Why Stop at One Error? Benchmarking LLMs as Data Science Code Debuggers for Multi-Hop and Multi-Bug Errors

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Abstract

LLMs are transforming software development, yet current code generation and code repair benchmarks mainly assess syntactic and functional correctness in simple, single-error cases. LLMs' capabilities to autonomously find and fix runtime logical errors in complex data science code remain largely unexplored. To address this gap, we introduce **DSDBench**: the **D**ata **S**cience **D**ebugging **Bench**mark, the first benchmark for systematic evaluation of LLMs on multi-hop error tracing and multi-bug detection in data science code debugging. DSDBench adapts datasets from existing data science task benchmarks, such as DABench and MatPlotBench, featuring realistic data science debugging tasks with automatically synthesized multi-hop, multi-bug code snippets. DSDBench includes 1,117 annotated samples with 741 cause-effect error pairs and runtime error messages. Evaluations of state-of-the-art LLMs on DSDBench show significant performance gaps, highlighting challenges in debugging logical runtime errors in data science code. DSDBench offers a crucial resource to evaluate and improve LLMs' debugging and reasoning capabilities, enabling more reliable AI-assisted data science in the future.

1 Introduction

Recent advancements in Large Language Models (LLMs) have significantly reshaped software development practices, particularly in automating code generation and debugging. Benchmarks like DebugBench (Tian et al., 2024), CodeEditorBench (Guo et al., 2024a), and DebugEval (Yang et al., 2025) have played a pivotal role in evaluating LLMs' capabilities in code repair. However, these benchmarks largely rely on simplified programming exercises from platforms like *LeetCode*, which prioritize **syntactic correctness** and **functional accuracy** in **isolated** and **single-error** scenarios, far removed from real-world software complexity.

Meanwhile, growing research efforts are exploring LLMs' potential in data science coding (Yang et al., 2024b; Hu et al., 2024; Zhang et al., 2024b; Hong et al., 2024), where practitioners routinely tackle challenges involving black-box library functions, intricate data transformations, and statistical modeling. Yet, a critical gap persists: despite this emerging focus, there remains a striking lack of investigation into LLMs' ability to *debug dynamic logical errors in data science code*. Such errors, manifesting only at runtime, are endemic to this domain due to hidden dependencies in data pipelines, implicit assumptions in mathematical operations, and unpredictable interactions with external resources.

As illustrated in Figure 1, unlike constrained programming exercises, debugging data science codebases presents unique challenges: 1) Its heavy reliance on external libraries (e.g., pandas, NumPy, scikit-learn, matplotlib) means subtle misuses or incorrect data processing steps can easily trigger downstream runtime exceptions. 2) Data scientists often work in interactive environments like Jupyter Notebooks, which lack robust debugging tools. This makes it harder to identify and fix runtime bugs, especially when **multiple subtle errors**, such as incorrect data transformations or misaligned indices, coexist and interact within the code, complicating the debugging process. 3) Standard debugging tools offer limited assistance in diagnosing **multi-hop logical errors** within complex workflows. The root cause of these errors can be distantly located from the point of error manifestation. Standard debuggers typically report the *symptom* (the line of error manifestation in the stack trace) rather than the *root cause* responsible for the program's termination. Overall, a dedicated benchmark for rigorously assessing LLMs' dynamic debugging of multi-hop logical errors in complex multi-bug data science code is still lacking.

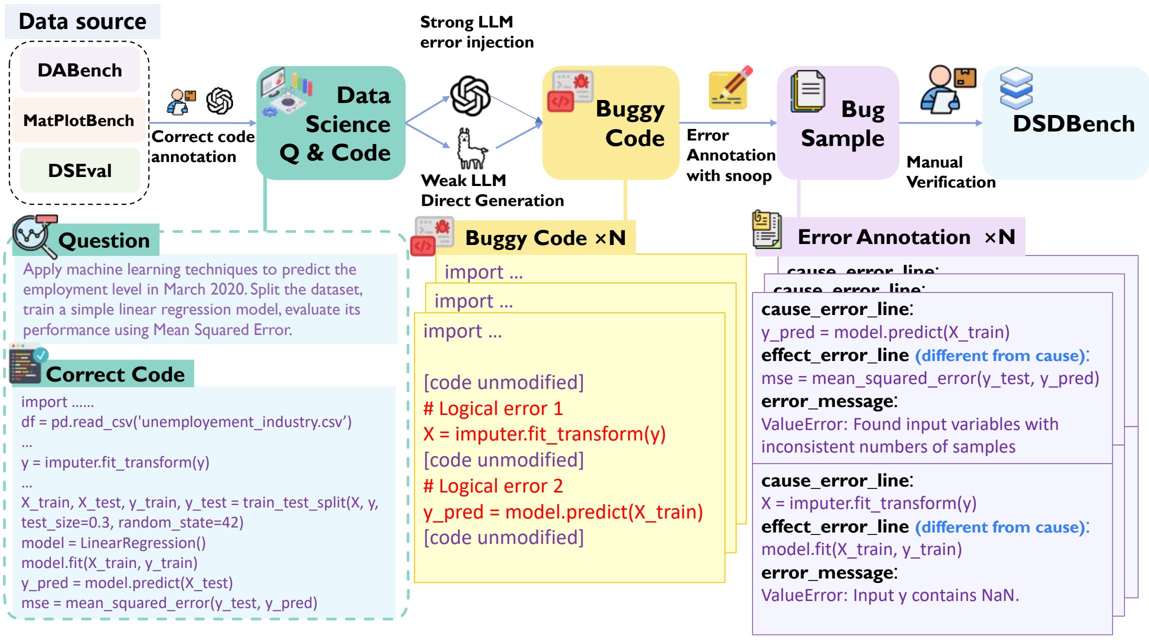

Figure 1: Dataset construction pipeline of DSDBench.

Benchmark	Domain	Error Complexity	Multi-Hop Error	Error Type
DebugBench	General	Multi-Bug	✗	Static
DebugEval	General	Multi-Bug	✗	Static
CodeEditorBench	General	Single-Bug	✗	Static
DSDBench	**Data Science**	Multi-Bug	✓	**Runtime**

Table 1: Comparison with existing benchmarks.

Motivated by this evident gap in evaluating LLMs' dynamic debugging skills for data science, we introduce **DSDBench**: the **D**ata **S**cience **D**ebugging **Bench**mark. Distinct from prior works that primarily focus on repairing single, syntactic and static errors, where these errors are easily caught by interpreters or compilers, DSDBench is the first benchmark to systematically evaluate LLMs on: (1) **Multi-Hop Error Tracing**: requiring models to trace runtime errors back through multiple lines of data science code to identify the root cause; and (2) **Multi-Bug Error Detection**: assessing their ability to concurrently detect and reason about multiple logical errors within a single data science code snippet. Table 1 summarizes the comparisons between DSDBench and existing code debugging benchmarks.

DSDBench leverages datasets and tasks from established data science coding benchmarks like DABench (Hu et al., 2024), MatPlotBench (Yang et al., 2024b), and DSEval (Zhang et al., 2024b). We systematically inject errors into data science code, synthesizing multi-error scenarios by combining individual bugs. Our dataset comprises 1,117 meticulously annotated samples, complete with ground-truth cause-effect error line pairs and captured runtime error messages.

In summary, our contributions are threefold:

- **DSDBench Benchmark:** We release the first dedicated benchmark and dataset for evaluating LLMs in runtime, multi-bug debugging of data science code. DSDBench features realistic logical errors, multi-hop error scenarios, and detailed annotations, addressing a critical gap in current debugging benchmarks.
- **Automated Error Injection and Annotation Framework:** We develop a robust pipeline for automated error injection, runtime execution tracing, and alignment of interpreter outputs with error-originating code lines, facilitating scalable benchmark creation and future expansion.
- **Empirical Analysis and Insights:** We present a comprehensive empirical evaluation of state-of-the-art closed-source and open-source LLMs on DSDBench. Our findings reveal significant performance gaps and highlight critical challenges in dynamic debugging for complex, real-world data science code.

2 DSDBench Construction

The creation of a high-quality dataset is paramount for a robust benchmark. As illustrated in Figure 1, DSDBench is meticulously constructed through a multi-stage process encompassing data sourcing, correct code preparation, error injection, error annotation, and quality assurance.

2.1 Data Collection

We build the DSDBench upon three widely-adopted data science coding benchmarks for their realistic data science tasks and diverse scenarios, including DABench (Hu et al., 2024), MatPlotBench (Yang et al., 2024b), and DSEval (Zhang et al., 2024b). We focus on the hard subset of DABench because error injection in its easy and medium subsets rarely produces runtime exceptions. MatPlotBench and DSEval supplement DABench, expanding task diversity and library coverage (`pandas`, `sklearn`, `scipy`, `matplotlib`, `numpy`) to represent typical data science workflows. These benchmarks cover data manipulation, statistical analysis, machine learning, and visualization.

However, some of these datasets mainly contain the natural language instructions and the final results after running the data science code, while the ground-truth correct codes are not provided. As the first step, we prepare the correct and error-free codes for each benchmark as follows:

DABench We design an agent-based annotation framework, which includes a self-debugging code agent and an error verifier agent. Annotation begins by feeding benchmark questions and metadata to the self-debugging code agent, which generates initial code and debugs it based on error messages. Subsequently, the error verifier agent analyzes this code to correct logical errors, meanwhile ensures the code produces correct answers according to DABench's ground truths. The details of the agent-based annotation framework are presented in Appendix A.

MatPlotBench Similar agent-based code generation is adopted, but automated verification is challenging due to the visual nature of plot outputs. Therefore, manual expert verification is employed, comparing plots to ground truth images and correcting code for accurate visualizations.

DSEval We extract and concatenate code blocks from ground truth Jupyter notebooks provided by DSEval, using concatenated code as our benchmark's correct code.

2.2 Error Injection

To systematically introduce errors, we employ two error injection methodologies. The details regarding the error injection prompts are provided in Appendix B.

Strong LLM-based Error Injection One primary method is called strong LLM-based error injection, which utilizes a strong LLM, *i.e.*, GPT-4o, to inject runtime-interrupting errors. This involves a two-stage process: 1) We identify code lines using data science libraries (`numpy`, `scipy`, `matplotlib`, `sklearn`, `pandas`) by instructing GPT-4o to extract relevant core library functions. 2) We inject runtime errors into these lines using GPT-4o by introducing plausible, contextually relevant runtime errors within code identified in the first step, causing programs to halt. In terms of multi-hop errors, error injection on one line could cause a runtime error to manifest on a later line due to sequential code execution.

Weak LLM-based Direct Error Generation Across our three data sources, we explore weak LLM-based direct error generation using Llama-3.1-8B. We instruct Llama-3.1-8B to directly generate Python code from benchmark questions. Due to the limitations of weaker LLMs, the generated code often contains errors. In terms of multi-hop errors, in directly generated code with functions, an error in a sub-function could trigger an error reported in the `main` function during execution.

2.3 Error Annotation

For each buggy code snippet, we annotate three ground truths, `cause_error_line`, `effect_error_line`, and `runtime error messages`. Our annotation process can be divided into single-error and multi-error phases.

Single-Error Annotation We commence dynamic error capture with `snoop`[1], a Python debugging library that logs execution details, for single-error ground truth. `snoop` monitors the execution of both injected and direct generated error code. We first filter out successfully executed ones. For error-triggering snippets, we analyze `snoop`'s execution traces to extract: `cause_error_line` (error origin), `effect_error_line` (error manifestation), and `runtime error messages`, providing ground truths for single-error annotation.

Multi-Error Annotation Multi-error annotations are generated based on single-error annotations. For each question, we systematically gen-

[1]https://pypi.org/project/snoop/

Dataset Size			Example Type		Multi-Error Examples	Code Complexity	Question Complexity
Total # Examples	# Single-Error	# Multi-Error	# Single-hop	# Multi-hop	Avg Errors/Example	Avg Code Length	Avg Question Length
1,117	741	376	385	356	2.87 ± 1.14	65.31 ± 21.31	92.42 ± 55.86

Table 2: Dataset statistics of DSDBench.

erated all combinations of the already annotated single errors to create a pool of candidate multi-error annotations. From each question's candidate pool, we randomly sample a subset to form our multi-error dataset.

2.4 Human Verification and Quality Control

To ensure the quality and correctness of the constructed dataset, we perform a two-stage verification process: **code-based checks** and **LLM-assisted verification**. 1) Code checks involve printing and manually inspecting annotated cause and effect lines to correct nonsensical annotations by human annotators. We also print error messages, identifying and resolving a common `plt.show()` backend issue by adding backend settings to the MatPlotBench correct code examples. 2) LLM-assisted verification is used to review all annotations, flagging remaining inconsistencies that require human intervention to correct the annotations. Overall, the pass rates of the human verification for the two stages are 83% and 87%, respectively. The high pass rates also validate the effectiveness of the automated annotation process.

2.5 Dataset Characteristics

This section presents a statistical overview of the DSDBench dataset, characterizing its composition, diversity, and complexity. Table 2 provides a statistical overview of the DSDBench dataset. The **dataset size and splits** are as follows: the total number of examples is 1,117, of which 741 are single-error examples and 376 are multi-error examples. For single-error examples, the number of examples with multi-hop cause and effect error lines is 356, the rest 385 examples contain identical cause and effect error lines *i.e.*, single-hop errors). For multi-error examples, the number of errors per example ranges from 2 to 9, with an average of 2.87 errors per example. Regarding complexity, the average code length is 65.31 lines, and the average question length is 92.42 words. For a more detailed breakdown of these statistics, please refer to Table 2.

Figure 2 illustrates the **error type distribution** in DSDBench. Figure 3 shows the **data science library coverage** within the dataset.

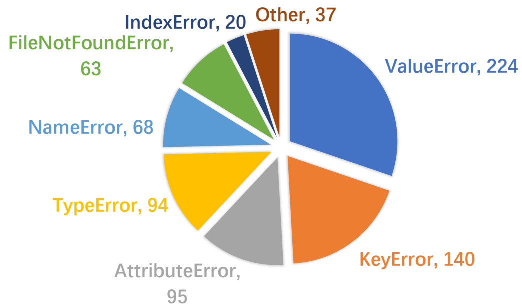

Figure 2: Distribution of different error types. Details of error types are described in Appendix C.

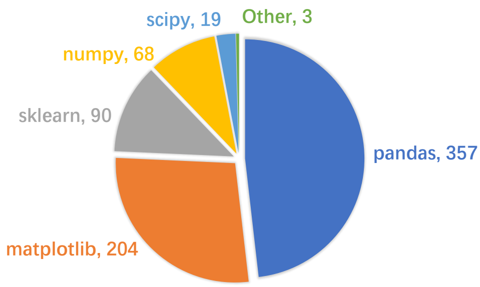

Figure 3: Distribution of different data science libraries.

3 Problem Formulation

3.1 Task Definition

This section formally defines the task of **Data Science Code Debugging** for the DSDBench benchmark, outlining the input, desired output, and evaluation settings. The primary objective of DSDBench is to evaluate the capability of LLM-based debuggers to identify and explain **logical errors** in **data science Python code** during simulated **runtime execution**.

The benchmark is specifically designed to assess two critical dimensions of debugging proficiency: **multi-hop error detection** and **multi-bug error detection**. Multi-hop error detection evaluates the LLMs' ability to trace errors to their **root cause** (**`cause_error_line`**), which may precede the **interpreter's error point** (**`effect_error_line`**) by several lines of code. Multi-bug error detection assesses the LLMs' ability to identify and explain **multiple, concurrent logical errors** within a single code snippet, rather than solely the initial error encountered. A further goal is to evaluate the quality of **error message reproduction**, specifically the ability of LLMs to accurately reproduce the **er-**

ror messages thrown by the Python interpreter for each identified error.

Formally, for each task instance i, the input is a pair (Q_i, C_i), where Q_i is a natural language question describing a data science task, and C_i is a Python code snippet intended to perform task Q_i, but containing logical errors. The task of the LLM is to predict a structured output $O_i = (L_{cause,i}, L_{effect,i}, M_i)$, where $L_{cause,i}$ is the exact line of code for the cause error, $L_{effect,i}$ is the exact line of code for the effect error, and M_i is the error message that would be produced by a Python interpreter when executing C_i. The DSDBench benchmark dataset can be represented as $D = \{(Q_i, C_i, L^{GT}_{cause,i}, L^{GT}_{effect,i}, M^{GT}_i)\}^N_{i=1}$, where GT denotes the ground truth annotation. The objective is to evaluate LLMs' capabilities to perform the task of $f : (Q_i, C_i) \mapsto O_i$ which localizes and interprets the error.

3.2 Evaluation Metrics

This section details evaluation metrics for LLM debugger performance on DSDBench, focusing on error localization accuracy and description quality. Model performance is evaluated across four dimensions, including **Cause Line Matching**, **Effect Line Matching**, **Error Type Matching**, and **Error Message Matching**.

Specifically, we calculate `cause_line_score`, `effect_line_score`, and `error_type_score` as binary metrics (1 for exact match with ground truth, 0 otherwise). `error_message_score` is evaluated by GPT-4o on a scale in [0.0, 0.25, 0.5, 0.75, 1.0] based on the relevance and correctness of the reproduced error message compared to the ground truth error message.

Dimension-Level Definitions: For each evaluated dimension:

- **TP (True Positives):** Number of instances with correct LLM predictions (exact match for lines/types, `error_message_score` ≥ 0.75 for error messages).
- **FP (False Positives):** Number of instances with specific incorrect LLM predictions (commission errors).
- **FN (False Negatives):** Number of instances where LLM failed to provide a relevant prediction, (omission errors) e.g., incorrect output format ; $FN = GT\_Instances - (TP + FP)$.
- ***GT_Instances*:** Total Ground Truth Instances for the dimension.

Evaluation Metrics (per dimension): We employ Precision, Recall, F1-score, and Accuracy to evaluate performance across dimensions. Because DSDBench only contains test cases with errors, meaning there is no True Negatives in model predictions. Therefore, we calculate **Recall** by **(True Positive Rate - TPR)** to measure the completeness of error detection as:

$$\text{Recall (TPR)} = \frac{TP}{GT\_Instances}$$

making Recall (TPR) numerically equivalent to Accuracy. All metrics are calculated dimension-wise to provide a detailed performance profile.

4 Experiments

4.1 Setup

Models We benchmarked a diverse set of state-of-the-art models on the DSDBench dataset, including both closed-source models and open-source models. Specifically, the closed-source models we employed were GPT-4o, GPT-4o-mini, o1-mini (OpenAI, 2024), Gemini 2.0 Flash Thinking (Google, 2024), and Claude 3.5 sonnet-20240620. Open-source model consisted of Llama-3.1-8B-instruct, Llama-3.1-70B-instruct, Llama-3.1-405B-instruct (Meta, 2024), Qwen2.5-7B-Instruct, Qwen2.5-32B-Instruct, Qwen2.5-72B-Instruct (Qwen, 2025), DeepSeek-V3, DeepSeek-R1 (DeepSeek-AI, 2025). Notably, we categorize Gemini 2.0 Flash Thinking, DeepSeek-R1 and o1-mini as Large Reasoning Models (LRMs). All models were used with their default decoding parameters apart from setting temperature to 0. Zero-shot setting were used. We used OpenRouter's API services for all models.

Evaluation Protocol The prompt used to evaluate all models are identical, including task description, buggy Python code snippet from DSDBench, and instructions to output the debugging analysis in a structured JSON format. The precise prompt template is in Appendix D. This zero-shot evaluation approach allows us to assess the inherent debugging abilities of each model. We utilized the metrics defined in Section 3.2 for quantitative assessment.

4.2 Main Results

Table 3 and Table 4 present the primary results of our experiments, showing the accuracy of various models in detecting single and multi-bug scenarios across the full and subset DSDBench datasets.

Model	Cause Line		Effect Line		Error Type		Error Message	
	Single-Bug	Multi-Bug	Single-Bug	Multi-Bug	Single-Bug	Multi-Bug	Single-Bug	Multi-Bug
GPT-4o	39.0	20.3	34.3	10.4	30.6	**3.6**	31.4	**4.7**
GPT-4o-mini	40.2	11.2	23.9	2.7	21.7	2.2	21.3	0.8
Claude 3.5 sonnet	43.7	12.3	35.2	4.1	**36.3**	1.9	34.0	2.5
Deepseek-V3	**48.3**	15.1	34.5	6.6	35.9	3.3	**34.7**	**4.7**
Llama-3.1-8B-instruct	25.2	3.0	14.2	0.0	7.7	0.0	7.2	0.0
Llama-3.1-70B-instruct	42.5	0.0	29.3	0.0	20.4	0.0	20.9	0.0
Llama-3.1-405B-instruct	41.7	18.6	31.3	8.5	29.3	1.1	29.3	2.5
Qwen2.5-7B-Instruct	29.3	4.7	19.3	1.1	10.7	0.3	10.9	0.0
Qwen2.5-32B-Instruct	40.9	17.5	30.5	6.3	24.7	2.2	24.7	2.2
Qwen2.5-72B-Instruct	41.6	**21.4**	**36.2**	**11.2**	27.5	3.0	27.4	3.6

Table 3: Overall evaluation results of LLMs on DSDBench. The reported score is the Accuracy (%), while full metrics are presented in Appendix E.

	Model	Cause Line		Effect Line		Error Type		Error Message	
		Single-Bug	Multi-Bug	Single-Bug	Multi-Bug	Single-Bug	Multi-Bug	Single-Bug	Multi-Bug
LLMs	GPT-4o	35.4	12.5	31.2	5.0	33.3	2.5	33.3	2.5
	GPT-4o-mini	39.6	7.5	29.2	5.0	25.0	2.5	22.9	0.0
	Deepseek-V3	**44.8**	12.5	28.1	7.5	**34.4**	5.0	**34.4**	7.5
LRMs	Gemini 2.0 Flash Thinking	42.7	20.0	**32.3**	12.5	33.3	0.0	35.4	2.5
	Deepseek-R1	**49.0**	32.5	**49.0**	**25.0**	**53.1**	**15.0**	**54.2**	**17.5**
	o1-mini	43.8	**35.0**	36.5	22.5	43.8	**17.5**	46.9	**17.5**

Table 4: Comparison with large reasoning models (LRMs). The reported score is the Accuracy (%), while full metrics are presented in Appendix E. Due to the unstableness of certain LRM APIs, we randomly sample a subset of DSDBench for this evaluation, which comprises of 96 Single-Error and 40 Multi-Error instances.

Single-Bug Debugging Performance As shown in Tables 3, top-performing LLMs like Deepseek-V3 and Claude 3.5 sonnet achieve reasonable accuracy across all tasks, indicating a degree of error tracing capability. Conversely, smaller models such as Llama-3.1-8B-instruct and Qwen2.5-7B-Instruct exhibit significantly lower accuracy. Notably, Qwen2.5-72B-instruct demonstrated strong performance, on par with state-of-the-art closed-source LLMs such as GPT-4o and Claude 3.5 sonnet. In general, effect line accuracy is consistently lower than cause line accuracy across models, showing LLMs' deficiency to reason about code execution traces and find the exact location where the program would trigger an error. Error type and error message accuracy vary across different models, suggesting varying levels of understanding and interpretation of runtime errors.

Challenges in Multi-Bug Debugging The results reveal a dramatic decrease in accuracy when models are challenged with multi-bug scenarios, models fails to identify an correct set of errors within a code snippet with multiple bugs. Even for the best-performing models, cause line accuracy drops to around 20% on the full dataset and 30% on the subset. This substantial performance degradation underscores the increased complexity of debugging multiple bugs concurrently. Furthermore, the low accuracy in error type and error message prediction in multi-bug cases suggests that models struggle to correctly interpret error messages within these more complex contexts.

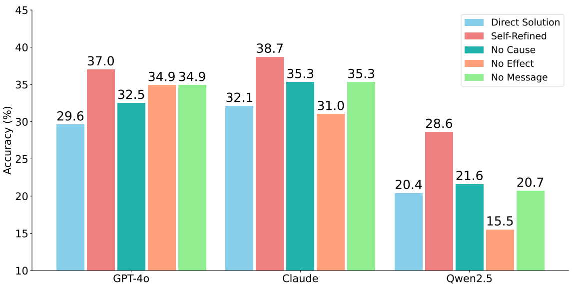

Figure 4: Impact of Self-Refinement.

LRMs Show Promise in Multi-Bug Debugging Comparing LLMs and LRMs on the subset dataset (Table 4) reveals that LRMs generally outperform standard LLMs, particularly in the more demanding multi-bug scenarios, indicating superior reasoning capabilities in LRMs are crucial for tackling complex debugging tasks. A more detailed analysis and case study can be found in Figure 7.

4.3 Impact of Self-Debugging

To further investigate the impact of LLM-as-debuggers on real-world coding tasks, we explored using LLM-generated debugging information in data science coding tasks as a self-refining mechanism. In this experiment, models were tasked with solving DABench-Hard either directly or by

Error Type	Cause Line			Effect Line		
	GPT-4o	Qwen	DeepSeek	GPT-4o	Qwen	DeepSeek
ValueError	57.9	61.6	**66.1**	50.5	**59.6**	54.0
TypeError	30.8	39.5	**50.0**	31.9	34.6	**37.8**
NameError	68.2	64.0	**85.4**	56.1	**60.0**	52.1
KeyError	22.7	28.4	**37.8**	**22.7**	17.6	27.9
AttributeError	35.1	**40.5**	40.0	**22.3**	14.9	15.0
IndexError	36.8	**41.2**	38.9	36.8	**58.8**	55.6
FileNotFoundError	0.0	9.6	**13.0**	1.6	9.6	**11.1**
Other	38.5	53.3	**66.7**	23.1	**46.7**	33.3

Table 5: Precision w.r.t. different error types. The **bold** scores represent the best model performance across error types and prediction tasks.

Library	Cause Line			Effect Line		
	GPT-4o	Qwen	DeepSeek	GPT-4o	Qwen	DeepSeek
matplotlib	46.6	48.4	**55.6**	45.6	52.2	**55.6**
numpy	41.4	40.4	**44.0**	**37.9**	36.8	32.0
pandas	28.1	37.0	**41.0**	21.6	22.0	**24.3**
sklearn	65.1	72.5	**87.7**	58.1	**63.8**	53.8
scipy	36.4	54.5	**72.7**	18.2	36.4	**45.5**

Table 6: Precision w.r.t. different libraries.

refining their initial code using self-generated debugging information.

Table 4 presents the accuracy of GPT-4o, Claude 3.5 sonnet, and Qwen2.5-72B-Instruct in various settings. Across models, **Self-Refinement significantly improves accuracy compared to the Direct Solution**. Furthermore, performance drops when either the cause line (*No Cause*) or effect line (*No Effect*) is removed from the debugging information. Removing only the error message (*No Message*) has less negative impact.

4.4 Detailed Analysis

This section analyzes model performance across error types, libraries, error counts, and multi-hop/single-hop to identify strengths and weaknesses. We adopt GPT-4o, Qwen-72B-Instruct, and DeepSeek-V3 for analysis.

Performance by error types Table 5 shows error type precision. Models exhibit varying performance on different error types. Generally, models perform better on more common error types and less on more obscure error types. Low performance on FileNotFoundError is possibly attributed to models not having access to the coding environment and file system. DeepSeek-V3 performs best on identifying Cause Lines, scoring the highest on every error type except AttributeError and IndexError. Qwen-72B-Instruct performs best on identifying Effect Lines.

Performance by data science libraries Table 6 shows library-specific precision. Pandas is the most difficult library to debug, due to its intricate

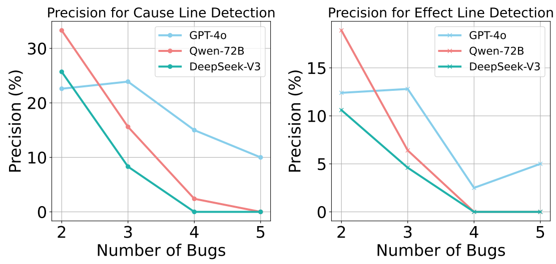

Figure 5: Precision for multi-Bug detection with different number of errors.

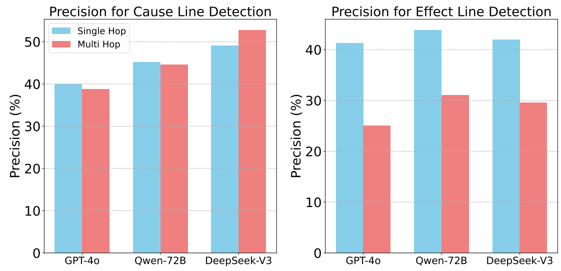

Figure 6: Precision for single-bug detection comparing multi-hop and single-hop errors.

and black-box data manipulation. Models demonstrated best performance on scikit-learn and reasonable performance on matplotlib, numpy and scipy, with significant room for improvement. DeepSeek-V3 demonstrated consistently better performance than other models across all libraries, showing robustness on all kinds of data science coding tasks.

Performance by number of errors Figure 5 shows precision by error count. Precision decreases significantly with more errors for all models. Precision drops sharply when there exists more than 3 errors, highlighting difficulty in multi-error scenarios. GPT-4o performs best on retaining precision on more than 2 bugs, showing potential in concurrent debugging.

Performance on single-hop vs. multi-hop errors Figure 6 compares single-hop vs. multi-hop error precision. Cause Line precision is similar for both types of errors across models. Effect Line precision is significantly lower for multi-hop errors, indicating increased difficulty when locating the point where the program triggers an exception. DeepSeek-V3 demonstrated best performance on Cause Line detection on both single-hop and multi-hop errors, while Qwen2.5-72B-Instruct performs slightly better on Effect Line detection.

4.5 Case Study

According to Figure 7, LRMs have demonstrated intriguing capabilities on reasoning multi-hop er-

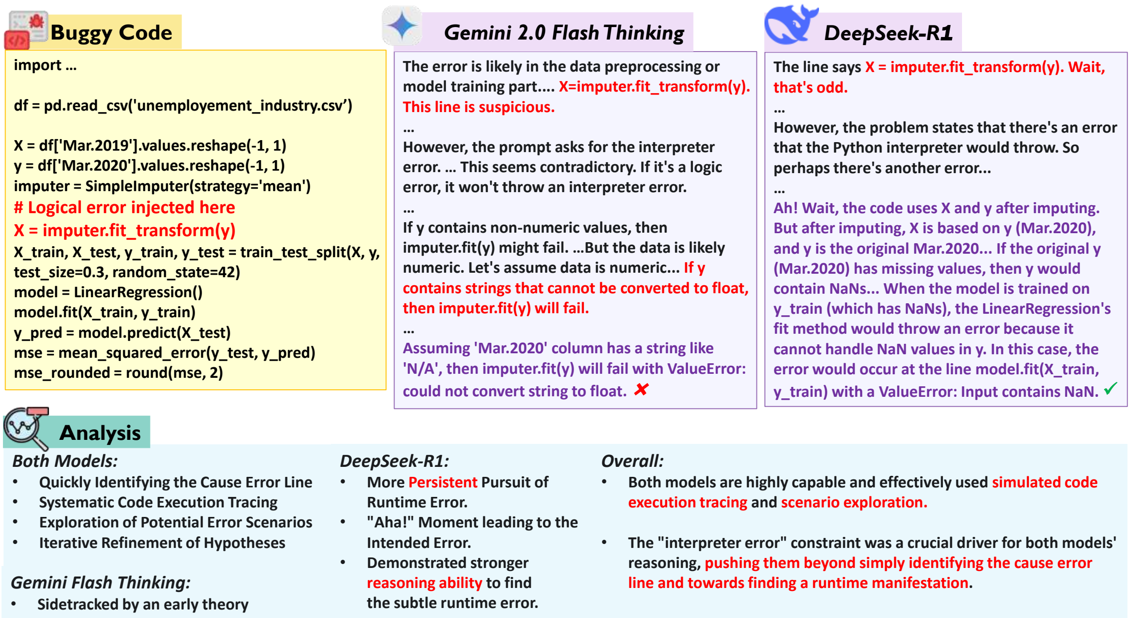

Figure 7: Case study of LRMs.

roneous code. Both Gemini 2.0 Flash Thinking and DeepSeek-R1 can promptly identify the cause `error line`, then mentally simulate code execution trace and explore multiple possible scenarios that could lead to runtime exception. However, Gemini 2.0 Flash Thinking was distracted by one of its early theories and produced an incorrect answer. On the other hand, DeepSeek-R1 ruled out all implausible possibilities after relentlessly pursuing an explanation for triggering a runtime error, eventually came up with the correct answer.

5 Related Work

LLMs Coding and Debugging Early benchmarks like HumanEval (Chen et al., 2021) and MBPP (Austin et al., 2021) focus on assessing code generation correctness. Recent works use reinforcement learning to improve code generation (Wei et al., 2025; Zeng et al., 2025). Runtime information is being used in LLM debuggers (Zhong et al., 2024). Multiple benchmarks (Yang et al., 2025; Tian et al., 2024; Jimenez et al., 2024; Ni et al., 2024; Yang et al., 2024a; Zan et al., 2025; Li et al., 2025a) have focused on LLM code reasoning.

In data science coding, general tools like the Data Interpreter (Hong et al., 2024) and specialized agents such as MatPlotAgent (Yang et al., 2024b) and DSAgent (Guo et al., 2024b) are proposed. Benchmarks such as DSBench (Jing et al., 2024), InfiAgent-DABench (Hu et al., 2024), DSEval (Zhang et al., 2024b), and PyBench (Zhang et al., 2024a) are emerging to evaluate the performance of LLMs in data science coding.

However, DSDBench shifts the focus to dynamic debugging of *logical* errors in real-world data science code (e.g. runtime exceptions, data mismatch), which remain challenging to state-of-the-art LLMs.

LLM Self-Verification Self-correction enhance LLM reliability (Liang et al., 2024). But, LLMs struggle to identify their own errors, especially in complex reasoning (Stechly et al., 2024; Tyen et al., 2024; He et al., 2025). While some intrinsic self-correction exists (Liu et al., 2024), its effectiveness for subtle logical errors is debated (Stechly et al., 2024). Approaches to improve self-correction include confidence-guided methods (Li et al., 2024), critique-focused training (Lin et al., 2024; Li et al., 2025b) and reinforcement learning (Ma et al., 2025).

However, self-verification research mainly targets general language tasks or simplified reasoning. DSDBench uniquely targets dynamic debugging of runtime errors in data science code.

6 Conclusion

We introduced DSDBench, a novel benchmark filling a critical gap in LLM evaluation by focusing on dynamic debugging of logical runtime errors in data science code, specifically multi-hop error tracing and multi-bug detection, built with a rigorous dataset construction process, reveals significant performance limitations of current state-of-the-art LLMs in these complex debugging scenarios.

Limitations

Our proposed DSDBench benchmark primarily focuses on the data science coding domain. While data science is a complex real-world task, our benchmark can be further expanded to encompass a wider range of practical coding scenarios, enabling a more comprehensive evaluation of LLMs' debugging performance in real-world coding pipelines. Additionally, future work could prioritize investigating LLMs' performance in debugging repository-level code with multi-file dependencies.

Ethical Considerations

To construct the DSDBench benchmark, we employed human annotators for data labeling and verification tasks. We recruited annotators from our research institution holding at least a master degree in Computer Science. All annotators participated voluntarily and were provided with comprehensive information regarding the task's purpose, content, workload, and compensation prior to annotating.

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Appendix

A Data Annotation Agent

Our automatic data annotation agent is comprised of two components, a self-debugging code agent

SYSTEM PROMPT: You are a cutting-edge super capable code generation LLM. You will be given a natural language query, generate a runnable python code to satisfy all the requirements in the query. You can use any python library you want. When you complete a plot, remember to save it to a png file.

USER PROMPT: Here is the query: """ {{query}} """ If the query requires data manipulation from a csv file, process the data from the csv file and draw the plot in one piece of code. When you complete a plot, remember to save it to a png file. The file name should be """{{file_name}}""".

Figure 8: The code generation prompt for code agent in Data Annotation.

USER PROMPT: There are some errors in the code you gave: {{error_message}} please correct the errors. Then give the complete code and don't omit anything even though you have given it in the above code.

Figure 9: The self-debugging prompt for code agent in Data Annotation.

and an error verifier agent. The prompts used for these agents are in Figure 8, 9, 10.

the code agent receives benchmark questions as input, generate a draft code according to the requirements in the questions. Then, the system environment in which the agent framework operates executes the draft code. If not successfully executed, the interpreter error message will be passed to the self-debugging code agent, prompting the agent to generate another draft code according to the error message and original benchmark question. The agent will be given a set amount of chances to refine its code according to the error message, if the code is still not executable after 5 rounds, the agent stops. If the code successfully executed within 5 retry times, then the error verifier agent will step in and check the code for further logical errors that may not elicit an interpreter error. If the error verifier agent deems the code correct, the system environment will execute the code and extract the answers from the code. Then we will compare the model generated answers with ground truth answers in each benchmark, if the answers match, we will collect the code that produces these answers as the correct code for our subsequent annotation process.

B Prompts for Error Injection

Figure 11 demonstrates the prompt for error injection, the LLM injector is required to inject plausible runtime logical error into existing correct code with meta information such as benchmark question, data file information. The output format should be a well-formatted JSON dict.

C Error Types

The error types collected in our benchmark are all Python Built-in Exceptions, more information can be accessed at: `https://docs.python.org/3/library/exceptions.html`

D Prompts for Evaluation

Figure 12 and 13 demonstrates the prompts used for evaluating LLMs and LRMs on single bug and multi bug detection. The models are provided with a benchmark question and a snippet of buggy code. The models should identify the error and locate cause and effect error line of code and reproduce error message thrown by the Python Interpreter. The output for single bug detection should be a well-formatted JSON dict, the output for multi bug detection should a list of aforementioned JSON dict.

E Full Evaluation Results

We provide the full results of Single-Bug and Multi-Bug evaluation with all four metrics in Table 7, 8, 9 and 10.

```
You will be provided with an original query and a data analysis code. Your task is to:
1. Read the Question carefully, determine whether the code has followed the query requirements, if so, further identify any errors in its data analysis process. If the code faithfully followed seemingly wrong data analysis practices explicitly stated in the Question. Deem it as correct.
2. Explain any errors found, including: Explanation: Explain why this is an error and what issues it may cause. Expected Outcome: Explain how this error will affect the data analysis results, such as misleading outcomes, degraded performance, or incorrect interpretations.
Output Format:
json
"is_error": "true/false",
"error_explanation":
"error_type": "Describe the type of error",
"explanation": "Detailed explanation of why this is an error and its impact",
"expected_outcome": "How this error will affect model performance or results",
"suggestions": "Specific suggestions for fixing the error",
"error_type": "Another error type if multiple errors exist",
"explanation": "Explanation for the second error", "expected_outcome": "Expected outcome for the second error",
"suggestions": "Suggestions for fixing the second error"
Important Notes:
1. Always provide the output in the exact JSON format specified above
2. Set "is_error" to "false" if no errors are found
3. If "is_error" is "false", provide an empty array for error_explanation
4. If "is_error" is "true", include all identified errors in the error_explanation array
5. Consider the original query requirements carefully, if the code follows the query's explicit requirements, even if they seem incorrect, consider it correct
```

Figure 10: The error verifying prompt in Data Annotation.

```
You will receive three components:
1. Original Query: A user query that contains specific requirements related to data analysis.
2. Correct Data Analysis Code: A working code snippet designed to analyze the data according to the original query.
3. CSV Information: Details about the structure content and sample data from the CSV file being analyzed.
Your task is to:
1. Identify sklearn and pandas code: Analyze the provided code and extract all lines where sklearn or pandas libraries are used. Organize these lines in a structured format.
2. Inject errors that will cause runtime interruptions: For EACH AND EVERY identified sklearn and pandas lines inject errors with the following guidelines:
Error Type: Inject errors that lead to runtime interruptions such as syntax errors attribute errors type errors or value errors.
Plausibility: The modified lines should still appear logical and plausible at first glance but contain mistakes that will cause the code to fail during execution.
Contextual alignment: Ensure the errors take into account the structure and content of the CSV file to create mistakes that are realistic and aligned with potential data issues.
Impact downstream processes: Errors should trigger runtime interruptions effectively halting the program before it completes execution.
3. Explain each error: For every injected error:
Describe why this is an error and the conditions under which it would fail.
Provide details on the likely runtime error e.g. KeyError ValueError AttributeError etc..
4. Output the structured results:
Provide the original sklearn and pandas code in a structured list.
Include the complete modified code with runtimeinterrupting errors injected.
Clearly explain each injected error in a concise and structured format.
Return your output in the following JSON format:
original_sklearn_pandas_code:
Original sklearn or pandas code line
...
errors:
code: Modified whole code file with the injected error
error_type: Specify the type of runtimeinterrupting error e.g. KeyError ValueError etc.
explanation: Describe why this is an error and the conditions under which it will cause a runtime interruption
```

Figure 11: The error injection prompt in Data Annotation.

SYSTEM PROMPT: You will be provided with an original query and a data analysis code. Your task is to:
1. Read the question carefully and identify if there are any logic error injected into the code.
2. For each logic error:
- Locate the Cause: Specify the exact line of code that causes the issue.
- Locate the Effect: Identify the line of code where the error will be triggered and the interpreter will throw an error.
- Error Description: Provide a concise description of the error message thrown by the Python Interpreter (not the full traceback).
Output Format:
json
cause_line: Specify the exact line of code causing the issue
effect_line: Specify the exact line of code where the error will be triggered
error_message: Provide a concise description of the error message thrown by the Python Interpreter not the full traceback
There will be only one error in the code. Output only ONE json dict in your response.

Figure 12: The single error evaluation prompt for tested models.

SYSTEM PROMPT: You will be provided with a data analysis code. Your task is to:
1. Read the code carefully and identify all logic errors injected into the code. There will be two or more logic errors in the code.
2. For each logic error you identify:
- Locate the Cause: Specify the exact line of code that causes the issue.
- Locate the Effect: Identify the line of code where the error will be triggered and the interpreter will throw an error or where the incorrect behavior is observed.
- Error Description: Provide a concise description of the error message thrown by the Python Interpreter not the full traceback. Focus on the type of error and the reason if possible from the output.
Output Format:
json
cause_line: Specify the exact line of code causing error 1
effect_line: Specify the exact line of code where error 1 is triggered
error_message: Concise error message for error 1 cause_line: Specify the exact line of code causing error 2
effect_line: Specify the exact line of code where error 2 is triggered
error_message: Concise error message for error 2 ... and so on for all identified errors There will be more than one error in the code. BUT output only ONE json block in your response.

Figure 13: The multi error evaluation prompt for tested models.

Model	Cause Line				Effect Line				Error Type				Error Message			
	P	R	F1	Acc	P	R	F1	Acc	P	R	F1	Acc	P	R	F1	Acc
gpt-4o	39.5	39.0	39.2	39.0	34.7	34.3	34.5	34.3	31.0	30.6	30.8	30.6	31.8	31.4	31.6	31.4
gpt-4o-mini	43.3	40.2	41.7	40.2	25.7	23.9	24.8	23.9	23.4	21.7	22.5	21.7	23.0	21.3	22.1	21.3
claude-3-5-sonnet	45.4	43.7	44.6	43.7	36.6	35.2	35.9	35.2	37.7	36.3	37.0	36.3	35.3	34.0	34.7	34.0
llama-3.1-8b-instant	32.4	25.2	28.4	25.2	18.2	14.2	15.9	14.2	9.9	7.7	8.6	7.7	9.2	7.2	8.0	7.2
llama-3.1-70b-versatile	45.7	42.5	44.0	42.5	31.4	29.3	30.3	29.3	21.9	20.4	21.1	20.4	22.5	20.9	21.7	20.9
llama-3.1-405b-instruct	46.9	41.7	44.1	41.7	35.2	31.3	33.1	31.3	32.9	29.3	31.0	29.3	32.9	29.3	31.0	29.3
Qwen2.5-7B-Instruct	31.0	29.3	30.1	29.3	20.4	19.3	19.8	19.3	11.3	10.7	11.0	10.7	11.6	10.9	11.2	10.9
Qwen2.5-32B-Instruct	43.5	40.9	42.1	40.9	32.4	30.5	31.4	30.5	26.3	24.7	25.5	24.7	26.3	24.7	25.5	24.7
Qwen2.5-72B-Instruct	43.8	41.6	42.6	41.6	38.1	36.2	37.1	36.2	29.0	27.5	28.2	27.5	28.8	27.4	28.1	27.4
deepseek-chat	50.6	48.3	49.4	48.3	36.2	34.5	35.4	34.5	37.6	35.9	36.7	35.9	36.4	34.7	35.5	34.7

Table 7: Overall evaluation results of Single-Bug Detection on DSDBench. P=Precision, R=Recall, F1=F1-Score, Acc=Accuracy.

Model	Cause Line				Effect Line				Error Type				Error Message			
	P	R	F1	Acc	P	R	F1	Acc	P	R	F1	Acc	P	R	F1	Acc
gpt-4o	20.5	20.3	20.4	20.3	10.5	10.4	10.5	10.4	3.6	3.6	3.6	3.6	4.7	4.7	4.7	4.7
gpt-4o-mini	11.3	11.2	11.2	11.2	2.7	2.7	2.7	2.7	2.2	2.2	2.2	2.2	0.8	0.8	0.8	0.8
claude-3-5-sonnet	12.5	12.3	12.4	12.3	4.2	4.1	4.1	4.1	1.9	1.9	1.9	1.9	2.5	2.5	2.5	2.5
llama-3.1-8b-instant	5.1	3.0	3.8	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
llama-3.1-70b-versatile	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
llama-3.1-405b-instruct	24.2	18.6	21.1	18.6	11.0	8.5	9.6	8.5	1.4	1.1	1.2	1.1	3.2	2.5	2.8	2.5
Qwen2.5-7B-Instruct	5.9	4.7	5.2	4.7	1.4	1.1	1.2	1.1	0.3	0.3	0.3	0.3	0.0	0.0	0.0	0.0
Qwen2.5-32B-Instruct	17.6	17.5	17.6	17.5	6.3	6.3	6.3	6.3	2.2	2.2	2.2	2.2	2.2	2.2	2.2	2.2
Qwen2.5-72B-Instruct	21.4	21.4	21.4	21.4	11.2	11.2	11.2	11.2	3.0	3.0	3.0	3.0	3.6	3.6	3.6	3.6
deepseek-chat	15.2	15.1	15.1	15.1	6.6	6.6	6.6	6.6	3.3	3.3	3.3	3.3	4.7	4.7	4.7	4.7

Table 8: Overall evaluation results of Multi-Bug Detection on DSDBench. P=Precision, R=Recall, F1=F1-Score, Acc=Accuracy.

Model	Cause Line				Effect Line				Error Type				Error Message			
	P	R	F1	Acc	P	R	F1	Acc	P	R	F1	Acc	P	R	F1	Acc
gpt-4o	35.8	35.4	35.6	35.4	31.6	31.2	31.4	31.2	33.7	33.3	33.5	33.3	33.7	33.3	33.5	33.3
gpt-4o-mini	42.7	39.6	41.1	39.6	31.5	29.2	30.3	29.2	27.0	25.0	25.9	25.0	24.7	22.9	23.8	22.9
claude-3-5-sonnet	37.0	35.4	36.2	35.4	27.2	26.0	26.6	26.0	34.8	33.3	34.0	33.3	32.6	31.2	31.9	31.2
llama-3.1-8b-instant	24.1	13.5	17.3	13.5	20.4	11.5	14.7	11.5	11.1	6.2	8.0	6.2	9.3	5.2	6.7	5.2
llama-3.1-70b-versatile	36.7	34.4	35.5	34.4	23.3	21.9	22.6	21.9	20.0	18.8	19.4	18.8	20.0	18.8	19.4	18.8
llama-3.1-405b-instruct	51.2	43.8	47.2	43.8	37.8	32.3	34.8	32.3	36.6	31.2	33.7	31.2	40.2	34.4	37.1	34.4
Qwen2.5-7B-Instruct	30.8	29.2	29.9	29.2	24.2	22.9	23.5	22.9	12.1	11.5	11.8	11.5	13.2	12.5	12.8	12.5
Qwen2.5-32B-Instruct	35.2	32.3	33.7	32.3	28.4	26.0	27.2	26.0	33.0	30.2	31.5	30.2	26.1	24.0	25.0	24.0
Qwen2.5-72B-Instruct	26.7	25.0	25.8	25.0	32.2	30.2	31.2	30.2	30.0	28.1	29.0	28.1	27.8	26.0	26.9	26.0
deepseek-chat	49.4	44.8	47.0	44.8	31.0	28.1	29.5	28.1	37.9	34.4	36.1	34.4	37.9	34.4	36.1	34.4
gemini-2.0-flash	49.4	42.7	45.8	42.7	37.3	32.3	34.6	32.3	38.6	33.3	35.8	33.3	41.0	35.4	38.0	35.4
deepseek-r1	51.6	49.0	50.3	49.0	51.6	49.0	50.3	49.0	56.0	53.1	54.5	53.1	57.1	54.2	55.6	54.2
o1-mini	46.2	43.8	44.9	43.8	38.5	36.5	37.4	36.5	46.2	43.8	44.9	43.8	49.5	46.9	48.1	46.9

Table 9: Comparison with large reasoning models (LRMs) on Single-Bug Detection. P=Precision, R=Recall, F1=F1-Score, Acc=Accuracy.

Model	Cause Line				Effect Line				Error Type				Error Message			
	P	R	F1	Acc	P	R	F1	Acc	P	R	F1	Acc	P	R	F1	Acc
gpt-4o	12.8	12.5	12.7	12.5	5.1	5.0	5.1	5.0	2.6	2.5	2.5	2.5	2.6	2.5	2.5	2.5
gpt-4o-mini	7.5	7.5	7.5	7.5	5.0	5.0	5.0	5.0	2.5	2.5	2.5	2.5	0.0	0.0	0.0	0.0
claude-3-5-sonnet	10.3	10.0	10.1	10.0	7.7	7.5	7.6	7.5	5.1	5.0	5.1	5.0	7.7	7.5	7.6	7.5
llama-3.1-8b-instant	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
llama-3.1-70b-versatile	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
llama-3.1-405b-instruct	23.3	17.5	20.0	17.5	16.7	12.5	14.3	12.5	6.7	5.0	5.7	5.0	6.7	5.0	5.7	5.0
Qwen2.5-7B-Instruct	3.3	2.5	2.9	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Qwen2.5-32B-Instruct	17.5	17.5	17.5	17.5	0.0	0.0	0.0	0.0	5.0	5.0	5.0	5.0	2.5	2.5	2.5	2.5
Qwen2.5-72B-Instruct	22.5	22.5	22.5	22.5	17.5	17.5	17.5	17.5	2.5	2.5	2.5	2.5	5.0	5.0	5.0	5.0
deepseek-chat	12.8	12.5	12.7	12.5	7.7	7.5	7.6	7.5	5.1	5.0	5.1	5.0	7.7	7.5	7.6	7.5
o1-mini	37.8	35.0	36.4	35.0	24.3	22.5	23.4	22.5	18.9	17.5	18.2	17.5	18.9	17.5	18.2	17.5
gemini-2.0-flash	21.1	20.0	20.5	20.0	13.2	12.5	12.8	12.5	0.0	0.0	0.0	0.0	2.6	2.5	2.6	2.5
deepseek-r1	32.5	32.5	32.5	32.5	25.0	25.0	25.0	25.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0

Table 10: Comparison with large reasoning models (LRMs) on Multi-Bug Detection. P=Precision, R=Recall, F1=F1-Score, Acc=Accuracy.