Towards Effectively Leveraging Execution Traces for Program Repair with Code LLMs

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Abstract

Large Language Models (LLMs) show promising performance on various programming tasks, including Automatic Program Repair (APR). However, most approaches to LLM-based APR are limited to the static analysis of the programs, while disregarding their runtime behavior. Inspired by knowledge-augmented NLP, in this work, we aim to remedy this potential blind spot by augmenting standard APR prompts with program execution traces. We evaluate our approach using the GPT family of models on three popular APR datasets. Our findings suggest that simply incorporating execution traces into the prompt provides a limited performance improvement over trace-free baselines, in only 2 out of 6 tested dataset / model configurations. We further find that the effectiveness of execution traces for APR diminishes as their complexity increases. We explore several strategies for leveraging traces in prompts and demonstrate that LLM-optimized prompts help outperform trace-free prompts more consistently. Additionally, we show tracebased prompting to be superior to finetuning a smaller LLM on a small-scale dataset; and conduct probing studies reinforcing the notion that execution traces can complement the reasoning abilities of the LLMs.

1 Introduction

Automatic Program Repair (APR) is a critical challenge in software engineering, aiming to reduce human effort in debugging and fixing software defects. Software bugs can lead to significant security vulnerabilities, financial losses, and system failures, necessitating efficient repair mechanisms. While large language models (LLMs) have demonstrated remarkable capabilities in generating and modifying code, their effectiveness in APR remains constrained by their reliance on static code analysis.

```
9
   ### Buggy Program:
10 def search(x, seq):
       index = 0
11
       def helper(index):
12
           if not seq:
13
14
               return 0
           elif x <= seq[index]:</pre>
15
               return index
16
17
           else:
18
               if index + 1 >= len(seq):
                   return index + 1
19
20
               else:
21
                   return helper(index+1)
22
23 ### Failing test case:
24 result = search(42, (-5, 1, 3, 5, 7, 10))
25 assert result == 6,
   → 'Expected 6 but got %s' % result
26 AssertionError: Expected 6 but got None
27
28 ### Execution trace:
29 Starting var:.. x = 42
30 Starting var:.. seq = (-5, 1, 3, 5, 7, 10)
31
   call
              10 def search(x, seq):
32 line
               11
                      index = 0
33 New var:.... index = 0
              12
                     def helper(index):
34 line
35 New var: ..... helper = <function search.<locals>
   \hookrightarrow .helper at 0x7fd455b89040>
              12
                      def helper(index):
36 return
37 Return value:.. None
```

Figure 1: Example buggy program, a failing test case and its execution trace. While the failure message simply indicates the output is wrong, the execution trace provides a detailed explanation how it was produced.

Debugging complex software issues often necessitates a deeper understanding of the program's execution behavior, including variable modifications and control flow changes, which conventional Deep Learning-based and LLM-based APR approaches fail to capture effectively (Xia and Zhang, 2022; Jiang et al., 2023; Tian et al., 2023; Sutton et al., 2023).

Recent advancements in knowledge-augmented NLP have emphasized integrating external information into language models to enhance reasoning and

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accuracy. Inspired by this, our research explores augmenting LLM-based automated program repair (APR) with program execution traces—structured runtime data that reveal a program's actual behavior. These traces provide diagnostic insights beyond static code analysis. By embedding them into repair prompts, we aim to bridge the gap between static and dynamic program understanding, aligning with trends in knowledge-augmented NLP that leverage external sources to enhance language model capabilities.

We frame our work in terms of three research questions (RQs). In RQ1 (Section 3.2), our objective is to quantify the gains from incorporating execution traces into the APR prompt over the prompts only containing the failing test case as well as the trace-free chain-of-thought prompting baseline (Chen et al., 2023). We find that simply adding the execution trace does not consistently outperform trace-free prompts.

To inform a more finegrained approach, in RQ2 (Section 3.3), we analyze the relationship between trace complexity and the likelihood of the LLM producing a working fix. To measure this complexity, we consider two parameters: trace length and the number of variable modifications. We find that the effectiveness of trace-based prompts decreases with the growing length and number of variable assignments.

Motivated by this finding, in RQ3 (Section 4), we aim at improving the consistency of trace-based APR by experimenting with three different representations of execution traces: traces in a collated format, LLM-optimized traces, and a trace representation conditionally selected based on querying the LLM's confidence. We find that LLMoptimized trace-based prompts provide the most consistent results with respect to program repair.

We additionally perform two follow-up studies: in the first, we compare our trace-based prompting approach with a fine-tuned baseline inspired by TraceFixer (Bouzenia et al., 2023); and in the second one, we directly probe the LLM on two trace understanding tasks.

The rest of the paper is organized as follows. In Section 2, we discuss the related work and how it differs from our approach. Section 3 details our methodological setup and covers RQ1 and RQ2. Section 4 covers RQ2 and in Section 5, we discuss the additional studies.

2 Related Work

Recent work looked into augmenting code LLMs with execution information to improve performance on downstream tasks, including APR.

SelfAPR (Ye et al., 2022) proposed to use compiler and test diagnostics during self-supervised training of the language model for improving APR. Additionally, several works have proposed the use of execution traces for pretraining code LLMs. In TRACED (Ding et al., 2023), authors finetuned a BERT-like model to predict execution paths and quantized values, which allowed it to outperform an AST-based UniXcoder (Guo et al., 2022) on clone detection and vulnerability detection. Whereas, Liu et al.'s program state prediction pre-training improved code search and generation (Liu et al., 2023). Finally, TraceFixer, based on CodeT5 and finetuned with execution traces, showed a 13% improvement in APR on synthetic bugs over the codeonly baseline but struggled with real bugs, hinting at potential generalization limitations (Bouzenia et al., 2023).

Among training-free approaches, Self-Debug (Chen et al., 2023) improved program generation by generating code explanations directly from the LLM, in a chain-of-thought fashion, as part of solving the APR task.

To the best of our knowledge, all of these works do not consider the effect of putting execution traces in the prompt of a pretrained LLM.

3 Analyzing the Impact of Execution Traces on Program Repair

In this section, we analyze the effects of adding traces in the LLM prompt on APR performance, compared to two trace-free baselines (Ye et al., 2022), (Chen et al., 2023). Additionally, we perform a differentiated analysis of APR performance based on trace complexity. We formulate the corresponding two research questions as follows.

RQ1. Are prompts with execution traces more effective at program repair than prompts without traces?

RQ2. How does trace complexity affect the effectiveness of trace-based prompts?

3.1 Set Up

Datasets. We surveyed 15 popular datasets across Python, Java, C++, and other major languages, focusing on dataset size, program diversity, unit test availability, and dataset origin (e.g., self-contained algorithmic problems like CodeNet (Puri et al., 2021) or full open-source projects like PyTrace-Bugs (Akimova et al., 2021)). While realistic datasets are ideal, evaluating them requires significant manual effort due to complex dependencies. Algorithmic datasets offer advantages like manageable length and easily testable, self-contained functions, enabling trace generation through execution.

We selected three APR datasets: Refactory (Hu et al., 2019), RunBugRun (Prenner and Robbes, 2023), and HumanEval-Java (Jiang et al., 2023). Refactory includes nearly 2000 faulty Python programs submitted by students, enabling coverage of diverse mistakes. RunBugRun, derived from CodeNet, contains a quarter million submissions for 4000 distinct problems; we sampled 1000 Python bugs for evaluation. HumanEval, originally for Python, was adapted into HumanEval-Java, injecting synthetic bugs for APR testing.

Each dataset includes at least 5 test cases per problem. For RunBugRun, we implemented a wrapper to handle input/output via standard input and print statements for accurate result comparison. Models. With the landscape of state-of-the-art code LLMs rapidly changing, we chose use two most widely studied commercial models from OpenAI for ease of comparison with other work: GPT-3.5 Turbo (Ouyang et al., 2022) and GPT-4 (OpenAI, 2023). These two models represent two different performance tiers both in terms of the number of parameters and different release timelines, hence, studying these models could shine the light on the LLMs' evolving ability to reason about program execution across product generations. While there is undoubtedly scope for including more proprietary as well as open source models, given our narrow focus on traces, we leave this to be explored in future work.

Execution Traces Generation. As the program is being executed, it is possible to step through it programmatically, while also capturing every change to the function's variables, akin to interactive debugging. PySnooper(pys) library for Python provides this functionality via a decorator that can be added to a function of interest to automatically log state changes, such as variable initialization and modification, subroutine calls, returned values, and runtime exceptions. Crucially, each state change reference a specific line of code on which it occurred. Examples of execution traces are given in the Appendix A.2. Before appending traces to

the prompt we perform basic postprocessing, including the removal of timestamps and stripping of terminal formatting command sequences.

Prompt Types. We follow the instruction template for complete function generation used by Xia et al. (2023), expanding it with two additional types of information, namely, a failing test case (henceforth, referred to as *Error Prompts*) and a program execution trace (referred as *Trace Prompts*). We offer our rationale for these choices, along with other prompt types considered, in Appendix B.

To ensure the prompt and response fit within the GPT model context size, we truncate the content of the prompt if the number of lines exceeds 200. We have added an example of all the prompts in Section A in the Appendix.

Baseline. We consider the Prompt-based baseline Self-Debug. With this baseline, we explore prompting LLMs using execution traces generated by LLMs themselves (instead of actual program execution traces). This baseline inspired by Self-Debugging (Chen et al., 2023) where LLMs are prompted to debug their own generated code. In particular, we draw inspirations from the Explanation step of this work where the model is asked to generate execution traces for a predicted code. We tailored Self-Debugging's prompts to fit our usecase: in our prompts, we provide LLMs with a program and a test case feedback, and ask them to trace through the execution of the program and determine the needed fix, and correct the function accordingly. We perform these experiments with both GPT-3.5 and GPT-4.

Metrics. In previous work on APR, models are evaluated either at the granularity of distinct bugs solved (Xia et al., 2023; Jiang et al., 2023) or individual test cases passed (Tian et al., 2023). In contrast, we generate multiple prompts for each program tailored to a specific failing test case and its corresponding execution trace (e.g., A.1, A.2). Rather than aggregating predictions from multiple samples, we generate a single prediction per test case-specific prompt and aggregate across prompts when computing metrics. The key metrics are Correct Fix Accuracy (CFA), the percentage of fixes passing all test cases, and Correct Program Accuracy (CPA), the percentage of programs with at least one correct fix. We do not report test caselevel accuracy, as it can be too lenient and doesn't account for variations in the number of test cases per program.

Model	Dataset	Method	# FPs	# Fixes	# CF	# CP	CFA	CPA
	Refactory	Self-Debug	138	579	244	73	0.421	0.529
		Error Prompt			304	91	0.525	0.659
		Trace Prompt			295	87	0.509	0.630
	HumanEval-Java	Self-Debug	157	634	210	75	0.331	0.477
GPT-3.5		Error Prompt			241	85	0.380	0.541
		Trace Prompt			212	86	0.334	0.547
	RunBugRun	Self-Debug		559	151	132	0.270	0.289
		Error Prompt	456		260	221	0.465	0.484
		Trace Prompt			249	216	0.445	0.473
	Refactory	Self-Debug	138	579	414	117	0.715	0.847
		Error Prompt			458	122	0.791	0.884
		Trace Prompt			427	113	0.737	0.818
	HumanEval-Java	Self-Debug	157	634	312	105	0.492	0.668
GPT-4		Error Prompt			313	104	0.493	0.662
		Trace Prompt			324	112	0.511	0.713
	RunBugRun	Self-Debug	456	559	337	287	0.602	0.629
		Error Prompt			296	264	0.529	0.578
		Trace Prompt			312	266	0.558	0.583

Table 1: **RQ1 Quantitative Results.** FP = Faulty Programs, CF = Correct Fixes, CP = Correct Programs, CFA = Correct Fix Accuracy, CPA = Correct Program Accuracy.

3.2 RQ1. Are prompts with execution traces more effective at program repair than prompts without traces?

In this research question, our objective is to evaluate the effectiveness of including program execution traces into LLM prompts, for solving APR tasks, compared to the baselines. The effectiveness is measured through reporting CPA and CFA. The evaluation results can be found in Table 1. The number of faulty programs, number of fixes, and total test cases are the same for all types of prompts per each dataset.

Across the board, the Self-Debug baseline performs the worst except in one configuration using GPT-4 on the RunBugRun dataset. This general outcome is unsurprising as having the LLM generate an execution trace could introduce hallucination and thus undermine the resulting fixes. For both GPT-3.5 and GPT-4 on the Refactory dataset, prompts including just a failing test case decisively outperform ones with execution traces by multiple percentage points on both fix accuracy and program accuracy.

On the HumanEval-Java dataset with GPT-3.5, error-only prompts are only ahead of trace-based prompts in terms of fix accuracy but are slightly behind in program accuracy. Meanwhile, with GPT-4, trace-based prompts consistently outperform error-only prompts on both metrics. Results on RunBugRun paint a similar picture, where GPT- 3.5 doesn't seem to benefit from including traces, while GPT-4 gets a tangible lift over the error-only prompts. Overall, on two out of three datasets, trace-based prompts significantly improve the ability of GPT-4 to generate working bug fixes.

While GPT-3.5 lagging behind in terms of absolute scores irrespective of prompt type is expected, more broadly, its inability to benefit from execution traces (even degraded performance) could highlight a qualitative generational gap when it comes to emergent abilities of LLMs. Notwithstanding, there remain a few unexplained results, such as the lack of performance gain from using traces on the Refactory dataset and the unusually strong performance of the Self-Debug baseline in one particular configuration. To gain a fine-grained understanding, in the next research question, we focus on studying the varying complexity of execution traces and how they affect downstream APR performance.

RQ1 Summary. Trace prompts do not consistently outperform Error Prompts on program repair.

3.3 RQ2. How does trace complexity affect the effectiveness of trace-based prompts?

Unlike other elements of the prompt, execution traces are dynamic in nature and are highly dependent on a particular input as much as the program itself. Additionally, execution traces can be dramat-

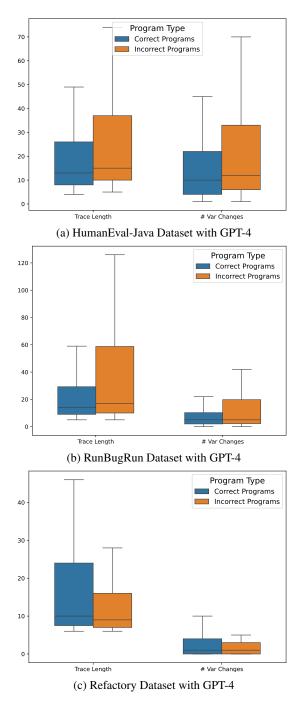


Figure 2: Distributions of trace lengths and variable changes across correct vs incorrect program fixes generated by GPT-4. Analysis for GPT-3.5, showing a similar trend, is given in the appendix.

ically different in the presence of a runtime error, compared to when the function finishes executing correctly (even if the returned value itself is wrong). Thus, variations in trace complexity could be a crucial factor in how beneficial their inclusion is in the prompt. On the one hand, traces that are too short may not provide much information beyond what is already conveyed by the program itself and the failing test case. On the other hand, overly long and complex traces may overwhelm LLMs' long context and ultimately confuse it. We believe there is a sweet spot at which the inclusion of traces is most beneficial. As such, we observed great variability with respect to the overall trace length, as well as in the number and type of individual state changes.

To gain insights into nuanced differences among our evaluated datasets, we compute the statistics of overall trace length and the number of variable modifications in all prompts, while differentiating by whether the resulting fix was correct (Figure 2). For both the HumanEval-Java and RunBugRun datasets, median¹ trace length and number of variable modifications were significantly higher for failing fixes than for the correct ones. This corroborates our presupposition that longer traces could undermine rather than help APR. Conversely, in the Refactory dataset, somewhat contrary to our intuitions, for failing fixes median trace length were actually lower than for successful fixes. Regarding the number of variable modifications, the median was just one, compared to 5 in RunBugRun. This disparity implies variable modifications could play a key role in the effectiveness of a trace for APR.

RQ2 Summary. The prompts having longer execution traces have a lower chance of generating a correct fix.

4 Impact of Modified Traces

As we find that longer trace length could have a negative impact in the effectiveness of GPT models, we focus on modified trace strategies and their impact on the effectiveness of the model. In this section, we discuss one research question.

RQ3. Can the format of traces be optimized to guarantee gains for APR?

4.1 Modified Traces

Collated Execution Traces. Even though execution traces for both languages reference code lines from the original program, they are placed in the standalone section of the prompt, separate from the program itself. In order to thoroughly ablate

¹In all datasets and for both correct and failing fixes we observed the presence of extremely long traces in excess of 10,000 entries. Additionally, a significant number of trace prompts got truncated (5% for Refactory and almost 10% for RunBugRun).

trace format, we experimented with combining the two by placing each trace entry directly to its corresponding line of code as an inline comment ². The rationale behind this design choice is to consolidate the two types of information in the common location, potentially freeing the LLM from having to constantly cross-reference between them.

LLM-Optimized Execution Traces (OPT). While in a general case deterministic traces provide valuable information regarding variable changes, logging every single event is not always ideal. In scenarios such as infinite loops, traces end up repeating the same information, while also unboundedly growing in length. It can thus be desirable to optimize potentially lengthy traces by condensing superfluous information. To optimize execution traces, we prompt a long context GPT4-32k model with the deterministic execution trace and an instruction to generate a shorter version of it, optimized for downstream APR.

Confidence Based Prompt Selection (Conf OPT). In addition to modifying the format or content of the prompt itself, we experimented with a simple prompt routing mechanism based on pre-querying LLM's confidence about correctly solving a program repair task using the deterministic trace. If the confidence level is low, we fallback onto using an LLM-optimized trace instead.

We have considered multiple ways to find the confidence value of the model. One possible way is to prompt the model to find whether it's confident or not (boolean) to use a specific prompt to repair a program. But on a small prompt set, we find that the model outputs that it is always confident for all inputs. Additionally, another way is to feed both prompts and ask the model for which prompt it is more confident to repair the program. However, based on the findings of recent work (Huang et al., 2023), LLM might be biased for a specific position (prompt one or prompt two). Hence, based on the findings of Huang et al. (Huang et al., 2023), we use a Likert-scale based confidence score. Given a score range of 1-5, if the confidence score provided by the model is less than 3, we consider that the model has low-confidence. The approach is shown in Figure 3.

Trace-length Based Prompt Selection (TRL OPT). As we have found through investigating

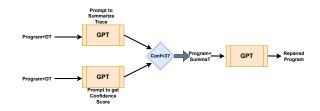


Figure 3: The Flow of Conditional Selection of Traces

RQ2 that trace prompts work well if the trace length is within a specific range; hence, switching to a different prompt given a longer trace might be beneficial. In this technique, instead of using a confidence score like Conf OPT, we use trace length for routing between prompts. The routing is investigated in two settings: trace prompt and OPT prompt, and trace prompt and error prompt. If the trace length is less than N, we use trace prompt, or we use OPT prompt or error prompt based on the setting. We use the following N values for the experiment: 25,30,35,40,45,50.

4.2 RQ3 Results.

The results could be found in Table 2. For ease of comparison, for each dataset and model we include the best performing strategy from RQ1, which could be either error prompt, trace prompt or the Self-Debug baseline. Of the three trace modification strategies, LLM-Optimized prompts (OPT) provide the most consistent performance gains on both CFA and CPA metrics. With respect to CPA, for all dataset and model pairs, OPT is among the top three performing prompting techniques. The CFA values for OPT are even more commendable, whereas, for three out of six model-dataset pairs, OPT has the best CFA (second best in the other three). Furthermore, this confirms our implication from RQ2 that less complicated traces are better for prompting for program repair tasks.

For confidence-based prompt selection, while we find the CFA and CPA values are comparatively better for GPT4, the performance in GPT3.5 is worse. This would imply that GPT-4 is significantly better in providing confidence scores for prompts than GPT-3.5. But, as the performance is significantly worse than OPT on average, the application of the method for GPT-4 is still not reliable.

For trace length-based prompt selection, we only report the best results in the table. We have two findings here; first, although routing could improve the CFA and CPA values more than individual

²In case of multiple passes through the same line e.g., variable changes within a loop, we concatenate each of the traced events by a new line, providing a full history of state changes at that line.

Metric	Method		GPT-3.5		GPT-4			
Metric	Method	Refactory	HumanEval-Java	RunBugRun	Refactory	HumanEval-Java	RunBugRun	
	Collated Trace	0.452	0.391	0.381	0.656	0.531	0.483	
CFA	OPT Trace	0.502	0.430	0.472	0.753	0.572	0.570	
CFA	Conf OPT Trace	0.368	0.380	0.429	0.735	0.549	0.527	
	TRL OPT Trace (EP)	0.490	0.312	0.457	0.742	0.492	0.549	
	TRL OPT Trace (OPT)	0.493	0.353	0.466	0.737	0.473	0.574	
	RQ1 Best	0.525	0.380	0.465	0.791	0.511	0.602	
	Collated Trace	0.587	0.497	0.407	0.818	0.681	0.508	
СРА	OPT Trace	0.601	0.535	0.497	0.862	0.713	0.589	
CPA	Conf OPT Trace	0.384	0.522	0.453	0.847	0.732	0.550	
	TRL OPT Trace (EP)	0.623	0.528	0.484	0.826	0.694	0.589	
	TRL OPT Trace (OPT)	0.623	0.573	0.491	0.826	0.675	0.603	
	RQ1 Best	0.659	0.547	0.484	0.884	0.713	0.629	

Table 2: RQ3 Quantitative Results. CFA = Correct Fix Accuracy, and CPA = Correct Program Accuracy.

prompts, we find that only for the GPT-3.5 model and HumanEvalJava dataset could routing get the best CPA score among all considered techniques. Second, changing the value of N would have a limited impact on CFA and CPA values. Overall, we could not find any strong result suggesting that routing between techniques based on trace length might be significantly beneficial. Detailed results could be found in Figures 6 and 7 (in Appendix).

Lastly, collated trace prompts disappointingly do not provide an improvement over trace prompts. One possible explanation is a lack of exposure to this format during LLM training as code doesn't normally include inline comments about state changes. Second, inline traces within loops can "stretch" the length of the program quite a bit, possibly diluting LLMs attention to the continuation of the program after the loop. In our probing studies of LLM trace understanding, we find that, indeed, LLMs struggle to keep up with variable changes across multiple iterations. Finally, the problem of truncation becomes more severe with collated traces, as not just the trace but also part of the original problem could be excluded from the prompt.

RQ3 Summary. Optimized trace prompt is the most consistent type of prompting technique, specifically for CFA metric.

5 Additional Studies

5.1 Trace-based prompting compared to finetuning a smaller model.

In this RQ, we focus on evaluating if fine-tuning a small-sized LLM would generate better results w.r.t program repair rather than prompting GPT models with different prompts. For that purpose, we

fine-tune the deepseek-coder-1.3b-instruct ³ model with training data extracted from HumanEval-Java and RunBugRun datasets. Finally, we compare the program repair performance of fine-tuning and prompting-based techniques on test data.

Finetuning Setup. Our finetuning approach is inspired by TraceFixer (Bouzenia et al., 2023), which finetunes a CodeT5 model using the buggy program's code, its execution trace, and the desired state of the program. As we didn't have access to TraceFixer's code, we implemented our own finetuning pipeline. In our case, the input to the model consists of a buggy program, the failing test case results, and corresponding execution traces. During training, the correct version of the program is included in the prompt, while during inference it is omitted, to be filled in by the model. For each dataset, 80% of the problems are randomly selected for training, and the rest are reserved for testing. This accounts for 459 samples for RunBugRun and 517 samples for HumanEval-Java datasets. We use the training settings and parameters suggested by deepseek-coder developers to finetune this model. Details of these parameters can be found in the model's repo.

Result. Figure 4 shows the results. For comparison purposes, we calculate CPA and CFA for prompting-based techniques on the same test programs. It can be noted that all the prompting techniques outperform fine-tuned model's CPA and CFA. It is observed that models fine-tuned with and without trace show lower CPA and CFA than prompting-based techniques. One of the reasons behind the results might be the limited training data for each task. Also, the TraceFixer technique showed better results in the original work, but the number of training examples for TraceFixer was

³https://github.com/deepseek-ai/DeepSeek-Coder

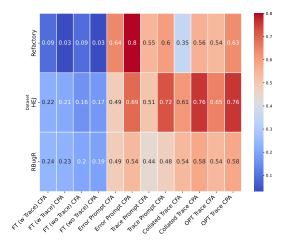


Figure 4: CPA and CFA of Prompting-Based Techniques vs. Model Fine-Tuned for APR Tasks.

significantly higher, too. In our future work, we plan to use a larger training dataset and larger models for finetuning.

5.2 Probing Studies of Trace Understanding

To gain insights into the observed lack of improvement in APR performance using collated traces and results from using traces for APR in general, we investigate two additional questions via small-scale probing experiments.

Can the LLM align the program with its execution trace? We directly measure the LLM's ability to perform trace collating given a standalone program and its execution trace. The rationale behind this experiment is that if an LLM can do this task with high accuracy, then there is no added benefit of adding collating traces into prompts.

Can the LLM infer the execution trace from the program alone? Although the Self-Debug approach implicitly traces through the program's execution, it is never formally evaluated. If an LLM can accurately generate a program's execution trace, then adding such a trace into the prompt would understandably not provide additional value for APR. Prompts used for each task can be found in Appendix C.2.

For both of these experiments we used GPT-4 on a subset of programs from the Refactory dataset. Since trace prediction behavior can be different depending on whether a function executes successfully or raises an error, for each experiment we differentiate between traces produced for working and failing programs. In addition, due to a limited number of distinct problems in Refactory, we additionally evaluate on the Geeks-for-geeks dataset⁴. To evaluate the LLM's output, we compute a diff against the ground truth trace or collated trace/program and report the exact match rate, after light post-processing, in Table 3 of Appendix C.1.

Based on these results, trace collating accuracy reaches 88% on reference Refactory programs, however it degrades by nearly ten percent on programs containing failures. Furthermore, on the more diverse Geeks for geeks dataset, which also eliminates the possibility of prompt leakage, collating performance sharply decreases to just 45%.

Prediction of a program's execution trace by an LLM from scratch is a significantly more challenging task compared to merely modifying the format of the trace. As a result, the rate of zero-diff trace predictions does not exceed 50% in the case of reference Refactory programs and is further halved for programs containing failures. Across the Geeks for geeks dataset, only 15% of generated traces perfectly match the ground truth. We provide qualitative analysis of a manually reviewed sample of diffs in the appendix.

Despite the impressive ability of GPT-4 at manipulating execution traces neither of the two tasks appear to be trivially solvable. Hence, we conclude real execution traces can contribute information for downstream tasks not yet easily inferrable by strong LLMs such as GPT-4.

6 Conclusion

In this study, we examined the impact of incorporating program execution traces into prompts on the program repair capabilities of the GPT model family. Our findings indicate that trace-based prompts do not consistently outperform error-based prompts; their effectiveness varies with the dataset and LLM used. Analysis reveals that longer traces and more variable assignments reduce prompt effectiveness. Using this insight, we developed variations of trace-based prompts, finding that LLMoptimized traces offer more consistent improvements without limiting trace complexity heuristically. We validated our results against a fine-tuned baseline and found that LLMs have limited capacity for trace generation, explaining the weaker performance of the Self-Debug baseline and highlighting the potential utility of traces in code tasks.

⁴https://github.com/facebookresearch/ TransCoder

7 Disclaimer

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A Different Prompt Types

A.1 Error Prompt

```
1 ### Provide a fix for the buggy function.
   ### Buggy Function:
2
   def sort_age(lst):
3
       return lst.sort(key = lambda x: x[1])
4
5
6 ### Failing Test Case:
    Traceback (most recent call last):
7
     File "temp.py", line 13, in <module>
8
        result = sort_age([('F', 18), ('M', 23), ('F', 19), ('M', 30)]); assert result == [('M', 30),
        \rightarrow ('M', 23), ('F', 19), ('F', 18)], 'Expected [(\'M\', 30), (\'M\', 23), (\'F\', 19), (\'F\', \rightarrow 18)] but got %s' % result
10 AssertionError: Expected [('M', 30), ('M', 23), ('F', 19), ('F', 18)] but got None
11
```

A.2 Trace Prompt

```
1 ### Provide a fix for the buggy function.
2 ### Buggy Function:
   def sort_age(lst):
3
        return lst.sort(key = lambda x: x[1])
4
5
   ### Failing Test Case:
6
    Traceback (most recent call last):
7
      File "temp.py", line 13, in <module>
8
        result = sort_age([('F', 18), ('M', 23), ('F', 19), ('M', 30)]); assert result == [('M', 30),

→ ('M', 23), ('F', 19), ('F', 18)], 'Expected [(\'M\', 30), (\'M\', 23), (\'F\', 19), (\'F\',
9
        10 AssertionError: Expected [('M', 30), ('M', 23), ('F', 19), ('F', 18)] but got None
11
12 ### Function Execution Trace:
   Source path:... temp.py
13
14 Starting var:.. lst = [('F', 18), ('M', 23), ('F', 19), ('M', 30)]
                 10 def sort_age(lst):
15 call
16 line
                     return lst.sort(key = lambda x: x[1])
                 11
17Modified var:..lst = [('F', 18), ('F', 19), ('M', 23), ('M', 30)]18return11return lst.sort(key = lambda x: x[1])
19 Return value:.. None
```

A.3 Collated Prompt

```
1 ### Provide a fix for the buggy function, annotated with its execution trace of the below failing
   → test case.
2 ### Buggy Function (execution states indicated via inline comments):
3 # Starting var:.. lst = [('F', 18), ('M', 23), ('F', 19), ('M', 30)]
4 def sort_age(lst): # Call def sort_age(lst):
     lst.sort(key=lambda x: x[1],reverse=True) # Modified var:.. lst = [('M', 30), ('M', 23), ('F',
5
     \rightarrow 19), ('F', 18)]
     print(lst) # Return print(lst)
6
     # Return value:.. None
7
8
9 ### Failing Test Case:
10 [('M', 30), ('M', 23), ('F', 19), ('F', 18)]
11 Traceback (most recent call last):
     12
13
       \rightarrow ('M', 23), ('F', 19), ('F', 18)], 'Expected [(\'M\', 30), (\'M\', 23), (\'F\', 19), (\'F\', \rightarrow 18)] but got %s' % result
14 AssertionError: Expected [('M', 30), ('M', 23), ('F', 19), ('F', 18)] but got None
```

```
A.4 OPT Prompt
```

```
2 ### Provide a fix for the buggy function.
3 ### Buggy Function:
4 def sort_age(lst):
5 lst.sort(key=lambda x: x[1],reverse=True)
6 print(lst)
7
```

- 8 ### Failing Test Case:
- 9 [('M', 30), ('M', 23), ('F', 19), ('F', 18)]
- 10 Traceback (most recent call last):
- II File "temp.py", line 15, in <module>
- 13 AssertionError: Expected [('M', 30), ('M', 23), ('F', 19), ('F', 18)] but got None
- 14 ### Function Execution Trace:Source path: temp.py
- 15 Function: sort_age(lst)
- 16 Input: lst = [('F', 18), ('M', 23), ('F', 19), ('M', 30)]
- 17 Line 12: Sorted list based on age in descending order
- 18 Updated 1st: [('M', 30), ('M', 23), ('F', 19), ('F', 18)]
- 19 Line 13: Printed sorted list
- 20 Return: None
- 21

B Rationale behind prompt choice and other prompts considered.

In our preliminary experiment error-based prompts always performed better than program-only prompts. Hence, we use Error Prompts as a point of comparison for Trace Prompts, foregoing prompts only containing the buggy program. Furthermore, we explored the option of including all failing test cases in the same prompt, however that did not provide a lift compared to a single test case, and overall performed slightly worse. We hypothesize multiple test cases could be more helpful for program generation to help define the space of valid solutions, whereas in APR the buggy function itself provides a bulk of information for fixing a bug, and a single failing test case, while inexhaustive, is generally sufficient for setting the LLM on the right path to finding a fix. The use of few-shot prompts, while feasible for improving the accuracy of error-based prompts, is problematic for traces as it can greatly increase the overall length of the prompt, potentially exceeding the 8k context window.

C Comparison of Refactory Fixes Generated by GPT 3.5 for Error and Trace Prompts

```
### Provide a fix for the buggy function.
1
2 ### Buggy Function:
   def sort_age(lst):
3
       return lst.sort(key = lambda x: x[1])
4
5
6 ### Failing Test Case:
   Traceback (most recent call last):
7
8
     File "temp.py", line 13, in <module>
       result = sort_age([('F', 18), ('M', 23), ('F', 19), ('M', 30)]); assert result == [('M', 30),

↔ ('M', 23), ('F', 19), ('F', 18)], 'Expected [(\'M\', 30), (\'M\', 23), (\'F\', 19), (\'F\',

↔ 18)] but got %s' % result
9
10 AssertionError: Expected [('M', 30), ('M', 23), ('F', 19), ('F', 18)] but got None
11
12
   ### Function Execution Trace:
13 Source path:... temp.py
14 Starting var:.. lst = [('F', 18), ('M', 23), ('F', 19), ('M', 30)]
15 call
               10 def sort_age(lst):
   line
                11
                      return lst.sort(key = lambda x: x[1])
16
   Modified var:.. lst = [('F', 18), ('F', 19), ('M', 23), ('M', 30)]
17
18 return 11 return lst.sort(key = lambda x: x[1])
19 Return value:.. None
1 # GPT 3.5 EP Response:
                                                        1 # GPT 3.5 TP Response:
   '''The issue with the buggy function is that
                                                        2 '''To fix the buggy function, we need to make
2
3 the `lst.sort()` method modifies the list
                                                        3 two changes: 1. Instead of returning the
4 in-place and does not return a sorted list.
                                                        4 result of the `lst.sort()` method, we need
5 To fix this, we can modify the function to
                                                        5 to return the sorted list itself. 2. We need
6 first sort the list using `lst.sort()` and
                                                        6 to sort the list in descending order by
7 then return the sorted list by simply
                                                        7 modifying the sorting key lambda function to
                                                        8 `lambda x: -x[1]`. Here is the fixed version
9 of the function:'''
8 returning the original list `lst`. Here's
9 the fixed function:''
10
                                                        10
11 def sort_age(lst):
                                                        ii def sort_age(lst):
       lst.sort(key=lambda x: x[1])
                                                                lst.sort(key=lambda x: -x[1])
12
                                                       12
       return 1st
                                                                return 1st
13
                                                        13
14
                                                        14
   '''Now, running the failing test case
                                                        15 '''This will return the correct sorted
15
16 should give us the expected output:'''
                                                            \rightarrow list.''
```

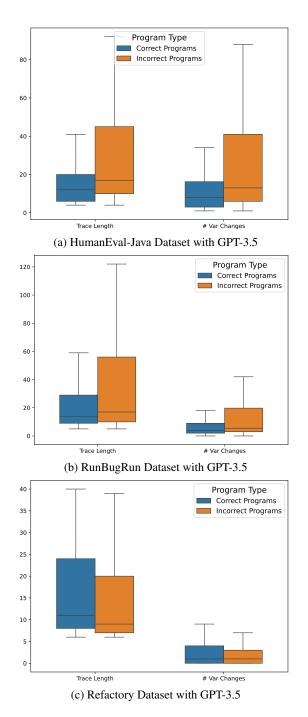
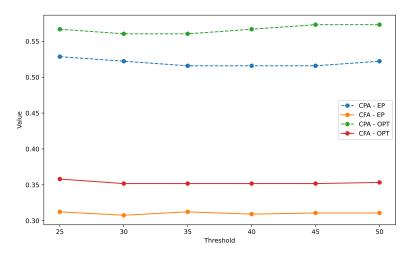
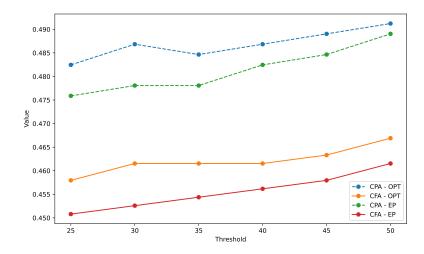


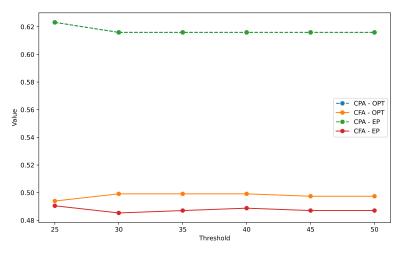
Figure 5: Distributions of trace lengths and variable changes across correct vs incorrect program fixes generated by GPT-3.5



(a) HumanEval-Java Dataset with GPT-3.5



(b) RunBugRun Dataset with GPT-3.5



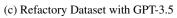
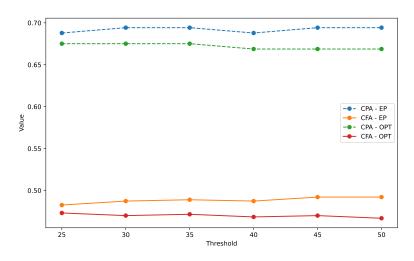
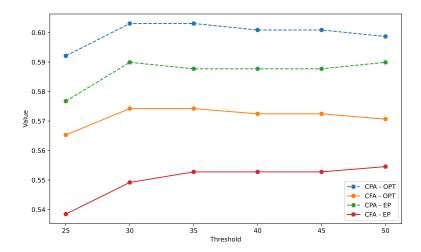


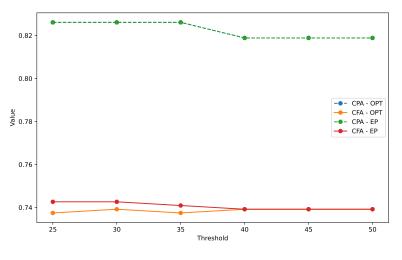
Figure 6: Ablations of trace length threshold values used with the routing strategy for GPT3.5



(a) HumanEval-Java Dataset with GPT-4



(b) RunBugRun Dataset with GPT-4



(c) Refactory Dataset with GPT-4

Figure 7: Ablations of trace length threshold values used with the routing strategy for GPT-4.

C.1 Trace Understanding Probing Studies Full Results and Qualitative Findings

Dataset partition (#prompts)	Trace Collating	Trace Prediction
Refactory reference (34)	88%	50%
Refactory fail (38)	79%	26%
Geeks for geeks (300)	45%	15%

Table 3: Trace Understanding Probing Results

We manually reviewed a sample of diffs to gain qualitative insights of LLM trace manipulation behavior. Most discrepancies between ground truth and either LLM-collated or predicted traces are due to additions or deletions of variable modifications from the trace. In particular, within loops, the LLM tends to either miss or add extra variable modifications., which could hit at a potential limitation in the depth of reasoning and memory. In the task of trace prediction from scratch, the second most erratic behavior is around predicting function returns, which can amount to both wrong value and wrong placement within the execution flow. Interestingly, in addition to generating traces, the LLM consistently attempts to fix code formatting, and in many cases optimizes away code branches not taken. Similarly, in the presence of execution failures, the LLM is unreliable at correctly predicting exceptions – either predicting exception types not commonly raised by a given operation, missing the exception altogether or, in some cases, patching the code to prevent an exception. Miscellaneous observed other discrepancies are due to the LLM adding superfluous commentary, trace formatting mistakes and hallucination of object hashes and other literals.

C.2 Prompts for Predicting and Collating Traces

```
1 ### Given a function and its invocation, trace the function's execution, using inline comments in
   \hookrightarrow the format shown in the below examples:
   ### Example program:
2
   def unique_day(day, possible_birthdays):
3
       count = 0
4
       for birthday in possible_birthdays:
5
            if birthday[1] == day:
6
                count += 1
7
       return count == 1
8
10 ### Example invocation:
unique_day(day = '1', possible_birthdays = (('January', '1'), ('February', '1')))
12
13 ### Example traced program:
14 # Starting var:.. day = '1'
15 # Starting var:.. possible_birthdays = (('January', '1'), ('February', '1'))
   def unique_day(day, possible_birthdays):
16
       count = 0 # New var:.... count = 0
17
       for birthday in possible_birthdays: # New var:..... birthday = ('January', '1')
18
       # Modified var:.. birthday = ('February', '1')
19
           if birthday[1] == day:
20
                count += 1 # Modified var:.. count = 1
21
                # Modified var:.. count = 2
22
23
       return count == 1
       # Return value:.. False
24
25
26 ### Example program with exception:
   def remove_extras(lst):
27
       result = []
28
29
       for i in 1st and not result:
           result += result + i
30
       return result
31
32
33 ### Example invocation with exception:
   remove_extras(lst = [3, 4, 5, 1, 3])
34
35
36 ### Example traced program with exception:
37 # Starting var:.. lst = [3, 4, 5, 1, 3]
   def remove_extras(lst):
38
       result = [] # New var:.... result = []
39
       for i in lst and not result: # Exception:..... TypeError: 'bool' object is not iterable
40
41
           result += result + i
       return result
42
43
44 ### Valid traces types the following: 'Starting var', 'Modified var', 'New var', 'Return value',
   \leftrightarrow 'Exception'. Do not insert any other comments.
45
46
   ### Program:
47
   def search(x, seq):
       for i in range(len(seq)):
48
49
           if x <= seq[i]:</pre>
                return i
50
       return len(seq)
51
52 ### Invocation:
53 search(-100, ())
54
```

```
↔ shown in the below examples:
### Example program:
   2
         def unique_day(day, possible_birthdays):
    count = 0
   3
                 for birthday in possible_birthdays:
    if birthday[1] == day:
   5
   6
   7
                               count += 1
                return count == 1
   8
  9
 10
       ### Example trace:
         ### Example trace:
Source path:... temp.py
Starting var:.. day = '1'
Starting var:.. possible_birthdays = (('January', '1'), ('February', '1'))
call 10 def unique_day(day, possible_birthdays):
line 11 count = 0
 11
 12
 13
 14
 15
          New var:..... count = 0
line 12 for birthday in possible_birthdays:
 16
 17
         New var:.... birthday = ('January', '1')
line 13 if birthday[1] == day:
line 14 count += 1
 18
 19
         Modified var... count = 1
line 12 for birthday in --
Modified var...
 20
21
22
         Modified var... count - for birthday in possible_b
Modified var... birthday = ('February', '1')
line 13 if birthday[1] == day:
line 14 count += 1
                                             for birthday in possible_birthdays:
23
24
25
         line 13 In birtiday[1] -- day.

line 14 count += 1

Modified var:.. count = 2

line 12 for birthday in possible_birthdays:

line 15 return count == 1

return 15 return count == 1
 26
27
 28
 29
 30
          Return value:.. False
 31
 32
         ### Example aligned:
         ### Example aligned:
# Starting var:.. day = '1'
# Starting var:.. possible_birthdays = (('January', '1'), ('February', '1'))
def unique_day(day, possible_birthdays):
    count = 0 # New var:..... count = 0
    for birthday in possible_birthdays: # New var:..... birthday = ('January', '1')
    # Madified are birthdays: # New var:..... birthday = ('January', '1')
 33
 34
35
 36
 37
                 # Modified var:.. birthday = ('February', '1')
if birthday[1] == day:
 38
 39
                         count += 1 # Modified var:.. count = 1
# Modified var:.. count = 2
40
 41
 42
                 return count == 1
 43
                 # Return value:.. False
 44
 45
          ### Example program with exception:
        def remove_extras(lst):
    result = []
    for i in lst and not result:
        result + i
        result + i
        result + i

46
 47
 48
 49
 50
 51
          ### Example trace with exception:
 52
 53
          Source path:... temp.py
         Starting var:.. lst = [3, 4, 5, 1, 3]
call 10 def remove_extras(lst):
line 11 result = []
 54
 55
 56
         Ine II result = []
New var:..... result = []
line 12 for i in 1st and not result:
exception 12 for i in 1st and not result:
Exception:.... TypeError: 'bool' object is not iterable
 57
 58
 59
60
          Call ended by exception
 61
62
 63
         ### Example aligned with exception:
         ### Extering ariii bit = [3, 4, 5, 1, 3]
def remove_extras(lst):
    result = [] # New var:..... result = []
    for i in lst and not result: # Exception:.... TypeError: 'bool' object is not iterable
        result += result + i
64
 65
66
 67
 68
 69
                 return result
 70
 71
72
         ### Note aligned versions only include capitalized entries from the trace. Do not insert any other comments.
 73
          ### Program:
 74
         def search(x, seq):
                 for i in range(len(seq)):
    if x <= seq[i]:</pre>
 75
 76
 77
78
                               return i
                 return len(seq)
          ### Trace:
 79
 80
           Source path:... temp.py
        81
 82
83
 84
 85
 86
87
         line 11 for i in range(len(seq)):
Modified var:.. i = 1
line 12 if x <= seq[i]:
line 11 for i in range(len(seq)):
Modified var:.. i = 2
line 12 if x <= seq[i]:
line 11 for i in range(len(seq)):
Modified var:.. i = 2
 88
 89
 90
91
 92
93
                                             for i in range(len(seq)):

    Infe
    1
    Infe
    1

    Modified
    x1
    in
    ange(infection)

    line
    12
    if x <= seq[i]:</td>

    line
    11
    for i in range(len(seq)):

 94
95
 96
97

    Ine
    12
    if x <= seq[i]:</th>

    line
    11
    for i in range(len(seq)):

 98
 99
         Modified var:. i = 5
line 12 if x <= seq[i]:
line 11 for i in range(len(
100
101
                                             for i in range(len(seq)):
return len(seq)
102
                                                                                                                                           177
                           14
14
103
         line
104
         return 14
Return value:.. 6
                                             return len(seq)
105
```

1 ### Given a function and its execution trace, can you align each element in the trace with the corresponding line in the program, using the format

C.3 Qualitative Examples of Trace Prediction Errors

```
1 # Starting var:.. lst = [3, 4, 5, 1, 3]
                                                        1 # Starting var:.. lst = [3, 4, 5, 1, 3]
   def remove_extras(lst):
                                                         2 def remove_extras(lst):
2
       i = 0 # New var:.... i = 0
                                                                 i = 0 # New var:.... i = 0
3
                                                         3
       while i < len(lst):</pre>
                                                                 while i < len(lst):</pre>
4
                                                         4
            j = i + 1 # New var:.... j = 1
                                                                     j = i + 1 # New var:.... j = 1
                                                         5
5
            # Modified var:.. j = 2
                                                         6 # Modified var:.. j = 2
6
            # Modified var:.. j = 3
                                                         7 # Modified var:.. j = 3
7
            while j < len(lst):</pre>
                                                         8 # Modified var:.. j = 4
8
9
                if lst[i] == lst[j]:
                                                         9 # Modified var:.. j = 5
                                                                    while j < len(lst):</pre>
                     lst = lst[:j] + lst[j+1:] #
10
                                                         10
                     \hookrightarrow Modified var:.. lst = [3,
                                                         11
                                                                          if lst[i] == lst[j]:
                     \leftrightarrow 4, 5, 1]
                                                                              lst = lst[:j] + lst[j+1:] #
                                                         12
                j += 1 # Modified var:.. j = 2
                                                                              \leftrightarrow Modified var:.. lst = [3,
11
                # Modified var:.. j = 3
                                                                                 4, 5, 1]
12
                                                                               \rightarrow 
                                                                          j += 1
                # Modified var:.. j = 4
                                                         13
13
                                                                     i += 1 # Modified var:.. i = 1
                # Modified var:.. j = 5
                                                         14
14
                # Modified var:.. j = 3
# Modified var:.. j = 4
# Modified var:.. j = 4
                                                        15 # Modified var:.. i = 2
15
16
                                                         16 # Modified var:.. i = 3
                                                        17 # Modified var:.. i = 4
17
            i += 1 # Modified var:.. i = 1
                                                                 return lst # Return value:.. [3, 4, 5, 1]
18
                                                        18
            # Modified var:.. i = 2
19
                                                         19
20
            # Modified var:.. i = 3
                                                         20
            # Modified var:.. i = 4
21
        return lst # Return value:.. [3, 4, 5, 1]
22
```

Figure 8: Example of erroneous variable modifications within a nested loop (Ground truth - left, prediction - right)

```
1 # Starting var:.. date = '3'
                                         1 # Starting var:.. date = '3'
 2
 def unique_day(date, possible_birthdays):
                                         3 def unique_day(date, possible_birthdays):
3
     if date in possible_birthdays[1]:
                                         4 if date in possible_birthdays[1]:
4
        return False
                                                 return True # Return value:.. True
5
                                         5
6
     else:
                                         6
                                               else:
        return True # Return value:.. True
                                                  return False
                                         7
7
```

Figure 9: Example of wrong return value placement and code modification. (Ground truth - left, prediction - right)

```
1 # Starting var:.. lst = [('M', 23), ('F', 19),
1 # Starting var:.. lst = [('M', 23), ('F', 19),
  ↔ ('M', 30)]
                                                     → ('M', 30)]
                                                   2 def sort_age(lst):
 def sort_age(lst):
2
      return lst.sort(key = lambda x: x[1],
                                                         return lst.sort(key = lambda x: x[1],
3
                                                  3
      → reverse = True) # Modified var:.. lst
                                                         → reverse = True) # Return value:.. None
      ↔ = [('M', 30), ('M', 23), ('F', 19)]
                                                  4 # Exception:.... AttributeError: 'NoneType'
      # Return value:.. None
                                                     ↔ object has no attribute 'sort'
4
```

Figure 10: Example of a falsely predicted exception. (Ground truth - left, prediction - right)

1	# Starting var: lst = [('F', 19)]	2	<pre>def sort_age(lst):</pre>
2	<pre>def sort_age(lst):</pre>	3	sort1 = [] # New var: sort1 = []
3	sort1 = [] # New var: sort1 = []	4	while lst:
4	while lst:	5	largest = lst[0][1] # New var:
5	largest = lst[0][1] # New var:		↔ largest = 19
	↔ largest = 19	6	<pre>for i in lst: # New var: i =</pre>
6	<pre>if i[1] > largest: # Exception:</pre>		↔ ('F', 19)
	\hookrightarrow NameError: name 'i' is not defined	7	<pre>if i[1] > largest:</pre>
7	largest = i[1]	8	largest = i[1]
8	lst.remove(i)	9	<pre>lst.remove(i) # Modified var: lst =</pre>
9	<pre>sort1.append(i)</pre>		\hookrightarrow []
10	return sort1	10	<pre>sort1.append(i) # Modified var:</pre>
			↔ sort1 = [('F', 19)]
1	# Starting var: lst = [('F', 19)]	11	<pre>return sort1 # Return value: [('F', 19)]</pre>

Figure 11: Example of a code modification to fix an exception. (Ground truth – left, prediction – right)