evaluate the models based on both success rate and efficiency in function calling. A function call sequence is considered correct if it produces the expected output for the task. To measure efficiency, we record the number of function calls generated by each model. Given budget constraints, we cap the maximum number of calls at twice the minimum required number. A more detailed analysis of function-calling sequences is provided in Section 4.5.

#### 4.2 MAIN RESULTS (RQ1)

Table 2 shows the overall results of all models across different numbers of core nodes. The results are averaged over no extra and 10, 20, 40 irrelevant nodes (functions) of three connectivity types with five generated graphs for each setting.

GPT-5 outperforms all other models by a significant margin, but it reaches only 15% on extended function-call sequences, while general-purpose models fail to reliably solve even simpler tasks. Reasoning-optimized models, e.g., GPT-5 and Gemini-2.5-Pro, consistently surpass general-purpose models (GPT-4.1, GPT-4.1-mini) at every core size. With 5 core nodes, GPT-5 attains a 72.5% success rate versus 12.0% for GPT-4.1. However, success rates fall sharply as sequence length grows: GPT-5 drops from 72.5% (5 core nodes) to 15.0% (20 core nodes), and Gemini-2.5-Pro from 46.5% to 6.0%. These trends suggest limited effective planning depth and only modest self-correction via reflection as tasks require longer function-call sequences.

**GPT-5 invokes 10% more calls than necessary even when successful.** While GPT-5 demonstrates strong performance, it still exhibits inefficiencies in function calling. For example, with 10 and 20 core nodes (i.e., required function calls), GPT-5 averages 11.5 and 22.0 function calls respectively for successful cases. This indicates that even the best-performing models struggle to optimize their function call sequences, often making unnecessary calls.

The trends of average calls on failed cases depend on the model. We observe distinct patterns in the average number of function calls (ACs) for failed cases across different models. For example,

<sup>&</sup>lt;sup>1</sup>Since GPT-5 and GPT-5-mini do not support the temperature parameter, we use their default settings.

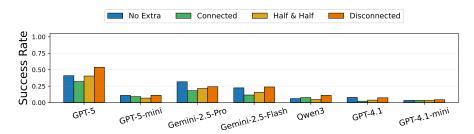


Figure 3: Success rate under different irrelevant node connection types. The results are averaged over  $\{5, 10, 20\}$  numbers of core nodes and  $\{0, 10, 20, 40\}$  irrelevant nodes. Connected, Half & Half, and Disconnected indicate that all, half, and none of the irrelevant nodes are connected to the core nodes, respectively.

GPT-5, GPT-5-mini, Gemini-2.5-Pro tend to make more function calls in failed cases than successful ones, indicating that they struggle to find the correct path once they deviate. In contrast, Gemini-2.5-Flash invokes significantly fewer function calls in failed cases compared to successful ones, suggesting that it gave up when it could not find the correct path.

# 4.3 EFFECT OF IRRELEVANT FUNCTIONS (RQ2)

**Connected irrelevant nodes (CINs) severely degrade performance for all models.** Figure 3 shows that CINs have the most negative impact on model performance compared to other types across most tested LLMs. We speculate that this is because CINs share variables with core nodes, making it challenging for models to distinguish relevant function paths from irrelevant ones.

Interestingly, the effect of disconnected irrelevant nodes (DINs) varies across models. For instance, GPT-5 achieves better performance in the "Disconnected" setting than in the "No Extra" setting, suggesting that the existence of DINs may prompt GPT-5 to carefully consider its function calls, potentially leading to better performance in the presence of irrelevant functions. In contrast, Gemini-2.5-Pro performs worse in the "Disconnected" setting than the "No Extra" setting, suggesting that it may struggle to ignore irrelevant functions even when they are disconnected from the core nodes.

We also observe that "Half & Half" settings often yield intermediate performance between the "No Extra" and "Connected" settings, indicating that the presence of some CINs is sufficient to significantly confuse the models.

# 4.4 EFFECT OF FUNCTION DEPENDENCY DEPTH (RQ3)

We break down the results by the dependency depth in Figure 4. We also show the results with 95% confidence intervals and more numbers of core nodes in Appendix B.

## Lower dependency depth is more manageable.

Lower dependency depth leads to higher success rates across all models. For instance, with 10 core nodes, GPT-5 achieves near a 90% success rate when the dependency depth is set to 1, where a graph has a star structure (see Figure 2), but this rate drops sharply to less than 30% when the dependency depth increases, i.e., between 4 and 8. This pattern is consistent across other reasoning-optimized models like Gemini-2.5-Pro and GPT-5-mini, suggesting higher dependency depth poses significant challenges for LLMs in function calling tasks.

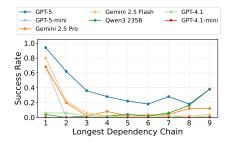


Figure 4: Success rates by the dependency depth. The number of core nodes is set to 10. The results are averaged over all irrelevant node settings.

**Fewer branches in the function call sequence are less harmful.** We observe that GPT-5, Gemini-2.5-Pro, and Qwen3 show a slight performance improvement when the dependency depth is set to 8 and 9, where a graph has a path structure, compared to dependency depth between 5 and 7. This suggests that having fewer branches in the function call sequence may be less harmful,

as it reduces the complexity of decision-making at each step. However, this trend is not observed in smaller models like GPT-5-mini and Gemini-2.5-Flash, indicating that this benefit may be more pronounced in larger, more capable models.

# 4.5 DISCUSSION (RQ4)

To better understand the behaviors of the best performing model, we conduct experiments using GPT-5 with larger function sets and different thinking budgets.

Larger sets of required nodes are generally more challeging even for the disconnected setting. Figure 5 shows results for each number of core nodes, where results are averaged across the numbers of irrelevant nodes.

Surprisingly, even in the disconnected setting where irrelevant functions are not type-compatible with core functions, GPT-5's performance degrades significantly (lower than 10% for 40 core nodes) as the number of core nodes increases. This poor performance of GPT-5 indicates that even the best models are not ready to be used over a large

function sets which is happening with existing MCP servers (Anthropic, 2025).

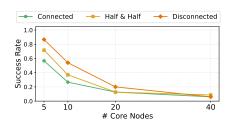


Figure 5: Success rate of GPT-5 with

various numbers of core nodes. The re-

sults are averaged across  $\{0, 10, 20, 40\}$ 

s irrelevant nodes.

Sufficient thinking budget is necessary in complex function calling tasks. To investigate in detail how the thinking budget affects the performance of GPT-5, we compare the medium thinking budget,<sup>2</sup> i.e., our default setting in other experiments, with the minimal thinking budget in Figure 6. We observe a significant drop from the medium thinking budget setting, indicating that the minimal budget severely limits the model's ability to reason through multi-step function calling tasks. Only for the no extra irrelevant nodes setting, GPT-5 with the minimal thinking budget obtains higher than 50% success rate. In other settings, the success rates are less than 20%. This result highlights the importance of providing

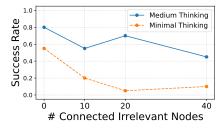


Figure 6: Thinking budget comparison for GPT-5 with 5 core nodes, averaged over all irrelevant node settings.

sufficient reasoning capacity for LLMs to effectively navigate complex function calling scenarios.

#### 4.6 FAILURE ANALYSIS AND MITIGATION STRATEGY (RQ5)

In analyzing model failures in function calling, we use complete execution traces from our in-house executor, which logs all calls, arguments, returns, and state updates, enabling deterministic, annotation-free attribution. The executor enforces four sequential, machine-checked predicates—name resolution, schema conformance, dataflow availability, and value consistency—designed to be minimal and collectively exhaustive. We categorize the failure cases into four types: 1) Function Not Found: The model attempts to call a function that does not exist in the provided function list. 2) Wrong Number of Inputs: The model provides more or fewer input arguments than the function schema allows. 3) Value Not Yet Known: The model tries to use a variable whose value has not been established through prior function calls or initial inputs. 4) Incorrect Value: The model uses a variable with an incorrect value, which has been established through prior function calls or initial inputs.

**Models attempt to use unknown variable values most frequently.** Table 3 summarizes the failure types of all models, where the results are aggregated over function calls made by each model. We observe that the most common failure mode across all models is attempting to use variable values

<sup>&</sup>lt;sup>2</sup>While GPT-5 has four options for its thinking budgets, high, medium (default), low, and minimal, we fucus on the medium and minimal thinking budgets in this paper due to the budget constraint.

Table 3: Failure types. The results are averaged  $\{5, 10, 20\}$  core nodes and all irrelevant node settings, with 5 trials each.

Failure type	GPT-5	GPT-5-mini	Gemini-2.5-Pro	Gemini-2.5-Flash	Qwen3	GPT-4.1	GPT-4.1-mini
Function Not Found	0.0%	0.0%	2.4%	0.0%	0.0%	0.0%	0.0%
Wrong Number of Inputs	0.0%	0.0%	0.2%	0.9%	0.1%	0.0%	0.0%
Value Not Yet Known	79.6%	66.8%	69.1%	81.3%	74.0%	73.2%	66.8%
Incorrect Value	20.4%	33.2%	28.3%	17.9%	25.8%	26.8%	33.2%
Total errors	6,054	13,180	5,756	235	9,472	3,597	8,560

that are not yet known, accounting for over 66% of failures in every model. This indicates that models often struggle to accurately track which variables have been established through function calls. While recent models have shown strong value retrieval capabilities (Hsieh et al., 2024) from given long documents, they still face challenges in maintaining context over multiple steps in function calling scenarios.

Interestingly, most models rarely attempt to call non-existent functions or provide too many inputs, suggesting that they generally understand the function schemas provided.

#### 4.6.1 MITIGATION STRATEGY

To address the most common failure types of using unknown variable values and incorrect values, we propose a simple mitigation strategy. Instead of each function just returning the value of its output variable, it also returns the list of all known variable values as well.

This provides no extra information to the model - it simply restates the values of all the variables the model has already discovered, including variables with wrong values that have been discovered through incorrect function calls. This provides the model with explicit context about which variables are available for use in function

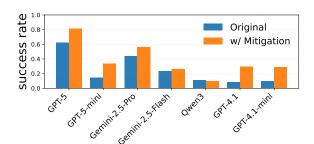


Figure 7: Comparison between the baseline and the proposed mitigation strategy. The number of core nodes is set to 5. The results are averaged across  $\{0, 10, 20, 40\}$  CINs, with 5 trials each.

calls. This lightweight approach does not rely on the FuncBenchGen framework, and can easily be implemented in real-world scenarios with a simple wrapper around the provided functions.

**Simple variable reminders dramatically improve performance.** Figure 7 compares the success rates of all models with and without the above mitigation strategy. We observe that the mitigation strategy improves performance over both reasoning and general models. Gemini-2.5-Flash and Qwen3 have a small improvement or a slight performance drop, suggesting that these models may struggle to effectively utilize the additional context provided. Overall, this result indicates that even a simple reminder of known variable values can significantly enhance LLMs' function calling capabilities by reducing errors related to variable usage.

## 5 CONCLUSION

We present FuncBenchGen, a novel framework for generating multi-step function calling benchmarks that address key limitations in existing evaluations. By enabling controllable complexity and contamination-free tasks, FuncBenchGen provides a robust platform for systematically assessing LLMs' function calling capabilities. Our extensive experiments reveal significant performance gaps between reasoning-optimized and general-purpose models. Results also highlight challenges posed by irrelevant functions and long call sequences – even GPT-5 struggles with longer function call sequences. We identify common failure types, and based on this analysis propose a simple yet effective mitigation strategy that significantly improves performance across various models. Overall, FuncBenchGen offers a valuable tool for advancing research into LLM function calling capabilities.

# REPRODUCIBILITY STATEMENT

We have made several efforts to ensure the reproducibility of our work. First, the design principles, methodology, and evaluation setup for FuncBenchGen are detailed in Section 3. All models used in the experiments are well-documented in Appendix A.1, with the prompt example in Appendix A.3. Upon paper acceptance, we will release the framework, codebase, and detailed documentation for both the experimental setup and data generation to promote ease of replication.

#### ETHICS STATEMENT

We made use of AI tools such as ChatGPT and Copilot to support coding and refining this paper, but all content was carefully reviewed and edited by us to ensure it adheres to our standards and aligns with our research objectives.

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# A Addional Experiment Details

#### A.1 MODEL DETAILS

Model	Size	Context	HuggingFace / API	License
GPT-5 (OpenAI, 2025b)	-	400k	gpt-5-2025-08-07	OpenAI Service Terms <sup>1</sup>
GPT-5-mini (OpenAI, 2025b)	-	400k	gpt-5-mini-2025-08-07	OpenAI Service Terms
Gemini-2.5-Pro (Comanici et al., 2025)	_	1M	gemini-2.5-pro	Gemini API Additional Terms of Service <sup>2</sup>
Gemini-2.5-Flash (Comanici et al., 2025)	_	1M	gemini-2.5-flash	Gemini API Additional Terms of Service <sup>2</sup>
Qwen-3 (Team, 2025)	235B	128k	Qwen/Qwen3-235B-A22B-Instruct-2507	Apache license 2.0
GPT-4.1 (OpenAI, 2025a)	_	1M	gpt-4.1-2025-04-14	OpenAI Service Terms
GPT-4.1-mini (OpenAI, 2025a)	_	1M	gpt-4.1-mini-2025-04-14	OpenAI Service Terms

Table 4: Models used in experiments. Model sizes are not publicly disclosed (-).

We summarize the details of the models used in our experiments in Table 4. All models are used via their respective APIs except for Qwen3, which is accessed through HuggingFace. We set the temperature and top-p parameters to 0.0 and 1.0, respectively, for all our experiments. For models that do not support the temperature parameter, we use their default settings.

# A.2 Types and Subtypes

We observed that if functions were linked based on exact variable names, the problem became too easy. In real-world scenarios, even if a function consumes the output of another function, the names of those variables are rarely the same. Instead these relationships are captured through semantic meaning and data types. For example, if function A outputs a variable of type SQLQuery and function B has an input of type SQLQuery, that often means that function B is designed to consume the output of function A. To reflect this, FuncGenBench links functions based on types, rather than direct variable names. The only exception to this are the input variables listed in the model prompt. Those are linked to function schemas based on direct variable name matching instead.

Additionally, each variable is given both a type and a subtype. A subtype is unique to that variable to allow for unambiguous linking between two functions, but types may be shared across many different variables of completely separate functions. We include both type and subtype to better reflect real-world scenarios where many functions operate on the same kind of data, but only some functions are able to consume the outputs of others in a meaningful way. For example, many functions could accept an argument of type "Employee", but some functions (such as num\_managed\_employees) would expect that "Employee" to have subtype "Manager."

# **Function Linking Strategies**

# Linking based on variable names:

Func\_yep processes variable mfmjsy to produce variable tcok.

Func\_ayj processes variable tcok to produce variable arpl.

# Linking based on types:

Func\_yep processes variable mfmjsy (type\_uxe with subtype\_muw) to produce variable aargww (type\_beo with subtype\_dej)

Func\_ayj processes variable riivq (type\_beo with subtype\_dej) to produce variable sjyav (type\_wdc with subtype\_uqq)

#### A.3 EXAMPLE MODEL INPUT

We provide an example of the model input used in our experiments below.

```
Example Model Input
User Prompt:
Using the tools at your disposal, use functions until you are able to give me the correct value of variable
bujxye.
Variable mfmjsy = 731
You have all the information you need to get the correct result.
Tool Prompt:
[{'type': 'function'
   function': {'name': 'func_yep',
   'description': 'Processes variable of (type_uxe with subtype_muw) to
   produce (type_beo with subtype_dej)',
    'strict': True,
    'parameters': {'type': 'object',
     'properties': {'mfmjsy': {'type': 'integer'}},
'required': ['mfmjsy'],
     'additionalProperties': False}}},
]
```

#### B ADDITIONAL RESULTS

# B.1 RESULTS OF NO EXTRA SETTING

Table 5 shows the results of all models in the no extra irrelevant node setting. We observe that the trends of success rates and ACs are consistent with those in Section 4 while the "No Extra" setting obtains higher success rates in general.

#### B.2 RESULTS OF DEPENDENCY DEPTH WITH ERROR BARS

Figure 8 shows the results for each dependency depth with error bars in which the results are averaged across the numbers of noisy connected nodes.

#### B.3 RESULTS OF OTHER DEPENDENCY DEPTHS

Figure 9 shows the results of all models for each dependency depth with 20 core nodes. We observe similar trends to those in Figure 4. Lower dependency depth leads to higher success rates across models.

Table 5: Success rates and average function calls (ACs) that were actually made by models. Results are aggregated across only no extra irrelevant node configurations and graph dependency depth  $\{1,...n^{\text{core}}-1\}$ , with 5 random trials per configuration. ACs (Succ.) and (Fail.) denote the ACs for successful and failed trials, respectively. "–" indicates that there are no successful trials.

# core nodes	5			10			20		
	Success Rate	ACs (Succ.)	ACs (Fail.)	Success Rate	ACs (Succ.)	ACs (Fail.)	Success Rate	ACs (Succ.)	ACs (Fail.)
GPT-5 GPT-5-mini Gemini-2.5-Pro Gemini-2.5-Flash Qwen3 GPT-4.1 GPT-4.1-mini	80.0% 20.0% 65.0% 35.0% 10.0% 15.0%	5.0 5.0 5.0 5.0 5.0 5.0 5.0	5.0 4.7 5.0 0.5 5.0 4.0 4.3	28.9% 8.9% 20.0% 22.2% 4.4% 6.7% 0.0%	10.4 10.0 10.0 10.0 10.5 10.0	9.6 8.9 12.1 0.3 9.9 6.9 8.6	14.0% 4.0% 10.0% 10.0% 4.0% 2.0% 0.0%	21.0 20.0 20.0 20.0 21.0 21.0	17.6 17.5 24.6 0.0 18.2 12.2 15.0

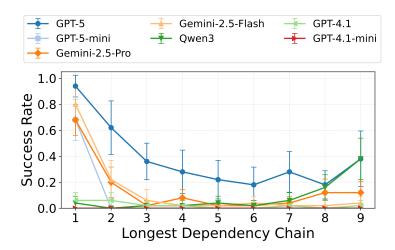


Figure 8: Success rates by the dependency depth with error bars. The number of core nodes is set to 10. Error bars indicate 95% confidence intervals.

Figure 10 shows the results of GPT-5 for each dependency depth with 40 core nodes. Since the core node size is large, the success rates are 0 when dependency depth is greater than or equals 9.

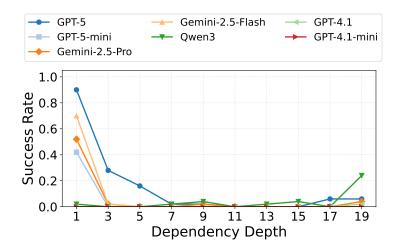


Figure 9: Success rates of all models by the dependency depth. The number of core nodes is set to 20 and the results are aggregated .

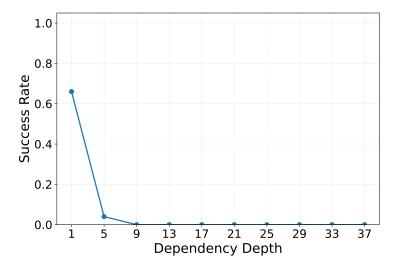


Figure 10: Success rates of GPT-5 by the dependency depth. The number of core nodes is set to 40.