CRUXEVAL: A BENCHMARK FOR CODE REASONING, UNDERSTANDING AND EXECUTION

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Abstract

We present CRUXEVAL (Code Reasoning, Understanding, and eXecution Evaluation), a benchmark consisting of 800 Python functions (3-13 lines). Each function comes with an input-output pair, leading to two natural tasks: input prediction and output prediction. First, we propose a general recipe for generating our execution benchmark by sampling from a model, which can be used for more challenging versions of the benchmark if needed. Second, we evaluate twenty code models on our benchmark and discover that many recent high-scoring models on HumanEval show no improvements on our benchmark. Third, we show that simple CoT and fine-tuning schemes can improve performance on our benchmark but remain far from solving it. The best setup, GPT-4 with chain of thought (CoT), achieves a pass@1 of 75% and 81% on input and output prediction, respectively. In contrast, Code Llama 34B achieves a pass@1 of 50% and 46% on input and output prediction. When it comes to reasoning about code, GPT-4 has a huge edge over other models but still fails consistently on some surprisingly simple Python programs.

1 INTRODUCTION

In recent months, software engineering and programming have become increasingly mainstream domains for language models (LMs) as they attempt to conquer a potpourri of tasks including code completion, program repair, debugging, test case generation, and code optimization (see Zan et al. (2023) and Fan et al. (2023) for surveys). Recent models including Code Llama (Roziere et al., 2023), GPT-3.5 (Brown et al., 2020; Ouyang et al., 2022), and GPT-4 (OpenAI, 2023) have shown promise in code-related tasks and are being used to develop tools to help programmers.

The primary evaluation for code LMs is via benchmarks such as HumanEval (Chen et al., 2021) and MBPP (Austin et al., 2021), which test the ability to generate short code snippets from natural language specifications. While HumanEval and MBPP capture code generation abilities on simple and fundamental tasks, there is an absence of benchmarks capturing other fundamental dimensions of code LMs such as code understanding and execution.

Motivated by this, we contribute a new benchmark, CRUXEVAL (Code Reasoning, Understanding, and eXecution Evaluation) with two tasks: 1) output prediction, CRUXEVAL-O to measure code execution following and 2) input prediction, CRUXEVAL-I to measure code reasoning and understanding. Two samples in CRUXEVAL are shown in Listing 1 (modified for readability). CRUXEVAL examines the abilities of code LMs to reason about the execution behaviour of *simple* Python programs. While LMs shouldn't be expected to replace an interpreter on arbitrarily complex problems, we ensure the samples in our benchmark are simple (maximum 13 lines, no complex arithmetic) and solvable by a university-level CS graduate without needing more memory than the output (in our opinion). CRUXEVAL provides a useful and important probe for better understanding the capabilities of code LMs, as following a few simple steps of code execution should be a basic requirement for

these models. The ability to reason about the execution behavior of code also paves the way to tackling more difficult tasks such as code repair with execution feedback and code summarization.

```
def f(string):
    string_x = string.rstrip("a")
    string = string_x.rstrip("e")
    return string
# output prediction, CRUXEval-0
assert f("xxxxaae") == ??
## GPT4: "xxxx", incorrect
# input prediction, CRUXEval-I
assert f(??) == "xxxxaa"
## GPT4: "xxxxaae", correct
```

def f(nums): count = len(nums) for i in range(-count+1, 0): nums.append(nums[i]) return nums # output prediction, CRUXEval-O assert f([2, 6, 1, 3, 1]) == ?? # GPT4: [2, 6, 1, 3, 1, 6, 1, 3, 1], incorrect # input prediction, CRUXEval-I assert f(??) == [2, 6, 1, 3, 1, 6, 3, 6, 6] # GPT4: [2, 6, 1], incorrect

Listing 1: Sample problems

At a high level, our benchmark is constructed as follows. First, we use CODE LLAMA 34B to generate a large set of functions and inputs. The outputs are generated by executing the functions on the inputs. Second, we filter the set so that our benchmark only consists of short problems with low computation and memory requirements, problems which a good human programmer should be able to do without extra memory in a minute or so. Third, we randomly select 800 samples passing the filter, ensuring the benchmark is both small enough to easily run but large enough to reliably see performance differences among various models. While it is difficult to come up with example where the strongest models like GPT-4 fail consistently, we observe that models actually fail often on random yet reasonable generated programs. We also highlight that as models improve, this generate-and-filter approach can be used to create future benchmarks that are more difficult and test different aspects of program execution.

The best model, GPT-4, achieves a pass@1 of 67% on CRUXEVAL-I and 63% on CRUXEVAL-O. In contrast, the best open-source models only achieve 47% on CRUXEVAL-I and 44% on CRUXEVAL-O, failing over half the time at simple execution prediction and code reasoning despite being trained on 100G of Python code and 1T of code data. We also observe that for base models, stronger HumanEval performance correlates with stronger CRUXEVAL performance. However, this trend breaks down for models distilled on GPT-4 like data such as WizardCoder, Phind, and Phi, which have impressively high HumanEval scores but no better than CodeLlama on CRUXEVAL.

We also observe that CoT and fine-tuning on input-output assertions are effective techniques for improving performance on CRUXEVAL, but are far from enough to ace it. Overall, our benchmark reveals that the gap between GPT-4 and open source models reflects GPT-4's stronger ability to reason about the behavior of code. As existing benchmarks like HumanEval and MBPP are insufficient for measuring code understanding and execution ability, capturing it through our benchmark is critical to make progress towards closing the gap between open models and GPT-4. Finally, we discover that despite its impressive abilities, GPT-4 consistently fails to understand the execution behavior of some surprisingly simple Python programs.

2 RELATED WORK

Benchmarks for Evaluating Code LMs: There are various benchmarks serving to evaluate different aspects of these code LMs. We survey a handful here and refer readers to the survey (Zhang et al., 2023g) for more. HumanEval (Chen et al., 2021) and MBPP (Austin et al., 2021) evaluate Python

code generation on relatively simple functions. HumanEval+ (Liu et al., 2023c) augments HumanEval with better test cases after discovering many passing solutions are incorrect. ReCode (Wang et al., 2022a) is a variant of HumanEval with perturbed function names and docstrings. HumanEval-X (Zheng et al., 2023), MultiPLe (Cassano et al., 2022), and MBXP (Athiwaratkun et al., 2022) are extensions of HumanEval and MBPP with a focus on including programming languages outside of Python. APPS (Hendrycks et al., 2021), CodeContests (Li et al., 2022), and LeetCode-Hard (Shinn et al., 2023) evaluate code generation on more difficult, interview or competition style problems.

There are also benchmarks to evaluate code generation in data science applications, such as DS-1000 (Lai et al., 2023), ARCADE (Yin et al., 2022), NumpyEval (Zhang et al., 2023b), and PandasEval (Jain et al., 2022). Going one step further, some benchmarks also measure ability to use API's or perform more general software engineering tasks, such as JuICe (Agashe et al., 2019), APIBench (Patil et al., 2023), RepoBench (Liu et al., 2023e), ODEX (Wang et al., 2022b), SWE-Bench (Jimenez et al., 2023), GoogleCodeRepo (Shrivastava et al., 2023), RepoEval (Zhang et al., 2023a), and Cocomic-Data (Ding et al., 2022).

To our knowledge, our CRUXEVAL is the first publicly available benchmark to measure the execution ability of code LMs. While some prior work has measured the output prediction ability of code LMs, we leverage our CRUXEVAL-O to perform a more thorough investigation of these capabilities. Our CRUXEVAL-I is the first to measure the ability of code LMs to perform input prediction.

Leveraging Test Cases and Code Execution: Another line of work uses test cases and code execution information to improve code generation. Some examples include Speculyzer (Key et al., 2022), CodeT (Chen et al., 2022), CodeGen-Test (Zhong et al., 2022), Coder-Reviewer reranking (Zhang et al., 2023f), MBR-EXEC (Shi et al., 2022) TCoT (Tian & Chen, 2023), Algo (Zhang et al., 2023d), Pangu-Coder2 (Shen et al., 2023), LEVER Ni et al. (2023), and Self-Play (Haluptzok et al., 2022). The idea of these works is to generate many programs and many test cases and select which programs and test cases seem correct based on the execution results. using execution info.

Most relevant to our work, a handful of works examine and improve the execution ability of code LMs. Austin et al. (2021), Scratchpad (Nye et al., 2021), and CodeExecutor (Liu et al., 2023a) train code LMs on execution information. Inspired by these works, we briefly touch on two primitive ways to improve performance on our benchmark, chain-of-thought and fine-tuning. Moving forward, we believe our CRUXEVAL could serve as a useful reference point as more techniques are designed to improve code execution abilities.

Failure modes of LM Reasoning: Another dream of the community is to better understand the failure modes of LMs on reasoning tasks. Bubeck et al. (2023); Liu et al. (2023b); Arkoudas (2023); Zhang et al. (2022); Dziri et al. (2023); Olausson et al. (2023a); Lee et al. (2023); Zhang et al. (2023e) all investigate and point out various failure modes of LMs on a wide variety of reasoning tasks. Other examples of reasoning failures include 1) understanding negation (Hosseini et al., 2021), 2) ignoring irrelevant context (Shi et al., 2023), 3) operating under counterfactual situations such as 1-indexed Python or base-9 addition (Wu et al., 2023), and 4) generating Python code after identifier swaps like print, len = len, print (Miceli-Barone et al., 2023). Taking a more theoretical perspective, Dziri et al. (2023); Zhou et al. (2023); Merrill & Sabharwal (2023); Giannou et al. (2023) characterize the types of reasoning tasks transformers can and cannot be expected to carry out. Merrill et al. (2021) argues that it is not possible to learn meaning from ungrounded form with context dependence and assuming that syntax is independent of semantics. In this work, we use CRUXEVAL to empirically examine failures in code execution / reasoning.

3 BENCHMARK CONSTRUCTION

CRUXEVAL consists of 800 distinct functions, each with an input-output pair such that executing the function on the input deterministically produces the output. Using these functions and input-output pairs, we derive two benchmark tasks. In the *output prediction* task, the goal is to predict the output of executing the function on its associated input. In the *input prediction* task, the goal is to find any input such that executing the function on that input produces the output. For both tasks, we use an execution-based correctness metric. For input prediction, a generated input passes if assert f(generated_input) == output passes, and for output prediction, a generated output passes

if assert f(input) == generated_output passes. A few statistics about the samples of CRUXEVAL can be found in Appendix B.3.

3.1 GENERATING CANDIDATES

We use CODE LLAMA 34B to generate all the candidate functions and inputs of CRUXEVAL. To do so, we prompt it with the name of a function in the Python standard library such as str.zfill and ask it to generate a Python function that makes use of the library function in addition to 5 test inputs. We provide two varying few-shot examples in our prompt for improved diversity of generations (see Appendix B.2 for more details). A sample prompt is shown in Listing 3.

We use a total of 69 different functions from the standard library: 47 from the str, 11 from dict, and 11 from list (see Appendix B.1 for the full list of functions). Overall, we generate a total of 102000 functions (46% str, 27% dict, 27% list) and 489306 input-output pairs.

3.2 FILTERING CANDIDATES

Next, we filter the generated candidates to ensure that the samples in the dataset are reasonable and of high quality. In order to avoid forcing the model to perform tasks such as arithmetic calculation, we design filters so that the benchmark only consists of samples that are solveable by a human without extra memory.

Concretely, we filter based on the following criteria: 1) Compile time: all arguments of the function must be used in the function, length of code is between 75 and 300 characters, no syntax errors, proper assertion assert f(input) == output. 2) Runtime: no floating point operations, true division, exp, other integer operations must have at least one argument ≤ 3 , string and list operations must have at least one argument with length ≤ 3 , finish running in 2 seconds, no uncaught exceptions. 3) Best effort to remove other undesirable code: function cannot have any imports (such as os, sys), must be deterministic (no random, set ordering), and cannot have side effects such as input, __builtins_-, etc.

3.3 DATA SIZE AND MEASURING NOISE

The success of HumanEval (164 examples) shows that evaluation benchmarks can be small, and having faster/cheaper evaluation is an overlooked advantage. We first overgenerate a larger set (~ 1700) of samples and then pick a minimal data size that leads to sufficiently small noise.

On the overgenerated set, CODE LLAMA 34B outperforms CODE LLAMA 13B (as expected), and we would like to retain this property with high confidence in our smaller dataset. To do this, we took bootstrap samples of size N out of ~1700 samples to measure the probability that the performance would be reversed, shown in Fig. 1. 800 examples are enough to test that CODE LLAMA 34B > CODE LLAMA 13B, CODE LLAMA COT > CODE LLAMA and as well as between DEEPSEEK 33B > CODE LLAMA 34B (output).

We measure two types of noise: 1) sampling which data points to include in the benchmark, and 2) sampling candidates from models for each data point (temperature > 0). Of these, 1) dominates 2). For 1) since model A does not always outperform model B on all data points even if model A > model B in aggregate, the measured performance depends on which data points are included. We measure both noise types on each model individually and type 1) noise on pairs of models using the bootstrap. Fortunately, we do not see major differences in noise level between models and the most important factor is just the size of the dataset. Type 1) noise is generally around 1.5% whereas type 2) noise is around 0.2% at N = 800. Type 1) noise usually becomes smaller on pairs of models due to correlation, yielding statistically significant results at the $\alpha = 0.025$ (one-sided) for many model pairs.

4 EVALUATION

We use N = 100 samples for all non-GPT models and N = 10 samples for GPT models. We report both pass@1 scores (T = 0.2) and pass@5 scores (T = 0.8). The results are shown in Fig. 2, and raw scores are provided in the Appendix in Table 2. In Fig. 2, we show the intervals generated by

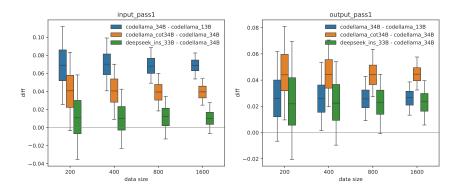


Figure 1: Difference between model pairs on bootstrap samples of various sizes. The whiskers show (2.5, 97.5) and boxes show (25, 75) percentiles.

10000 bootstrap samples from the dataset, where non-overlapping whiskers would be significant at the 2.5% level. To get more statistical power, we compare pairs of models on each bootstrapped sample. We show how each model compares to CODE LLAMA 34B in Fig. 15. The intervals generally decreases due to correlations. On all models vs. CODE LLAMA 34B, if the median bar clears the whisker in Fig. 2, then the difference actually holds with >97.5% probability under paired bootstrap. For example, CODE LLAMA 34B is better than WIZARD_34B on input and CODE LLAMA 34B is worse than DEEPSEEK_33B on output prediction with >97.5% probability.

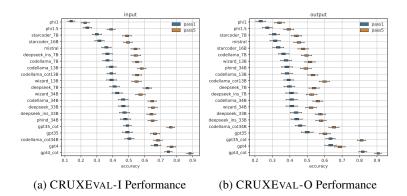


Figure 2: Main Results. Boxes show (25, 75) percentiles, whiskers show (2.5, 97.5), and the middle bar shows the median (\approx mean).

5 QUANTITATIVE ANALYSIS

Correlation between scores on HumanEval and CRUXEVAL: In Fig. 3, we plot reported HumanEval scores (we did not reproduce them ourselves) against scores on CRUXEVAL. Indeed, we spot some interesting outliers: when comparing the distilled models WizardCoder 34B and Phind 34B to CODE LLAMA 34B, we see that the distilled models score over 20% more than Code Llama on HumanEval but *do not show this drastic improvement when evaluated on either input or output prediction*. In addition, the Phi-1 model outperforms most of the bigger models on HumanEval, but performs among the worst of all our evaluated models on CRUXEVAL. Overall, this suggests that models optimized for the HumanEval task by distilling data from GPT-3.5 and GPT-4 (WizardCoder, Phind, Phi) may not have learned other code reasoning capabilities along the way. On the other hand, for models such as StarCoder, Mistral, CodeLlama, and DeepSeek-Base, we still see a positive trend between HumanEval score and CRUXEVAL score, suggesting that code generation and execution/understanding abilities are correlated.

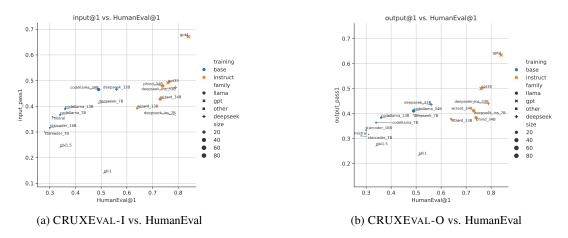


Figure 3: Correlation between HumanEval pass@1 scores and CRUXEVAL-O pass@1 scores

Relationship between input prediction and output prediction: In Fig. 4 (top), we compare the input prediction and output prediction pass@1 scores with each other. Conceptually, the two tasks seem relatively different: output prediction is directly testing code execution ability, while input prediction requires a higher-level understanding of the code's functionality. However, we discover that there is a strong correlation between their performance. This suggests the hypothesis that performance on relatively distinct coding-related tasks may be closely correlated. In addition, we see a relatively clear impact of scaling the model size on our two tasks.

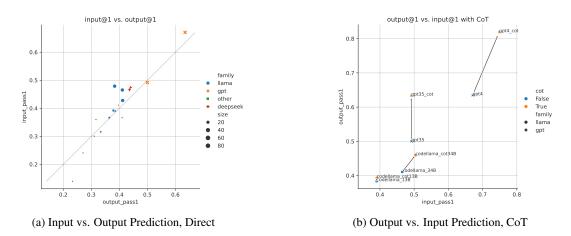


Figure 4: Correlation between Input and Output Prediction Scores, with and without CoT

5.1 CHAIN OF THOUGHT PROMPTING

Next, we evaluate how the popular chain-of-thought (CoT) prompting method (Wei et al., 2022) affects the performance of Code Llama, GPT-3.5, and GPT-4 models on CRUXEVAL. The full prompts can be found in Appendix E.3. All results are reported using N = 10 samples other than CodeLlama 13B and 34B without CoT, which are reported with N = 100 samples. As before, pass@1 is reported with T = 0.2 and pass@5 with T = 0.8. Additional results can be found in Appendix D.2.

Impact of CoT: We begin by focusing our attention on the pass@1 scores of models with and without CoT. In Fig. 4, we plot the input and output prediction scores of each model with and without CoT. First, GPT-4 benefits significantly more than other models. Second, output prediction boosts are generally larger than input prediction. In fact, CoT does not seem to improve Code Llama 13B and GPT-3.5 performance on input prediction. This is intuitive, as input prediction involves a more

difficult reasoning task, while output prediction only requires executing the program step by step. We defer raw numbers to the Appendix in Table 3.

CoT widens the gap between pass@5 and pass@1 scores: In Fig. 5, we plot the pass@5 scores against the pass@1 scores for all models. For models without CoT (shown in blue), there is a positive correlation between pass@1 and pass@5 scores. For models with CoT (shown in orange), we see an increase in the gap between pass@5 and pass@1 scores. We believe this phenomenon may be due to the additional diversity induced by CoT, which we analyze in detail in Appendix D.3.

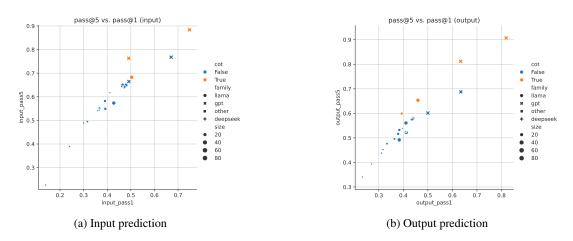


Figure 5: pass@5 score vs. pass@1 score with and without CoT

Predictions of CoT vs. Base Model: In Fig. 6, we show a confusion matrix over samples to better understand the correlations between direct output predictions and CoT predictions. For CodeLlama 13B (not shown), 34B, and GPT-3.5, we observe a large number of samples where direct prediction succeeds but CoT fails. However, with GPT-4, we observe that there are relatively few samples where this is the case.

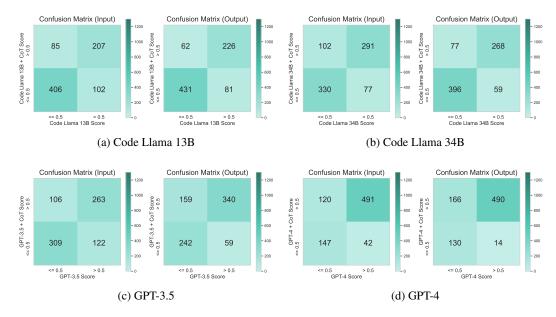


Figure 6: Confusion Matrix of Direct Prediction vs. CoT Prediction (T = 0.2)

5.2 FINE-TUNING EXPERIMENTS

Next, we do a preliminary analysis to understand the effect of simple fine-tuning schemes on CRUXEVAL performance. We fine-tuned CODE LLAMA 34B on nearly 140K samples of Python functions distilled with the procedure outlined in Sec. 3, without filtering. We perform weak decontamination, only removing samples where both the function and input-output pairs match samples in the benchmark.

In particular, we finetune on a mixture of 50% samples where the function is not in the benchmark and 50% samples where the function is in the benchmark but input-output pairs are not, a very liberal setup. The training and testing accuracy over time for output prediction is shown in Fig. 7. Despite finetuning on programs very similar to the benchmark, we still observe a plateauing effect in the test accuracy, suggesting that our execution tasks may be too difficult to learn from this simple fine-tuning scheme. We defer a few other insights from fine-tuning to Appendix D.7 and suggest a few fine-tuning ideas for improving our benchmark in Appendix A.

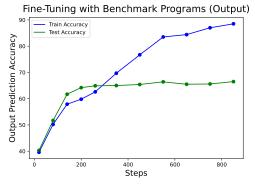


Figure 7: CRUXEVAL Performance after Fine-Tuning

6 QUALITATIVE ANALYSIS

All models except GPT-4 have over 50% failure rate, showing they cannot do simple executions. In this section, we focus on GPT-4 with CoT and verify that the remaining 20% failures are due to the model, are consistent and are indeed on *simple* programs. We refer the reader to Appendix F for further examples of the failures highlighted in this section as well as some impressive successes.

Failures of GPT-4 CoT. GPT-4 CoT scored 0/10 on 54 output prediction tasks and 65 input prediction tasks. On 22 problems, it scored 0/10 on both input and output prediction tasks. We manually check the 22 problems if they pass our criteria of being *simple* problems. Most failures are indeed on simple programs, like the one below.

```
def f(string, sep):
    cnt = string.count(sep)
    return((string+sep) * cnt)[::-1]
assert f('caabcfcabfc', 'ab') == 'bacfbacfcbaacbacfbacfcbaac'
# GPT4+CoT preds:
# f('baa', 'c')
# 'bacfbacfcbaabcabfbacfcbaabc'
```

Listing 2 shows GPT-4 CoT failures for output prediction only. In Listing 2 (bot), the model fails because it concludes that 6173 is not less than 1000. Small perturbations like changing to 0 < num and num < 1000 or changing the strings also failed. Both problems only have 2 possible answers and other models sometimes get them correctly whereas GPT-4 CoT is consistently wrong. We manually tested scratchpad Nye et al. (2021) style prompts, which failed in the same way as regular CoT (Appendix F.3).

```
def f(text, suffix):
    if suffix == '':
        suffix = None
    return text.endswith(suffix)
assert f('uMeGndkGh', 'kG') == ??
# GPT-4 CoT: True, should be False
```

```
def f(num):
    if 0 < num < 1000 and num != 6174:
        return 'Half Life'
    return 'Not found'
assert f(6173) == ??
# GPT-4 CoT: 'Half Life', should be 'Not found'
```

Listing 2: GPT-4 CoT output failures

Failures of GPT-4, Input Prediction: Below are two simple failures on input prediction where GPT-4 failed for concise and simple Python programs even with CoT.

```
def f(text, repl):
    trans = str.maketrans(text.lower(), repl.lower())
    return text.translate(trans)
assert f(??) == 'lwwer case'
# GPT4 CoT: 'lower case', 'ow'
# could be 'lower case', 'lwwer case'
```

```
def f(text):
    string = ''
    for char in text:
        string += char + char.lower()
    return string
assert f(??) == 'llaallaakk'
# GPT-4 CoT: 'LAK'
# should be 'lalak'
```

7 CONCLUSION

We propose CRUXEVAL, a new benchmark consisting of simple Python functions to evaluate the input and output prediction abilities of code LMs. First, we propose a three-part recipe to distill our benchmark consisting of large-scale distillation, filtering, and data size selection via a statistical noise analysis (Sec. 3). Second, we conduct a qualitative analysis by evaluating 20 models on our benchmark (Sec. 4). Our analysis leads to insights regarding the correlation between HumanEval and our benchmark, the correlation between input and output prediction, differences between various code LMs, and the diversity of different models. Third, we provide a qualitative analysis of GPT-4's successes and failures (Sec. 6 and Appendix F). Overall, we believe that CRUXEVAL provides a complementary perspective to classical code LM evaluation such as HumanEval and MBPP and encourage creators of future code LMs to try out our benchmark!

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A LIMITATIONS AND FUTURE WORK

Correlations between various code tasks: While our benchmark serves as an interesting lens to analyze code LMs, one might object that output prediction can simply be done with a Python interpreter and that input prediction abilities can be greatly enhanced by equipping a LM with an interpreter, like in GPT-4 Code Interpreter mode. While this is true, we believe that a good code LM still ought to have good code understanding and execution capabilities, similar to that of a strong programmer. We see that base models have a reasonably strong correlation between HumanEval, input prediction, and output prediction score. An interesting future direction is to more deeply investigate the correlations between performance on various code-related tasks such as code completion, execution, bug-finding, and code summarization.

Distilling future execution benchmarks: Our benchmark only measures the input and output prediction accuracy of relatively simple and self-contained Python functions distilled from a single model (Code Llama 34B). It would also be interesting to measure these capabilities on longer and more difficult code snippets, open-domain code samples, or code in other programming languages. As our distillation technique is relatively general, we welcome others to create their own benchmarks measuring the execution of code snippets from other distributions.

Variation due to prompt and temperature: The accuracy of a model on our benchmark may be very sensitive to the prompt and task format (Mizrahi et al., 2023). We try our best to address this by using prompts that are similar as possible across models (see Appendix E.2 and E.3) but understand that some prompts may improve the performance of certain models while decrease the performance on others. There are also countless prompting techniques (see (Liu et al., 2023d) for a comprehensive survey) that can be tried to improve the performance. We also run all our experiments with T = 0.2 and T = 0.8 due to budget constraints, but different temperatures will lead to different performance for all models. One must always be cautious and critical when using benchmarks to compare models. For example, for input prediction, while Phind v2's 47.9% pass@1 may seem to beat CodeLlama's 46.5%, the standard deviations of both models with respect to the 800 samples selected turns out to be around 1.5%, so this conclusion cannot be made.

Information loss due to pass@1: While the average pass@k metric is common in the code generation literature, it compresses a large amount of information into one number. While we suggest reporting pass@1 and pass@5 for our benchmark, we comment that pass@k is only one perspective of measuring execution ability. We try to shed more light on behaviour by including a bit more analysis throughout this work, but encourage the development of different evaluation and analysis techniques.

Fine-tuning: In our first fine-tuning experiment, we only check for exact string match when decontaminating the fine-tuning set, so there may still be semantic duplication or similar programs with small modifications, which may lead to a higher performance than if those examples were removed. In this work, we only consider the most direct and straightforward fine-tuning scheme. We believe there is room for improvement via more sophisticated techniques, such as using process supervision (Uesato et al., 2022), fine-tuning on correct CoT generations, or fine-tuning on snippets of code while including the program state after each step. Seeing that models like Phi, WizardCoder, and Phind outperformed Code Llama on HumanEval but not CRUXEVAL inspires the need for a deeper investigation of the utility of finetuning on distilled data from a more powerful model. Lastly, it remains a curiosity whether fine-tuning on execution information can help code generation abilities.

Jointly improving code generation and code execution: As we discovered, distilled models like Phi, Phind, and WizardCoder that are fine-tuned on code generation do not improve significantly on CRUXEVAL compared to their base models. It is unknown whether the opposite is true: does improved fine-tuning on code execution lead to better code generation abilities? It would also be interesting to explore techniques that can lead to improved performance on both code generation and code execution simultaneously.

Understanding reasoning from the lens of code: As future work, we believe that our benchmark serves as a good starting point towards understanding the code reasoning abilities of LM. Many further execution evaluations may be possible, such as testing execution of recursive functions, execution from a natural language description and an input, or execution of a composition of two functions. We find that output prediction serves as a good testbed for understanding CoT failures, because each step clearly corresponds to an operation with a ground truth, so reasoning failures can

be pinpointed. We observed many examples of CoT failures due to simple mistakes that the model seems to have knowledge about (see Appendix F.3.2 for examples), and it should be possible to analyze and characterize this behaviour more systematically.

Self-repair: Lately, self-repair has been used to improve the reasoning and programming abilities of LLMs (Chen et al., 2023; Olausson et al., 2023b; Madaan et al., 2023; Peng et al., 2023; Zhang et al., 2023c; Tyen et al., 2023). From our qualitative analysis, we find that when using CoT, many output prediction failures are recitation errors of information the model may already understand. Therefore, we believe that these mistakes may be easier to repair than when the correct reasoning path is not found in the first place, and that CRUXEVAL may be a simpler task to better understand model repair capabilities.

B BENCHMARK CONSTRUCTION AND STATISTICS

In this section, we provide more details about the process of constructing our benchmark. A sample prompt for generating functions and test cases is shown in Listing 3. The prompt is constructed by including two few-shot examples, one containing a specified str function and one containing a specified list function. The full list of specified functions is given in B.1, and the full list of few-shot examples chosen from is given in B.2. We learned that having random-looking inputs instead of common words and phrases in the few-shot prompts significantly increased the difficulty of the benchmark.

Listing 3: Sa	mple promr	ot for gene	rating fun	ctions and	test cases
Listing 5. Su	mpic promp	n ioi gene	raung ran	ctions une	i test euses

```
You will be given a function name between [TASK] and [/TASK] tags. Following the examples
     \hookrightarrow given, write a Python function that makes use of the given function and 5 test inputs
    \hookrightarrow for that function.
[TASK]
str.center
[/TASK]
[PYTHON]
def f(text):
   ls = list(text)
   for i in range(1, len(ls) - 1):
       ls.insert(i, '+')
    return ''.join(ls).center((len(ls) - 1) * 2)
[/PYTHON]
[TEST]
assert f('lynel') == ??
assert f('nzoh') == ??
assert f('u') == ??
assert f('anfsoixz') == ??
assert f('xzd') == ??
[/TEST]
[TASK]
list.append
[/TASK]
[PYTHON]
def f(nums):
   count = len(nums)
   for i in range(-count+1, 0):
       nums.append(nums[i])
   return nums
[/PYTHON]
[TEST]
assert f([2, 6, 1, 3, 1]) == ??
assert f([7, 1, 2, 6, 0, 2]) == ??
assert f([4, 3, 2, 1, 2, -1, 4, 2]) == ??
assert f([0, 6, 2, -1, -2]) == ??
assert f([-6, -2, 1, -3, 0, 1]) == ??
[/TEST]
[TASK]
str.zfill
[/TASK]
[PYTHON]
```

B.1 FUNCTIONS USED IN PROMPT

For each of str, list, and dict, we use all the non-dunder methods under that class. The resulting list of methods is as follows:

- str: capitalize, casefold, center, count, encode, endswith, expandtabs, find, format, format_map, index, isalnum, isalpha, isascii, isdecimal, isdigit, isidentifier, islower, isnumeric, isprintable, isspace, istitle, isupper, join, ljust, lower, lstrip, maketrans, partition, removeprefix, removesuffix, replace, rfind, rindex, rjust, rpartition, rsplit, rstrip, split, splitlines, startswith, strip, swapcase, title, translate, upper, zfill
- list: append, clear, copy, count, extend, index, insert, pop, remove, reverse, sort
- dict: clear, copy, fromkeys, get, items, keys, pop, popitem, setdefault, update, values

Motivated by seeing a GPT-4 failure of treating the ^ symbol as an exponential rather than an xor, we also attempted using all the non-dunder methods from operator. However, we found that the majority of the functions obtained were either too simple and uninteresting, or too computational, since many of the methods under operator are bit-manipulation or calculational operations. Therefore, we excluded it from our final benchmark.

B.2 FEW-SHOT EXAMPLES

We use 10 handwritten few-shot examples, 5 using str functions and 5 using list functions. For each prompt, we include two few-shot examples, one string few-shot example and one list few-shot example, for a total of 25 different combinations of few-shot prompts. We generate programs and inputs using CODE LLAMA 34B with temperature T = 1.

One interesting observation is that for a fixed pair of few-shot examples, there seems to be a limit to the number of diverse functions that can be generated: after about 60000 generations, only about 5000 of them were unique. Using all 25 combinations of few-shot prompts helps to overcome this duplication bottleneck.

The full set of few-shot examples can be found in Listing 5.

B.3 DATASET STATISTICS

In Fig. 8, we show the distribution of character count and line count of the 800 samples in our benchmark.

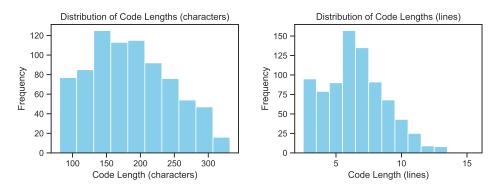


Figure 8: Dataset Distributions

In Fig. 9, we show the distribution of the "step count" of programs (with one outlier of 3175 steps excluded). Here, steps roughly correspond to Python bytecode operations during execution. The precise definition can be understood by checking the "numsteps" variable in our code here.

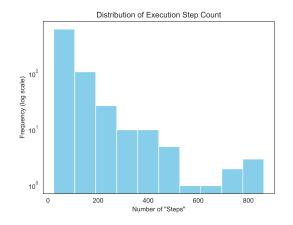


Figure 9: Number of steps

In Fig. 10, we plot the output prediction pass@1 scores against the input prediction pass@1 scores for each sample, observing little to no correlation between the difficulty of the two.

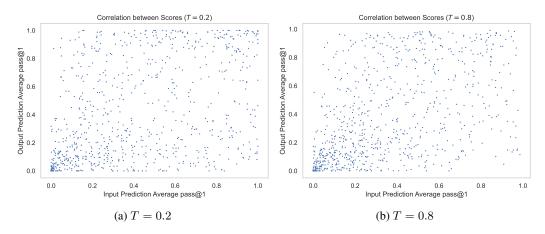


Figure 10: Sample-by-sample correlation between Input Prediction and Output Prediction

Method-level statistics: In Fig. 11, we show the number of samples containing each method in str, list, and dict. Even though we distilled the same number of samples using each str function and about twice as many for each list and dict functions, we observe that the resulting distribution is highly non-uniform. This is due to a few reasons. First, about 30% of the time, CODE LLAMA 34B sometimes fails to follow the instruction of including the library method in the resulting function. Second, some functions naturally lead to more operations that are removed by the filter. Third, common functions such as str/list.index or list.append are used in methods they are not prompted in.

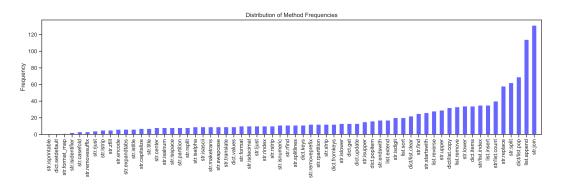


Figure 11: Frequency of various methods in CRUXEVAL

Next, we investigate trends of which methods are easier/harder for code LMs. For each method in the list, str, and dict libraries listed in Appendix B.1 with at least 5 samples, we calculate the average input prediction and output prediction score of benchmark samples containing that method. We show the 7 easiest and hardest methods for Code Llama 34B (Fig. 12), WizardCoder 34B (Fig. 13), and GPT-4 (Fig. 14). Some of the hardest methods, such as str.rsplit, str.maketrans, str.rfind, seem to be more obscure. We hypothesize that they may be underrepresented in pretraining corpora, explaining models' worse performance. While the distilled datasets of models like Phi, Phind, and WizardCoder are not yet available to the public, we speculate that they may include of fewer instances of these underrepresented functions and that distilling more obscure methods may help the model better learn their syntax and semantics.

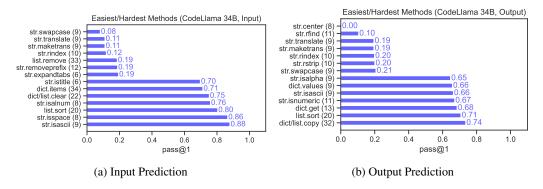


Figure 12: Easiest and hardest methods for Code Llama 34B input and output prediction, by pass@1 score (T = 0.2)

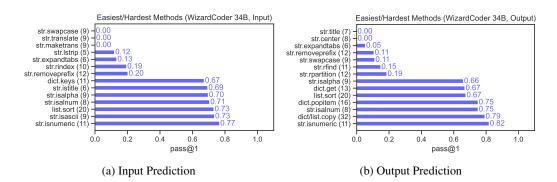


Figure 13: Easiest and hardest methods for WizardCoder 34B input and output prediction, by pass@1 score (T = 0.2)

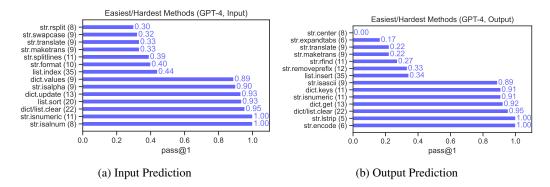


Figure 14: Easiest and hardest methods for Code Llama 34B input and output prediction, by pass@1 score (T = 0.2)

C MODEL URLS

For evaluation, we used the gpt-3.5-turbo and gpt-4 models on October 26, 2023. Note that this is before the OpenAI developer day release of GPT-4-Turbo. The corresponding HuggingFace model URLs for the rest of the evaluated models are listed in Table 1.

Table 1: Models and HuggingFace URLs

Model Name	HuggingFace URL
Mistral (7B)	https://huggingface.co/mistralai/Mistral-7B-v0.1
Phi-1 (1.3B)	https://huggingface.co/microsoft/phi-1
Phi-1.5 (1.3B)	https://huggingface.co/microsoft/phi-1_5
DeepSeek Instruct (6.7B)	https://huggingface.co/deepseek-ai/deepseek-coder-6.7b-instruct
DeepSeek Instruct (33B)	https://huggingface.co/deepseek-ai/deepseek-coder-33b-instruct
DeepSeek Base (6.7B)	https://huggingface.co/deepseek-ai/deepseek-coder-6.7b-base
DeepSeek Base (33B)	https://huggingface.co/deepseek-ai/deepseek-coder-33b-base
StarCoderBase (15.5B)	https://huggingface.co/bigcode/starcoderbase
StarCoderBase (7B)	https://huggingface.co/bigcode/starcoderbase-7b
WizardCoder (13B)	https://huggingface.co/WizardLM/WizardCoder-Python-13B-V1.0
WizardCoder (34B)	https://huggingface.co/WizardLM/WizardCoder-Python-34B-V1.0
Phind (34B)	https://huggingface.co/Phind/Phind-CodeLlama-34B-v2
CodeLlama 7B	https://huggingface.co/codellama/CodeLlama-7b-hf
CodeLlama (13B)	https://huggingface.co/codellama/CodeLlama-13b-hf
CodeLlama (34B)	https://huggingface.co/codellama/CodeLlama-34b-hf
CodeLlama Python (7B)	https://huggingface.co/codellama/CodeLlama-7b-Python-hf
CodeLlama Python (13B)	https://huggingface.co/codellama/CodeLlama-13b-Python-hf
CodeLlama Python (34B)	https://huggingface.co/codellama/CodeLlama-34b-Python-hf

D EVALUATION RESULTS

D.1 MAIN RESULTS

Table 2 shows the pass@1 and pass@5 results of all evaluated models on CRUXEVAL, and Fig. 15 shows them in box-plot form.

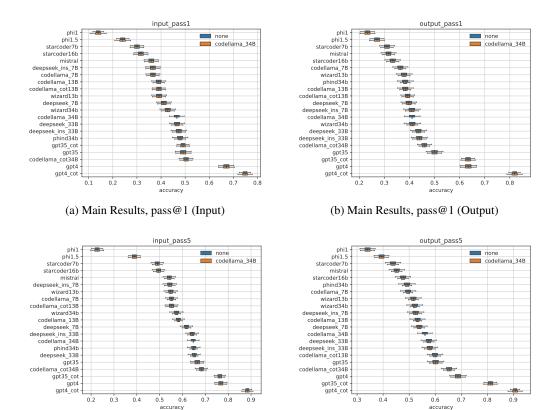
Model	Size	Input Prediction		Output Prediction	
Wither	Size	Pass@1	Pass@5	Pass@1	Pass@5
	7B	36.6%	55.2%	36.4%	49.6%
CodeLlama	13B	39.0%	58.2%	38.4%	53.2%
	34B	46.5%	64.7%	41.1%	56.1%
	7B	36.3%	56.0%	36.4%	49.7%
CodeLlama Python	13B	40.5%	58.0%	37.8%	50.8%
·	34B	41.5%	59.2%	40.7%	53.7%
Ct. C. L. D.	7B	30.0%	48.9%	31.1%	43.8%
StarCoder-Base	15.5B	31.6%	49.5%	33.3%	47.7%
WizardCoder	13B	39.2%	54.8%	37.9%	51.6%
wizardCoder	34B	42.8%	57.3%	41.2%	52.2%
Phi-1	1.3B	13.9%	22.6%	23.3%	34.0%
Phi-1.5	1.3B	24.1%	38.9%	27.1%	39.4%
Phind v2	34B	47.9%	64.9%	38.3%	49.2%
Desmande Carden Dese	6.7B	41.1%	61.7%	39.8%	53.9%
Deepseek Coder-Base	33B	46.6%	65.1%	43.6%	57.6%
Deenee als Carden Instance	6.7B	36.6%	54.4%	41.0%	52.5%
Deepseek Coder-Instruct	33B	47.4%	64.2%	44.0%	58.0%
Mistral	7B	36.0%	54.2%	31.7%	45.2%
GPT-3.5	-	49.2%	66.5%	50.0%	60.1%
GPT-4	-	67.1%	76.8%	63.4%	68.7%

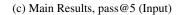
Table 2: Results of all models on CRUXEVAL

D.2 Additional Results on Impact of CoT

Table 3 shows the results of including CoT on Code Llama 13B, 34B, GPT-3.5, and GPT-4.

Sample-wide improvements from CoT: In Fig. 16, we show a histogram of how much CoT improves the pass@1 score of each sample (negative values means that CoT decreased the accuracy). We observe that CoT leads to little improvement for the majority of samples, this effect is partly due to samples already having high pass@1 scores. As evidenced by Fig. 16d, we see that CoT is much more effective for GPT-4 output prediction compared to both GPT-4 input prediction and other models. For the other models, however, we observe a large proportion of samples for which CoT actually decreases the pass@1.





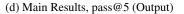
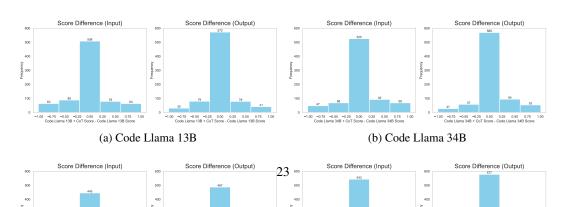


Figure 15: Main Results with confidence intervals compared to codellama_34B.

Model	СоТ	Input Prediction		Output Prediction	
With	COI	Pass@1	Pass@5	Pass@1	Pass@5
	×	39.0%	58.2%	38.4%	53.2%
Code Llama 13B	1	39.1%	55.2%	39.3%	59.9%
	-	+0.1%	-3.0%	+0.9%	+6.7%
	X	46.5%	64.7%	41.1%	56.1%
Code Llama 34B	\checkmark	50.4%	68.3%	46.0%	65.3%
	-	+3.9%	+3.6%	+4.9%	+9.2%
	X	49.2%	66.5%	50.0%	60.1%
GPT-3.5	\checkmark	49.1%	76.3%	63.3%	81.2%
	-	-0.1%	+9.8%	+13.3%	+21.1%
	X	67.1%	76.8%	63.4%	68.7%
GPT-4	1	74.8%	88.4%	81.9%	90.7%
	-	+7.7%	+11.6%	+18.5%	+22.0%

Table 3: Impact of CoT on CRUXEVAL



In Fig. 17, we show a more granular perspective of Fig. 6, which again highlights that CoT often decreases the pass@1 score of many samples. Again, we observe a stark difference between the impact of CoT on GPT-4 and other models.

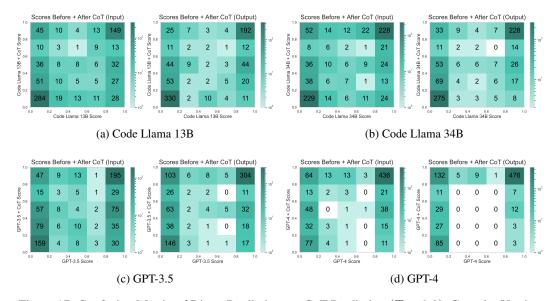


Figure 17: Confusion Matrix of Direct Prediction vs. CoT Prediction (T = 0.2), Granular Version

Qualitative example of CoT harming performance: Finally, we show one example of input prediction and one example of output prediction where GPT-4 succeeds without CoT and fails with CoT.

```
# Output Prediction
def f(phone_number):
    while phone_number.find('77777') != -1:
        phone_number = phone_number.replace('77777', 'seg', 1)
    return phone_number
assert f('7747777722') == '774seg22'
# GPT-4 CoT says that '77777' is not in '7747777722', returning '7747777722'
```

Correlations between failures of different models: Fig. 18 shows $P(Y \mid X = 0)/P(Y)$, the accuracy of model Y given that model X fails completely relative to the original accuracy of model Y. Although what is hard for a better model tend to be hard for worse models on average, worse models succeeded on some examples where the better models fail completely, showing idiosyncrasies in failures even for the best GPT-4 CoT model.

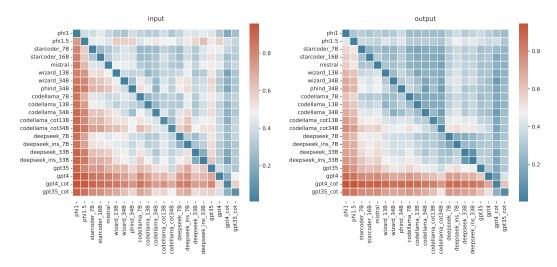


Figure 18: $P(Y \mid X = 0)/P(Y)$ where each Y is the accuracy of models in each row (X for column).

D.3 RESULTS ON DIVERSITY OF GENERATIONS

Diversity of generations across models: Next, we analyze the diversity of generated inputs and outputs across various models (without regard to correctness). In Fig. 19, we plot the mean and median number of unique answers generated across samples of CRUXEVAL for a selection of evaluated models. First, we observe the drastic increase in diversity between using T = 0.2 and T = 0.8. Second, by comparing Fig. 19a with Fig. 19b, we note that input prediction generally has a larger diversity of generations than output prediction. This may be due to the fact that output prediction only has one correct answer, but input prediction may have multiple correct answers. Third, we observe that at the same temperatures, Code Llama models have the highest diversity, while distilled models like Phind and WizardCoder have a lower diversity.

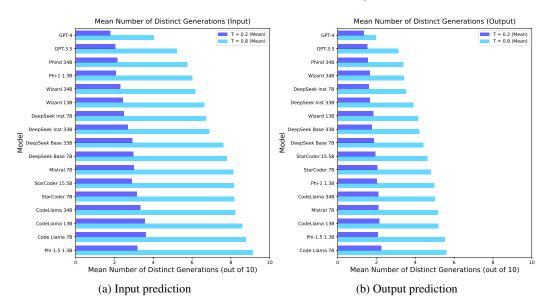


Figure 19: Number of distinct generations of various models (out of 10) at T = 0.2 and T = 0.8

CoT increase the diversity of generations: In Fig. 20, for each model, we plot the average number of distinct generations across all samples, where different chains of thought with the same input or output prediction are considered identical. We see again the trend of input prediction generations

being more diverse than output prediction generations. Interestingly, we observe that using CoT increases the diversity at both temperatures.

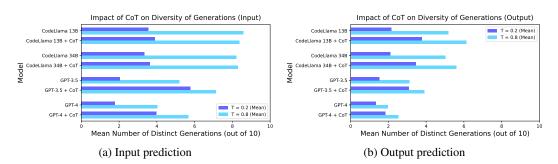


Figure 20: Number of distinct generations of various models (normalized to be out of 10) at T = 0.2and T = 0.8 with and without CoT. We observe that CoT increases the diversity of generations.

Functional diversity via distribution of pass@1 scores: In Fig. 21, for each model, we plot the percentage of samples where the pass@1 score (T = 0.2) is between 0.1 and 0.9, exclusive, indicating that the sample is neither "too easy" nor "too hard" for the model. This is a measure of functional diversity because models with more diversity are likely to generate both correct and incorrect samples, leading to more intermediate pass@1 scores. We make a few observations relatively consistent with our prior observations. First, the percentages are relatively low across the board, indicating that at a temperature of T = 0.2, models are generally producing a majority of correct or a majority of incorrect outputs. Second, distilled models have a much lower functional diversity than base models, for example comparing Phind 34B to CodeLlama 34B or DeepSeek Instruct 33B to DeepSeek Base 33B. Third, CoT greatly increases the functional diversity of models, which is very evident when looking at GPT-3.5 and GPT-4.

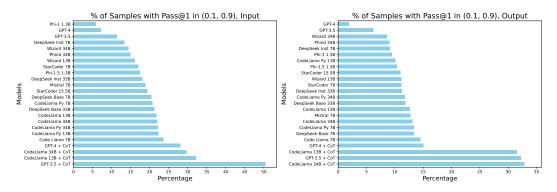


Figure 21: Percentage of samples where pass@1 score is in (0.1, 0.9), exclusive.

D.4 DIFFICULTY OF BENCHMARK SAMPLES

Distribution of sample difficulties: In Fig. 22, we show the average pass@1 score across all models for T = 0.2 in order to get a sense of the difficulty distribution of CRUXEVAL.

In Fig. 23, we show the pass@1 distributions of a few of the best-performing models at T = 0.8. Compared to the overall distribution, the distribution appears to be more bimodal. The output prediction distribution is more bimodal than the input prediction distribution, perhaps reflecting the differences in the tasks themselves. We also see the familiar trend of CoT increasing the number of samples with intermediate scores (in this case between 0.25 and 0.75).

Fully solved and unsolved samples: In Figs. 24 and 25, we examine a different metric, the percentage of examples with pass@1 score equal to 0 and 1, respectively, at T = 0.8. In a sense, this metric captures the ability of models to solve problems. It is also related to diversity, as with a higher

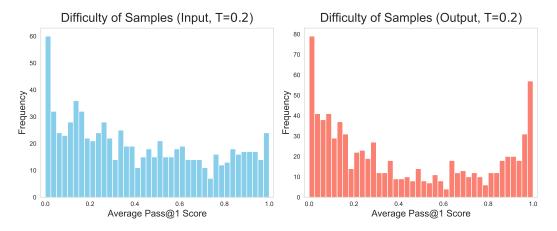


Figure 22: Difficulty of all samples of our benchmark, averaged across all models (T = 0.2)

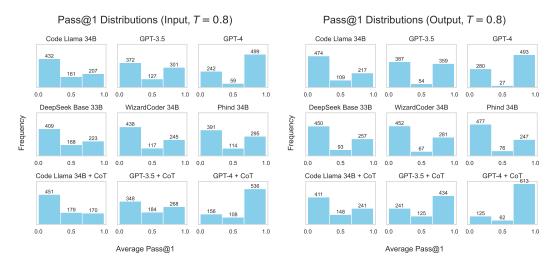


Figure 23: Pass@1 Distributions of Selected Models

diversity, the likelihood of solving the problem may increase. A few observations arise from looking at this metric.

Fig. 24, shows the percentage of samples that are completely unsolved by each model, i.e. with 0 pass@1. We analyze this metric for T = 0.8, because it leads to more diversity, which would improve this metric. First, when considering non-CoT modes, while GPT-3.5 and GPT-4 (red) are the two best-performing models at pass@1, they perform considerably worse at this metric than models such as Code Llama 34B and DeepSeek Base 33B. Second, instruction-tuned and distilled models (DeepSeek Instruct, Phind, WizardCoder) perform worse than their base counterparts, suggesting that their diversity may have been stifled from adherence to their instruction tuning datasets. Third, we observe that for the two Code Llama models, CoT actually makes this metric worse, but for GPT models, CoT makes it better. For GPT models, we hypothesize that this may be due to the increased diversity of CoT.

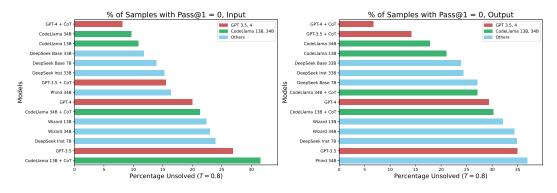


Figure 24: Percentage of samples unsolved, where pass@1 is 0 (T = 0.8)

In contrast, Fig. 25 shows the percentage of samples that models get fully correct, i.e. with a perfect pass@1. We analyze this metric for T = 0.2, as it would lead to more consistency, improving this metric. First, we see that GPT-4 excels, achieving over 60% for both input and output prediction. Second, when comparing base models with instruction tuned models, we see a trend matching the one before: since instruction tuned models are more consistent, they score better on this metric. Third, for output prediction, even though GPT-4 + CoT generally increases diversity, we see that consistency is not sacrificed!

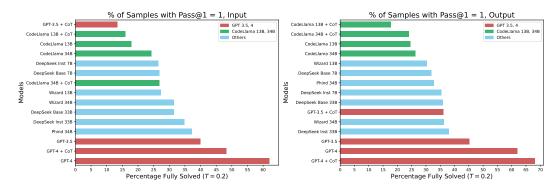


Figure 25: Percentage of samples fully solved, where pass@1 score is 1 (T = 0.2)

D.5 IMPACT OF ANONYMIZING FUNCTIONS

L

As a small ablation to understand the effect of variable names on execution ability, we also test CodeLlama 7B, 13B, and 34B on an anonymized version of a subset of the benchmark, where variable names are replaced with $\times 1$, $\times 2$, \ldots identifiers. An example of an anonymized function is shown in Listing 4. We use the same few-shot prompt without anonymization and report both pass@1 (T = 0.2) and pass@5 (T = 0.8) results on the anonymized benchmark with N = 10 samples. The results are shown in Table 4. This strengthens the case against memorization affects.

	benchmark		

```
Original:
def f(s):
    nums = ''.join(filter(lambda c:c.isdecimal(), s))
    if nums == '': return 'none'
    m = max([int(num) for num in nums.split(',')])
    return str(m)
assert f('01,001') == '1001'
Anonymized:
def f(x0):
    x1 = ''.join(filter(lambda x2: x2.isdecimal(), x0))
    if x1 == '':
        return 'none'
    x3 = max([int(x4) for x4 in x1.split(',')])
```

```
return str(x3)
assert f('01,001') == '1001'
```

Model	Anonymized	Input Prediction		Output Prediction	
	monymized	Pass@1	Pass@5	Pass@1	Pass@5
	×	36.6%	48.0%	36.4%	43.5%
CodeLlama 7B	\checkmark	37.5%	53.3%	34.0%	46.9%
	Δ	+0.9%	+5.3%	-2.4%	+3.4%
	×	39.0%	50.2%	38.3%	44.7%
CodeLlama 13B	\checkmark	40.0%	55.8%	36.1%	50.6%
	Δ	+1.0%	+5.6%	-2.2%	+5.9%
CodeLlama 34B	×	46.5%	57.4%	41.1%	47.5%
	1	48.0%	63.8%	39.1%	54.0%
	Δ	+1.5%	+6.4%	-2.0%	+6.5%

Table 4: Impact of Anonymization on CRUXEVAL

D.6 IMPACT OF DATA-GENERATING MODEL

In the early phases of this work, we were concerned that using Code Llama 34B to generate the benchmark would give the model an unfair advantage. Therefore, we checked the performance of a few models when generating data with Code Llama 13B, GPT-3.5, and GPT-4. The results are shown in Table 5.

These samples were generated using a different prompt and a much more relaxed filter, so the raw scores differ from those in the main text. Across all datasets, we see that the relative ordering of Code Llama 13B, Code Llama 34B, and GPT-3.5 are preserved. We also observed that generating data with GPT-3.5 led to a significantly easier benchmark. After looking at a few samples manually, we believe this is because the resulting inputs are much more predictable and guessable, such as f("abcde") rather than f("mai2!"). Including few-shot examples with random inputs did not improve this issue, and we believe this is an artifact of instruction tuning. We believe that together with the anonymization results in Appendix D.5, these results provide some evidence that evaluating a model on its own generated data does not seem to provide it a significant advantage.

Data Model	Evaluation Model	Input Pass@1	Output Pass@1
CL 13B	CL 13B	28.1%	28.4%
CL 13B	CL 34B	33.8%	29.2%
CL 34B	CL 13B	25.1%	24.3%
CL 34B	CL 34B	29.9%	25.4%
CL 34B	GPT-3.5	40.5%	36.6%
GPT-3.5	CL 13B	42.3%	49.7%
GPT-3.5	CL 34B	52.1%	50.7%
GPT-3.5	GPT-3.5	67.1%	67.2%
GPT-4	CL 13B	28.1%	42.4%
GPT-4	CL 34B	37.0%	44.6%

Table 5: Impact of Data Generating Model

D.7 FINE-TUNING

We discover three interesting insights from fine-tuning. In the main text, we only discuss insight 3. As a refresher, we fine-tuned CODE LLAMA 34B on 138889 samples of Python functions distilled with the procedure outlined in Sec. 3, without filtering. For the output prediction task, the model was fine-tuned on assertions of the form assert f(input) = output, and for the

input prediction task, the model was fine-tuned on assertions of the form assert output == f(input). During evaluation time, the fine-tuned model was asked to complete assertions of the same format as given in fine-tuning.

1. Direct fine-tuning leads to modest performance improvements: In the first setup, we analyze a stronger decontamination setup than that in the main text. Specifically, we remove samples that match functions used in the benchmark, even if the input-output pairs are different. In Fig. 26, we show the train and test accuracy of the model during the finetuning process. For ease of evaluation, the train accuracy is reported on a random subset of 500 samples from the finetuning set. The reported test accuracy is on a superset of CRUXEVAL.

First, we observe that fine-tuning is able to significantly increase performance on both input and output prediction tasks. Second, we observe that while the training accuracy is steadily increasing and the model is able to overfit the training set, the testing accuracy plateaus relatively quickly. This suggesting that simple fine-tuning may not be enough to achieve near-perfect scores on CRUXEVAL. Third, we observe that it is easier to overfit the training set on the output prediction benchmark than on the input prediction benchmark. We hypothesize this may be partially due to the fact that assert output == f(input) is a less natural format for assertions and partially due to the fact that input prediction requires a more sophisticated level of reasoning compared to output prediction.

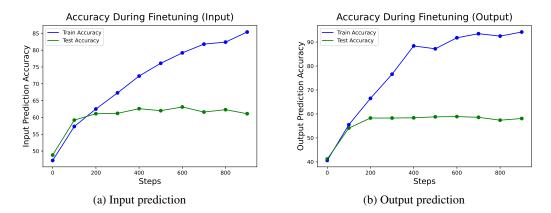


Figure 26: Train accuracy (500 random samples) and test accuracy (superset of CRUXEVAL) while finetuning. For both tasks, there is improvement, and the model steadily fits the training set while plateauing on the testing set.

2. The format of fine-tuning data greatly impacts its effectiveness: We also discovered that it is important that the finetuning assertions be formatted in the same way as when evaluating the model at test time. As evidence of this, we fine-tune CODE LLAMA 34B with two different sets of assertions, one on assert output == f(input) assertions and the other on assert f(input) == output assertions. We compare the accuracy of the two finetuned models on both input and output prediction in Fig. 27. We observe that when the format of the fine-tuning data and the testing data are different, the model even has difficulty overfitting the training set, showing that it may not have fully learned the equivalence of the two formats and the meaning of the == operator. This is perhaps another example of the "reversal curse" of LLMs (Berglund et al., 2023). The corresponding testing accuracy also plateaued at a lower accuracy when the format was misaligned. For example, in Fig. 27a, comparing the light green line with the light blue line shows almost a 10% difference in testing accuracy for input prediction when trained on a misaligned format. That being said, fine-tuning still improved performance relative to the base model, even with a mismatched format, showing that the fine-tuning with a mismatched format did still instill some information into the model.

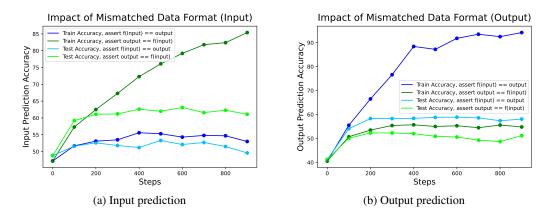


Figure 27: Aligning the fine-tuning data format with the evaluation data format is very important for benchmark performance.

3. Including benchmark programs still cannot improve test accuracy beyond 70%: Finally, we explore the upper limits of fine-tuning on functions and assertions via a "cheating" setup. We curate a small set of 7259 samples consisting only of programs in the benchmark but with different input-output pairs. We finetune on a mixture of 50% of the original finetuning set and 50% of this new set, showing the training and testing accuracy over time in Fig. 28. Despite finetuning on programs very similar to the benchmark, we still observe a plateauing effect in the test accuracy, suggesting that our execution tasks may be too difficult to learn from this simple fine-tuning scheme. Therefore, we suggest a few more fine-tuning ideas for improving our benchmark in Sec. A.

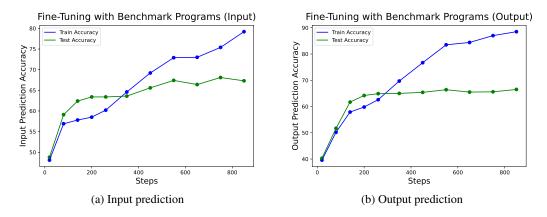


Figure 28: Finetuning 50% on the original finetuning set and 50% on "cheating" data

E PROMPTS

In this section, we list all the prompts we use throughout the paper. Other than ensuring that generations could be parsed properly, all prompts were not optimized towards any particular models.

E.1 BENCHMARK GENERATION FEW-SHOT PROMPTS

Listing 5: All few-shot examples used for benchmark generation

```
string_1 = """[TASK]
str.split
[/TASK]
[PYTHON]
def f(text):
     words = text.split()
     result = []
     for i in range(len(words)):
         if i % 2 == 0:
              result.append(words[i][::-1])
          else:
    result.append(words[i].upper())
return ' '.join(result)
[/PYTHON]
[TEST]
assert f("am7 fiDfd n") == ??
assert f("bnasadl") == ??
assert f("a j c n x X k") == ??
assert f("98 bask2 asoijdf9") = ??
assert f("") == ??
[/TEST]"""
string_2 = """[TASK]
str.capitalize
[/TASK]
 [PYTHON]
def f(text):
    a = []
     words = text.split(' ')
     for i in range(len(words)):
         if words[i][0].isdigit():
               return 'no'
          if i%2 == 0:
              a.append(words[i].capitalize())
          else:
              a.append(words[i])
     return ' '.join(a)
[/PYTHON]
[TEST]
assert f("20xk flkawhf") == ??
assert f("lkw hj sfaibw fi 9") == ??
assert f("abbot 2929 mbpu") == ??
assert f("rotor zisxrs fh29nx") == ??
assert f("pxk 5 bxD 9") == ??
[/TEST]"""
string_3 = """[TASK]
str.rindex
[/TASK]
[PYTHON]
def f(text, char):
     index = text.rindex(char)
     result = list(text)
     while index > 0:
         result[index] = result[index-1]
          result[index-1] = char
         index -= 2
     return ''.join(result)
[/PYTHON]
[TEST]
litbij
assert f('mnjs krupa', 'u') == ??
assert f('kqwomn0xj', 'm') == ??
assert f('qpfi jzm', 'j') == ??
assert f('102x0zoq', '0') == ??
assert f('nzu ei,', 'e') == ??
[/TEST]"""
string_4 = """[TASK]
str.rpartition
```

```
[/TASK]
[PYTHON]
def f(text, char):
    if char in text:
          pref, char, suff = text.rpartition(char)
suff = suff[:-len(char)] + char + suff[len(char):]
           return suff + pref
     return text
[/PYTHON]
[TEST]
assert f('smswfwe-r', '-') == ??
assert f('smswiwe'r', 'e') == ??
assert f('yz84701', '2') == ??
assert f('nviz0h2ja', 'c') == ??
assert f('aaa0a1', 'a') == ??
[/TEST]"""
string_5 = """[TASK]
str.center
[/TASK]
[PYTHON]
def f(text):
     ls = list(text)
     for i in range(1, len(ls) - 1):
    ls.insert(i, '+')
return ''.join(ls).center((len(ls) - 1) * 2)
[/PYTHON]
[TEST]
assert f('lynel') == ??
assert f('nzoh') == ??
assert f('u') == ??
assert f('anfsoixz') == ??
assert f('xzd') == ??
[/TEST]"""
list_1 = """[TASK]
list.pop
[/TASK]
[PYTHON]
def f(names, num):
    queue = names
     while len(queue) > 1:
         for _ in range(num):
                queue.append(queue.pop(0))
           queue.pop(0)
     return queue.pop()
[/PYTHON]
[TEST]
(lib);
assert f(['aiwn', 'xke', 'mpwiy'], 2) == ??
assert f(['y', 'z', 'cc', '2', '5', '.', 'zksdfjn'], 7) == ??
assert f(['98bfaj', 'cnll', 'fakldj', 'tjasl', 'a'], 10) == ??
assert f(['aghbvm'], 1) == ??
assert f(['mnv', 'fjw', 'fnk'], 0) == ??
[/TEST]""'
list_2 = """[TASK]
list.insert
[/TASK]
[PYTHON]
def f(text, position, value):
     length = len(text)
     index = position % (length + 1)
     if position < 0 or index < 0:
          index = length // 2
     new_text = list(text)
     new_text.insert(index, value)
     return ''.join(new_text)
[/PYTHON]
[TEST]
assert f('h grateful k', 3, 'h') == ??
assert f('ugiatedi x', 5, m') == ??
assert f('coscifysu', 0, 'd') == ??
assert f('fnmart', 4, 'o') == ??
assert f('rzti', -1, 'a') == ??
[/TEST]""
list_3 = """[TASK]
list.remove
[/TASK]
[PYTHON]
def f(array, elem):
```

```
array.reverse()
    try:
        while elem in array:
            array.remove(elem)
    finally:
       array.reverse()
    return array
[/PYTHON]
[TEST]
assert f([-1, 2, 1, -8, 2], 2) == ??
assert f([], 2) == ??
assert f([1], 1) == ??
assert f([3, 6, 4, -2, 5], 4) == ??
assert f([3, 2, 1, 2, 7, 1], 1) == ??
[/TEST]"""
list 4 = """[TASK]
list.append
[/TASK]
[PYTHON]
def f(nums):
    count = len(nums)
    for i in range(-count+1, 0):
       nums.append(nums[i])
    return nums
[/PYTHON]
[TEST]
assert f([2, 6, 1, 3, 1]) == ??
assert f([7, 1, 2, 6, 0, 2]) == ??
assert f([4, 3, 2, 1, 2, -1, 4, 2]) == ??
assert f([0, 6, 2, -1, -2]) == ??
assert f([-6, -2, 1, -3, 0, 1]) == ??
[/TEST]""'
list_5 = """[TASK]
list.index
[/TASK]
[PYTHON]
def f(nums, swap1, swap2):
    i1 = nums.index(swap1)
    i2 = nums.index(swap2)
    nums[i1], nums[i2], nums[i1 + 1], nums[i2 + 1] = nums[i2], nums[i1], nums[i2 + 1], nums[i1
     \hookrightarrow + 1]
    return nums
[/PYTHON]
[TEST]
assert f([6, 2, 1, 3, 4, 5], 3, 4) == ??
assert f([1, 1, 5, 3, 1, 2], 1, 2) == ??
assert f([1, 2, 1, 4, 1], 4, 2) == ??
assert f([6, 2, 3, 1, 7, 5, 7], 3, 7) == ??
assert f([2, 8, 8, 3, 8, 3, 9], 3, 2) == ??
[/TEST]""'
```

E.2 DIRECT PREDICTION PROMPTS

In Listings 6, 7, 8, 9, and 10, we include the prompts we use for our evaluation. We use a few-shot prompt for all models other than GPT models. For many models, we observed that using the zero-shot prompt leads to a generation that are not in a easily parsable format, and including the few-shot examples led to predictable formatting. For fairness, we also measured the performance of several few-shot prompts on the GPT models for a randomly sampled subset of the benchmark (instead of the full benchmark for cost reasons). However, we observed a decrease in performance compared to the zero-shot prompt for both input prediction and output prediction. Therefore, we decided to use the zero-shot prompt for GPT models and report numbers using that prompt. In addition, we use a separate output prediction prompt for Phind because the prompt in Listing 8 often led to explanation text before completing the assert.

Listing 6: Input Prediction (non-GPT)

You will be given a function f and an output in the form f(??) == output. Find any input such → that executing f on the input leads to the given output. There may be multiple answers, → but you should only output one. Think step by step before arriving at an answer. → Finally, surround the answer, with no additional words, with [ANSWER] and [/ANSWER] → tags. Express your answer as a function call that when executed will give the output. [PYTHON]

34

```
def f(my_list):
    count = 0
    for i in my_list:
      if len(i) % 2 == 0:
           count += 1
   return count
assert f(??) == 3
[/PYTHON]
[ANSWER]
f(["mq", "px", "zy"])
[/ANSWER]
[PYTHON]
def f(s1, s2):
   return s1 + s2
assert f(??) == "banana"
[/PYTHON]
[ANSWER]
f("ba", "nana")
[/ANSWER]
[PYTHON]
{function}
assert f(??) == {output}
[/PYTHON]
[ANSWER]
```

Listing 7: Input Prediction (GPT)

You will be given a function f and an output in the form output == f(??). Output the → completion of the last line so that the code will run without errors by finding any → input such that executing f on the input leads to the given output. There may be → multiple answers, and you can output any one. Do NOT output any additional information. → {function} assert {output} == f(

Listing 8: Output Prediction (non-GPT, non-Phind)

Listing 9: Output Prediction (GPT)

Listing 10: Output Prediction (Phind)

E.3 CHAIN OF THOUGHT PROMPTS

Below, we include the prompts we use for the chain of thought experiments. For the same reasons mentioned in Appendix E.2, use a one-shot prompt for Code Llama models and a zero-shot prompt for GPT models.

Listing 11: CoT input prediction prompt (Code Llama)

```
You will be given a function f and an output in the form f(??) == output. Your task is to find
     \hookrightarrow any input such that executing f on the input leads to the given output. There may be
    \hookrightarrow multiple answers, but only output one. First, think step by step. Then, surround the
    \hookrightarrow answer with [ANSWER] and [/ANSWER] tags. Express your answer as a function call that
    \hookrightarrow when executed will give the output.
def f(x):
   return x + 1
assert f(??) == 17
To find an input such that executing f on the input leads to the given output, we can work
     \hookrightarrow backwards from the given assertion. We know that f(??) == 17.
Since the function f(x) returns x + 1, for f(??) to be equal to 17, the value of ?? should be
     \hookrightarrow 16.
Therefore, the function call that will give the output as 17 is:
[ANSWER] f (16) [/ANSWER]
{function}
assert f(??) == {output}
```

Listing 12: CoT input prediction prompt (GPT)

You will be given a function f and an output in the form f(??) == output. Your task is to find → any input such that executing f on the input leads to the given output. There may be → multiple answers, but only output one. First, think step by step. Then, surround the → answer with [ANSWER] and [/ANSWER] tags. Express your answer as a function call that → when executed will give the output. {function}

Listing 13: CoT output prediction prompt (Code Llama)

Listing 14: CoT output prediction prompt (GPT)

What should the output of this code be so that the assertion is correct? Reason step by step \hookrightarrow before arriving at an answer. Finally, surround the answer, with no additional words, \leftrightarrow with [ANSWER] and [/ANSWER] tags.

{function}

assert f(??) == {output}

F QUALITATIVE ANALYSIS

In this section, we see some examples of interesting successes and failures of the best performing model, GPT-4, with and without CoT. GPT-4 is relatively sensitive to its prompt, and slight tweaks in the prompt may lead correct examples to fail or incorrect examples to succeed. However, we believe that these examples are nevertheless interesting and reveal insights into the operating modes of GPT-4. Note that some of these examples may not be in the benchmark and were taken from a larger set of generated examples.

F.1 OUTPUT PREDICTION WITHOUT COT

F.1.1 GPT-4 SUCCESSES WITHOUT COT, OUTPUT PREDICTION

Even without CoT, we found that GPT-4 achieves impressively high pass@1 scores on output prediction. We highlight a few GPT-4 successes below that we found impressive, suggesting that GPT-4 has the capability to perform somewhat complex reasoning and code execution.

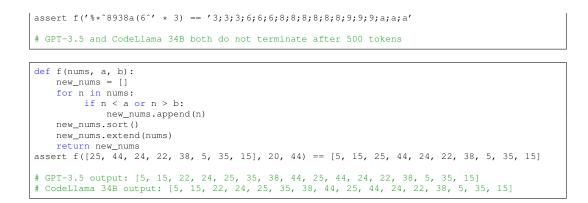
```
def f(text):
    if ',' in text:
        before, _, after = text.partition(',')
        return after + ' ' + before
        return ',' + text.partition(' ')[-1] + ' 0'
    assert f('244, 105, -90') == ' 105, -90 244'
    # GPT-3.5 output: '-90 244'
    # CodeLlama 34B output: '244, 105, -90 0'
```

```
def f(text):
    text = text.lower()
    count = 0
    for char in text:
        if char.isalpha():
            count += 1
    return count
assert f("The computer factory") == 18
# GPT-3.5 output: 3
# CodeLlama 34B output: 16
```

```
def f(text):
    d = {}
    updated = []
    for ch in text:
        if ch in d:
            d[ch] += 1
        else:
            d[ch] = 1
    while len(d) != 0:
        el = d.popitem()
        for i in range(el[1]):
            updated.append(el[0])
    return ''.join(updated)
    assert f('pdrq') == 'qrdp'
# GPT-3.5 output: 'pdrq'
# CodeLlama 34B output: 'gprd'
```

```
def f(a, b):
    b.reverse()
    c = b.copy()
    b.extend(a.copy())
    b.extend(c)
    return b
assert f([5, 2, 3], [4, 9, 3, 1]) == [1, 3, 9, 4, 5, 2, 3, 1, 3, 9, 4]
# GPT-3.5 output: [1, 3, 9, 4, 5, 2, 3]
# CodeLlama 34B output: [4, 9, 3, 1, 5, 2, 3, 4, 9, 3, 1]
```

def f(s):
 ret = ';'.join(sorted([c for c in s if c.isalnum()]))
 return ret



F.1.2 GPT-4 FAILURES WITHOUT COT, OUTPUT PREDICTION

We still find a set of relatively simple failures on output prediction, which we expect would be relatively simple without CoT.

```
def f(nums):
    nums.reverse()
    return "".join(map(str, nums))
assert f([-1, 9, 3, 1, -2]) == '-2139-1'
```

```
# GPT-4 output: "-2, 1, 3, 9, -1"
```

```
def f(nums, num):
    for i in nums:
        if nums[i]==num:
            return num
        return 'Not Found'
assert f({'elad': 186, 'colton': 162, '12': 5}, 5) == '5'
```

GPT-4 output: 'Not found'

```
def f(text):
    dups = list(text)
    dups.append(dups[0])
    return ''.join(dups)
assert f('u') == 'uu'
```

GPT-4 output: 'u'

```
def f(match, fill, n):
    return fill[:n] + match
assert f('9', '8', 2) == '89'
```

```
# GPT-4 output: '889'
```

```
def f(string, prefix):
    if string.startswith(prefix):
        return string.removeprefix(prefix)
        return string
assert f("Vipra", "via") == 'Vipra'
# GPT-4 output: ""
```

F.2 INPUT PREDICTION WITHOUT COT

Similarly, we highlight examples from input prediction.

F.2.1 GPT-4 SUCCESSES WITHOUT COT, INPUT PREDICTION

```
def f(l, elems):
    l.reverse()
    l.extend(elems)
```

```
l.extend(l)
l.reverse()
l.reverse()
del l[(len(l)-1):]
return l
assert f([], [-1, 2, 7, 2, 8]) == [-1, 2, 7, 2, 8, -1, 2, 7, 2]
# GPT-3.5 output: f([2, 7, 2, 8], [-1])
# CodeLlama 34B output: f([-1, 2, 7, 2, 8], [-1, 2, 7, 2])
```

```
def f(text, position):
    length = len(text)
    index = position % length
    if position < 0 or index < 0:
        index = length // 2
    new_text = list(text)
    new_text.pop(index)
    return ''.join(new_text)
assert f('voxnzcuo', 7) == 'voxnzcu'
```

GPT-3.5 output: f('voxnzcu', 42)
CodeLlama 34B output: f('voxnzcu', -4)

```
def f(data, num):
    new_dict = {}
    temp = list(data.items())
    for i in range(len(temp) - 1, num - 1, -1):
        new_dict[temp[i]] = None
    return temp[num:] + list(new_dict.items())
    assert f({2: 10, 3: 1}, 0) == [(2, 10), (3, 1), ((3, 1), None), ((2, 10), None)]
# GPT-3.5 output: f({(2, 10): None, (3, 1): None}, 0)
# CodeLlama 34B output: f({2: 10, 3: 1}, 2)
```

```
def f(nums):
    nums = [y for y in nums if y > 0]
    if len(nums) <= 3:
        return nums
    nums.reverse()
    half = len(nums)//2
    return nums[:half] + [0]*5 + nums[half:]
    assert f([10, -1, 3, 2, -5, -6, 2, 6]) == [6, 2, 0, 0, 0, 0, 0, 2, 3, 10]
```

```
# GPT-3.5 output: f([6, 2, 0, 0, 0, 0, 0, 0, 2, 3, 10])
# CodeLlama 34B output: f([6, 2, 3, 10])
```

```
def f(text):
    upper = 0
    lower = 0
    for i in range(len(text)):
        if text[i].islower():
            lower+=1
        else:
            upper+=1
        if lower > upper:
            return text.swapcase()
        return text
assert f('iAv,sual6eaParntEnthuhsisth, {kasae}') == 'IaV,SUAL6EAPARNTENTHUHSISTH, {KASAE}'
# GPT-3.5 output: f("\'iAv,sual6eaparnteNthuhsisth, {kasae}\'")
# CodeLlama 34B output: f("IaV,sual6eApArnTeNthuhsiStH, {KASAE}")
```

F.2.2 GPT-4 FAILURES WITHOUT COT, INPUT PREDICTION

```
def f(name):
    return [name[0], name[1][::-1][0]]
assert f(??) == ['m', 'a']
# GPT-4 output: f(['m', 'apple'])
```

```
def f(nums):
    if 0 in nums:
        nums.pop(nums.index(0))
        nums.insert(0, 0)
```

```
if 1 in nums:
    nums.pop(nums.index(1))
    nums.append(1)
    return nums
assert f(??) == [0, 0, 1, 0, 1]
# GPT-4 output: f([0, 0, 1, 0, 1])
```

```
def f(text, speaker):
    while text.startswith(speaker):
        text = text[len(speaker):]
    return text
assert f(??) == 'Do you know who the other was? [NEGMENDS]'
```

GPT-4 output: f('Do you know who the other was? [NEGMENDS]', '')

```
def f(text):
    if text.isdecimal():
        return text
    else:
        s = ''.join(sorted(text))
        if s.isdecimal():
            return 'true'
        else:
            return 'false'
assert f(??) == '133476815'
```

GPT-4 output: 134678315

```
def f(length, text):
    if len(text) == length:
        return text[::-1]
    return False
    assert f(??) == False
# GPT-4 output: f(5, "Hello")
```

F.3 OUTPUT PREDICTION WITH COT

F.3.1 GPT-4 SUCCESSES WITH COT, OUTPUT PREDICTION

We see that when equipped with CoT, GPT-4 has some abilities to simulate an execution process, similar to what was seen in (Nye et al., 2021).

In this example, we see both the ability to reason about the flow of the code and the ability to count uppercase letters.

In the next two examples, we see the ability of GPT-4 with CoT to do relatively complex string manipulation tasks.

```
def f(text):
    replaced = list(text)
    while ' ' in replaced: replaced.remove(' ')
```

```
def f(widths):
    reversed names = []
    for skill in sorted(widths, key=widths.get, reverse=True):
        reversed_names.append("{0}={1}".format(widths[skill], skill))
   return '&'.join(reversed_names)
assert f({'craftsmanship':2, 'upholstery':1, 'tailoring':3}) == '3=tailoring&2=craftsmanship
     ↔ &1=upholsterv'
GPT-4: The function f takes a dictionary as an argument. The dictionary keys are skill names
     \hookrightarrow and the values are their corresponding widths. The function sorts the dictionary based
    \hookrightarrow on the values in descending order. Then it creates a list of strings where each
    \hookrightarrow string is a combination of the value and the key separated by an equal sign. Finally,
     \hookrightarrow it joins all the strings in the list with an ampersand (&) and returns the resulting
    \hookrightarrow string.
Let's break down the steps:
1. The dictionary {'craftsmanship':2, 'upholstery':1, 'tailoring':3} is sorted based on the

→ values in descending order, resulting in the list ['tailoring', 'craftsmanship', '
     \hookrightarrow upholstery'].
2. For each skill in the list, a string is created with the format "{value}={key}". The
     ↔ resulting list is ['3=tailoring', '2=craftsmanship', '1=upholstery'].
3. The strings in the list are joined with an ampersand (\&), resulting in the string '3=
     \hookrightarrow \texttt{tailoring\&2=craftsmanship\&1=upholstery'}.
So, the output of the function f({'craftsmanship':2, 'upholstery':1, 'tailoring':3}) should be
```

```
[ANSWER]'3=tailoring&2=craftsmanship&1=upholstery'[/ANSWER]
```

In the next two examples, we see the ability to simulate and reason about for/while loops.

```
def f(nums):
    count = 0
    for i in range(len(nums)):
        if len(nums) == 0:
           break
        if count % 2 == 0:
           nums.pop()
        else:
           nums.pop(0)
        count += 1
    return nums
assert f([3, 2, 0, 0, 2, 3]) == []
GPT-4: The function `f(nums)` takes a list of numbers as input. It initializes a counter `
    \hookrightarrow count' to 0. Then it enters a loop that runs for the length of the list.
In each iteration, it checks if the length of the list is 0. If it is, it breaks the loop.
     \hookrightarrow This condition will never be true because the loop runs for the initial length of the
    \hookrightarrow list and not the current length of the list.
Then it checks if the counter is even. If it is, it removes the last element from the list. If
     \hookrightarrow it's not, it removes the first element from the list.
After each iteration, it increments the counter by 1.
So, for the input list [3, 2, 0, 0, 2, 3], the function will perform the following operations:
```

```
Remove the last element (3) because the counter is 0 (even). The list becomes [3, 2, 0, 0, 

→ 2].
Remove the first element (3) because the counter is 1 (odd). The list becomes [2, 0, 0, 2].
Remove the last element (2) because the counter is 2 (even). The list becomes [2, 0, 0].
Remove the first element (2) because the counter is 3 (odd). The list becomes [0, 0].
Remove the last element (0) because the counter is 4 (even). The list becomes [0].
Remove the first element (0) because the counter is 5 (odd). The list becomes [].
So, the function should return an empty list for the input [3, 2, 0, 0, 2, 3].
```

[/ANSWER]

```
def f(number):
   multiplier = 2
    power = 1
    while number > 0:
        remainder = number % multiplier
        number //= multiplier
        if remainder == 0:
            power += 1
        if number == 1:
            return f'{2 ** power}-free'
assert f(8) == '16-free'
# GPT-4: The function f takes a number as input and checks if it is divisible by 2. If it is,
     \hookrightarrow it increments the power by 1 and continues to divide the number by 2 until the number
    \hookrightarrow is no longer divisible by 2. The function then returns a string that says the number
    \hookrightarrow is "2 to the power of (power + 1)-free".
In the case of the number 8, the function will divide 8 by 2 three times before it is no
     \hookrightarrow longer divisible by 2. This means the power will be incremented three times, from 1 to
    \leftrightarrow 4. Therefore, the function will return the string "2 to the power of 4-free", or "16-
    \hookrightarrow free".
So, the output of the code should be "16-free" for the assertion to be correct.
[ANSWER] "16-free" [/ANSWER]
```

F.3.2 GPT-4 FAILURES WITH COT, OUTPUT PREDICTION

Now, we highlight some failure cases of GPT-4 output prediction with CoT. One interesting failure mode is that the CoT makes a mistake on information that GPT-4 seems to know when prompted independently. For example, in the first example below, the CoT insists that 6173 is less tan 1000. However, when prompted independently, GPT-4 knows this is not true. We provide a few examples of these paired mistakes with proof of knowledge below. The outputs are abbreviated for brevity and to highlight the failures.

The first example shows a failure in number comparison.

```
Prompt: If num = 6173, is it true that 0 < num < 1000 and num != 6174?
```

GPT-4: No, the statement is not true. The variable num is assigned the value 6173, so the → condition 0 < num < 1000 is false because 6173 is not less than 1000. The second → condition, num != 6174, is true because 6173 is indeed not equal to 6174. However, → since the first condition is false, the overall statement is false.

This example is showing a semantic misunderstanding of str.islower.

Prompt: What is the output of the code?

Prompt: What is "816a".islower()?

```
GPT-4: ... The string "816a" contains digits and a lowercase alphabetic character 'a'. Since \hookrightarrow the only alphabetic character in the string is lowercase, the 'islower()' method would \hookrightarrow return 'True' when called on this string...
```

This example shows a failure with sorting " $h \in l l \circ$ ", which seems like it could be a tokenization artifact.

This example shows a failure with the str.strip method.

```
Therefore, the assertion should be:

'''python

assert f('tcmfsmj', 'cfj') == 'mfsm'
```

The output of the code, if the assertion passes, is nothing since assertions do not produce \hookrightarrow output if the condition is true.

Prompt: In Python, what is "jmsfmct".strip("cfj")?

GPT-4: ... Here's what happens step by step:

 \hookrightarrow remove, so the stripping stops at the end of the string without removing anything.

The resulting string after the 'strip' operation will be '"msfmct"'.

In this example, we observe a list indexing error.

Prompt: In Python, what is the value at index -3 of [0, 6, 2, -1, -2, 6, 6]?

In this example, we see a string indexing error.

- <code>`text[-i:]`</code> is <code>`'o5'`</code> (the substring from the character after the current character to the \hookrightarrow end of the string).

Therefore, the function will return $^{\prime\prime}\,\text{BOo5'}\,^{\prime}\dots$

F.4 INPUT PREDICTION WITH COT

F.4.1 GPT-4 SUCCESSES WITH COT, OUTPUT PREDICTION

The following examples highlights code reasoning abilities.

```
def f(text, size):
    counter = len(text)
    for i in range(size-int(size%2)):
        text = ' '+text+' '
        counter += 2
        if counter >= size:
            return text
assert f(??) == '
GPT-4: The function f takes two arguments: a text and a size. It adds spaces to the beginning
    \hookrightarrow and end of the text until the length of the text is greater than or equal to the size.
    \hookrightarrow The function stops adding spaces when the length of the text is greater than or equal
    \hookrightarrow to the size.
In this case, the output is '
                                 7
                                          ', which is a string of length 11. The text in the
     \leftrightarrow middle is '7', which is of length 1. The function adds 5 spaces to the beginning and
    \hookrightarrow end of the text to reach a total length of 11.
So, the input to the function should be '7' and 11.
[ANSWER]
f('7', 11)
[/ANSWER]
```

```
def f(text):
   uppercase_index = text.find('A')
    if uppercase_index >= 0:
        return text[:uppercase_index] + text[text.find('a') + 1 :]
    else:
       return ''.join(sorted(text))
assert f(??) == '
                    DEGHIVjkptx'
GPT-4: The function f takes a string as input. It first checks if there is an uppercase 'A' in
    \hookrightarrow the string. If there is, it removes the first occurrence of lowercase 'a' from the
     \hookrightarrow string and returns the string. If there is no uppercase 'A', it sorts the string in
    \hookrightarrow alphabetical order and returns it.
In this case, the output is ' DEGHIVjkptx', which is a sorted string. This means that the
    \hookrightarrow input string did not contain an uppercase 'A', and the function sorted the string.
To get this output, we can input a string that contains the same characters but in a different
     \leftrightarrow order. For example, the string 'xtpkjVIGHED ' contains the same characters and when
    \,\hookrightarrow\, sorted by the function, it will give the output '
                                                                DEGHIVikptx'.
So, the answer is 'xtpkiVIGHED '.
[ANSWER]
'xtpkjVIGHED
               ,
[/ANSWER]
```

The next example shows some ability in hexadecimal conversion. This may be partially due to memorization and data contamination effects, but this exact hex string was not found after a cursory Google search.

```
def f(text):
    hex_string = text.encode('utf-16')
    result = "0x"
    for c in hex_string:
       result += "%.2X" % c
    return result
assert f(??) == '0xFFFE66006E007700200052006F006D0065002100'
GPT-4: The function f takes a string as input, encodes it in utf-16 format, and then converts
     \rightarrow each character into a hexadecimal representation. The output '0
     ↔ xFFFE66006E007700200052006F006D0065002100' is the hexadecimal representation of a
     \hookrightarrow string in utf-16 format.
To find the input, we need to convert the hexadecimal representation back to a string. We can
     \hookrightarrow do this by first removing the 'Ox' prefix and then converting each pair of hexadecimal
     \hookrightarrow digits back to a character.
The hexadecimal string 'FFFE66006E007700200052006F006D0065002100' corresponds to the utf-16 \hookrightarrow encoded string 'nw Rome!'.
So, the input to the function f that will give the output '0
     → xFFFE66006E007700200052006F006D0065002100' is 'nw Rome!'.
[ANSWER] f('nw Rome!') [/ANSWER]
```

Just like we see in output prediction, GPT-4 is able to reason about non-trivial string manipulation code.

```
def f(text):
     text = text.split(',')
     text.pop(0)
text.insert(0, text.pop(text.index('T')))
return 'T' + ',' + ','.join(text)
assert f(??) == 'T,T,Sspp,G ,.tB,Vxk,Cct'
GPT-4: The function f takes a string as input, splits it into a list of substrings divided by
      \hookrightarrow commas, removes the first element of the list, finds the index of the substring 'T',
      \hookrightarrow removes it from its current position and inserts it at the beginning of the list.
      \hookrightarrow Finally, it joins the list into a string separated by commas and adds 'T' at the
      \hookrightarrow beginning of the string.
To get the output 'T,T,Sspp,G ,.tB,Vxk,Cct', we need to have 'T' as the second element in the
     \leftrightarrow list after splitting the input string by commas. The rest of the elements can be in any \leftrightarrow order. So, one possible input could be 'any,T,Sspp,G,.tB,Vxk,Cct'.
Let's check this:
↔ find the index of 'T' (which is 0), remove it from the list and insert it at the
↔ beginning to get the same list ['T', 'Sspp', 'G', '.tB', 'Vxk', 'Cct'], join the list
↔ into a string 'T,Sspp,G,.tB,Vxk,Cct' and add 'T' at the beginning to get 'T,T,Sspp,G
      \hookrightarrow ,.tB,Vxk,Cct', which is the desired output.
So, the answer is 'any, T, Sspp, G ,.tB, Vxk, Cct'.
[ANSWER] 'any, T, Sspp, G , .tB, Vxk, Cct' [/ANSWER]
```

In the following example, GPT-4 shows simple code analysis abilities, understanding that the first case will produce an error.

```
def f(nums):
    count = len(nums)
    if count == 0:
        nums = [0] * int(nums.pop())
    elif count % 2 == 0:
        nums.clear()
    else:
        del nums[:count//2:]
    return nums
assert f(??) == []
```

F.4.2 GPT-4 FAILURES WITH COT, INPUT PREDICTION

As with output prediction, also notice some relatively simple failures of CoT. One observation is that GPT-4 often tries to check the incorrect input against the assertion and says that it passes, even when it does not. We believe this is not necessarily just due to the lack of execution ability, but a prior that the solution it found is more likely to be correct.

In these first three examples, the model goes directly to a wrong answer without much step-by-step reasoning.

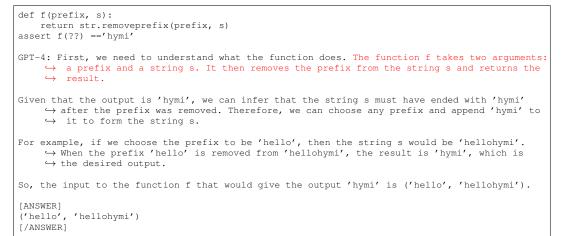
```
def f(text):
    odd = '
    even = ''
    for i, c in enumerate(text):
        if i % 2 == 0:
            even += c
        else:
            odd += c
   return even + odd.lower()
assert f(??) == 'Mmohamt'
GPT-4: The function f takes a string as input and separates the characters at even and odd
     \hookrightarrow indices. It then concatenates the characters at even indices with the characters at
    \hookrightarrow odd indices converted to lowercase.
To get the output 'Mmohamt', we can see that the even indexed characters are 'M', 'o', 'a', 't'
     \hookrightarrow and the odd indexed characters are 'm', 'h', 'm'.
So, the input string can be 'Mmohamt'.
[ANSWER]
f('Mmohamt')
[/ANSWER]
```

```
def f(text):
    string = ''
    for char in text:
       string += char + char.lower()
   return string
assert f(??) == 'llaallaakk'
GPT-4: The function f takes a string as input and for each character in the string, it appends
     \hookrightarrow the character itself and its lowercase version to a new string. The function then
    \hookrightarrow returns this new string.
Given the output 'llaallaakk', we can see that each character is repeated twice, once in its
    \hookrightarrow original form and once in lowercase. This means that the input string must have been
    \hookrightarrow LAK'.
So, the input that leads to the given output when passed to function f is 'LAK'.
[ANSWER]
'LAK'
[/ANSWER]
```

def f(nums, i):
 nums.append(nums.pop(i % len(nums)))
 nums[i % len(nums)] = '?'
 split = nums[::2]
 split.remove('?')

So, the input f([2, 4, 4, 4], 1) will give the output [2, 4, 4].

The following example is a bit tricky, because the naming of the variables does not match the semantics of str.removeprefix.



The following example shows a case where GPT-4 "checks" the forward execution incorrectly.

```
def f(text):
    count = len(text)
    for i in range(-count+1, 0):
        text = text + text[i]
    return text
assert f(??) =='wlace Alc 1 '
GPT-4: The function f takes a string as input and appends the characters from the end of the \hookrightarrow string to the string itself. The number of characters appended is equal to the length
     \hookrightarrow of the original string minus one.
To get the output 'wlace Alc l ', we need to find a string that when appended with its last
      By observing the output, we can see that the last 3 characters are spaces. This means that the
     \hookrightarrow last 3 characters of the original string must also be spaces.
The first character of the output is 'w', which is the first character of the original string. \hookrightarrow The second character of the output is 'l', which is the last character of the
     \hookrightarrow original string.
From this, we can infer that the original string is 'w l \ '.
Let's check this:
f('w l ') = 'w l ' + ' l ' = 'wlace Alc l '}
So, the input that gives the output 'wlace Alc l \, ' when passed to the function f is 'w l \, '.
```

So, the answer is: [ANSWER] 'w l ' [/ANSWER]

F.4.3 GPT-4 FAILURES WITH COT, EXAMPLES REQUIRING INSIGHTS

Unlike output prediction, where stepping through the code line by line suffices, some input prediction examples require insights and observations that can be difficult for models like GPT-4 to make. These examples are a bit more challenging, and passing them can require making these insights. Here, we highlight some of these examples, corresponding relevant insights, and GPT-4's failure modes.

In the following example, new_nums consists of a sorted portion and an unsorted portion. One insight is that the sorted portion must be a subarray of the unsorted portion. GPT-4 always takes [5, 15, 25, 44] to be the sorted portion and [24, 22, 38, 5, 35, 15] to be the unsorted portion, which cannot be the case because 44 (from the sorted portion) is not in the unsorted portion.

```
def f(nums, a, b):
    new_nums = []
    for n in nums:
        if n < a or n > b:
            new_nums.append(n)
        new_nums.sort()
        new_nums.extend(nums)
        return new_nums
    assert f(??) == [5, 15, 25, 44, 24, 22, 38, 5, 35, 15]
```

In the following example, the simplest solution is to bypass the while loop completely, but the model does not find it. However, the model chooses an output like "baec" because it back-translates the "a" to "i" using the translation table. Unfortunately, it does not take into account that other characters also get translated in the translation table.

```
def f(input_string):
    table = str.maketrans('aioe', 'ioua')
    while 'a' in input_string or 'A' in input_string:
        input_string = input_string.translate(table)
    return input_string
assert f(??) == 'biec'
```

In the following example, one must notice that x cannot end with a number and y cannot start with a number. Reasoning about x+y = 'nisou79-85233', GPT-4 incorrectly deduces that the y portion must be 85233, while in reality, it must be 79-85233 because x cannot end with a digit.

```
def f(urn):
    pieces = urn.split('--')
    x = pieces[0].rstrip('0123456789')
    y = pieces[1].lstrip('0123456789')
    return x+y
assert f(??) == 'nisou79-85233'
```

In the following example, it is very easy to solve the task by choosing source and target to make target in source false, going directly to the last line. However, GPT-4 tries to go down the more complicated path.

```
def f(source, target):
    if target in source:
        prefix, suff = source.split(target)
        prefix = prefix[:len(prefix) // 2] + target + prefix[len(prefix) // 2:]
        return prefix + suff
    return source
assert f('abcjava', 'python') =='abcjava'
```

In the following example, an important insight is that the last line of the function is a "....".join(), but that "...." does not occur in the output. This confuses the model.

```
def f(letters):
    letters_only = letters.strip("., !?*")
    return "....".join(letters_only.split(" "))
assert f(??) =='h,e,l,l,o,wo,r,ld'
```

F.5 SIMPLE AND ISOLATED GPT-4 FAILURES

Some of the failures from both input prediction and output prediction can be isolated to capabilities on smaller subtasks. Here, we highlight some interesting subtasks, as well as GPT-4's response to these subtasks.

```
Prompt: In Python, what is " BaB ".rfind(" B ")?
GPT-4: In Python, the `rfind()` method of a string object returns the highest index of the
     \hookrightarrow substring if found in the given string. If the substring is not found, it returns -1.
The string `" BaB "` has a space, followed by a capital 'B', followed by another space as the
     \hookrightarrow substring we are looking for with 'rfind(" B ")'.
Let's break down the string `" BaB "`:
- Index 0: space (' ')
- Index 1: 'B'
- Index 2: 'a'
- Index 3: 'B'
- Index 4: space (' ')
We are looking for the substring " B "' (space, 'B', space). This substring appears only once
     \leftrightarrow in the string, starting at index 3 and ending at index 5 (if we consider the space \leftrightarrow after the last 'B').
Therefore, '" BaB ".rfind(" B ")' will return 3, because that is the highest index at which
     \hookrightarrow the substring `" B "` starts.
Prompt: In Python, if I have a string s = 'iabnm""", what is s[1::2]?
GPT-4: In Python, the slicing operation `s[start:stop:step]` allows you to extract a substring
     \hookrightarrow from a string 's' by specifying a starting index 'start', a stopping index 'stop',
\hookrightarrow and a step 'step'. If 'start' is omitted, it defaults to the beginning of the string (
     \hookrightarrow index 0). If 'stop' is omitted, it defaults to the end of the string. If 'step' is
     \hookrightarrow omitted, it defaults to 1.
In your example, 's[1::2]' means that you want to start at index 1 of the string 's', go until
     \hookrightarrow the end of the string (since no stop index is provided), and select every second
     \hookrightarrow character (because the step is 2).
Given the string 's = 'iabnm" 'i let's break down what 's[1::2]' will return:
- Start at index 1: 'a'
```

```
- Every second character from index 1: 'abnm~~~~~~ -> 'an~'
```

```
So, `s[1::2]` will return the string `'an `'`.
```

Prompt: In Python, what is "+".join(['*', '+', 'n', 'z', 'o', 'h'])?

```
Prompt: In Python, if text = "!123Leap and the net will appear" and res = 123, what is text[
     \hookrightarrow len(str(res)):]?
GPT-4: In the given Python code snippet, you have a string 'text' and an integer 'res'.
'''python
text = "!123Leap and the net will appear"
res = 123
You want to know what 'text[len(str(res)):]' evaluates to. Let's break it down step by step:
1. 'str(res) ' converts the integer 'res' to a string, which is `"123"'.
2. `len(str(res))` calculates the length of the string `"123"`, which is `3`.
3. `text[len(str(res)):]` slices the string `text` starting from the index equal to the length
    \hookrightarrow of the string representation of `res` (which is `3`) to the end of the string.
So, `text[len(str(res)):]` will return the substring of `text` starting from the 4th character
    \hookrightarrow (since indexing in Python starts at 0) to the end of the string.
The 4th character in the string 'text' is the character ''L'' (the first three characters are
     \leftrightarrow `"!12"`), so the result will be:
''python
"Leap and the net will appear"
This is the substring of 'text' starting from the 4th character to the end.
Prompt: In Python, what is "pomodoro".replace("or", "pomodoro")?
```

F.6 FAILING GEMS

Next, we identify a collection of examples that we find GPT-4 often fails on, even with CoT. Some of these examples overlap with examples shown above, but others are new. Overall, we believe this collection of examples provides an interesting lens to understand the behaviour of GPT-4 on input and output prediction.

```
F.6.1 FAILING GEMS, OUTPUT PREDICTION
```

```
def f(nums):
   for i in range(-len(nums), 0):
       nums.insert(-i, nums[i])
   return nums
assert f([-6, -2, 1, -3, 0, 1]) == [-6, -6, -2, 1, 1, 1, -3, 0, 0, 1, 1, -6]
def f(text):
   if not text.islower():
       temp_text = '
       for i in range(len(text)):
           if text[i].islower():
               temp_text += text[i]
       return temp_text
   return text
assert f("816a") == '816a'
def f(list, separator):
   text = separator.join(list)
   return separator.join(reversed(text))
```

```
assert f(['is', 'it', 'top'], '0') == 'p0o0t000t0i000s0i'
def f(text, res):
   for c in '*\n"':
       text = text.replace(c, '!' + str(res))
    if text.startswith('!'):
       text = text[len(str(res)):]
   return text
assert f('"Leap and the net will appear', 123) == '3Leap and the net will appear'
def f(num):
   if 0 < num < 1000 and num != 6174:
       return 'Half Life'
   return 'Not found'
assert f(6173) == 'Not found'
def f(date):
   return date[6:] + date[4:6] + date[0:4]
assert f("08-10-2009") == '20090-08-1'
def f(text, suffix):
    if suffix and suffix[-1] in text:
       return f(text.rstrip(suffix[-1]), suffix[:-1])
    elset
return text
assert f('rpyttc', 'cyt') == 'rpytt'
def f(s, x):
   count = 0
    for i, c in enumerate(s):
       if x in s[i:] and x not in s[:i]:
           count += 1
   return count
assert f('fvyijrtwrjrsasgt', 'g') == 15
def f(text):
    segments = text.split()
    for i in range(len(segments)):
       segments[i] = segments[i][0].upper() + segments[i][1:-1] + segments[i][-1].upper()
   return ' '.join(segments)
assert f("hey !") == 'HeY !!'
def f(pattern, items):
    result = []
    for text in items:
       pos = text.rfind(pattern)
       if pos >= 0:
           result.append(pos)
   return result
assert f(" B ", [" bBb ", " BaB ", " bB", " bBbB ", " bbb"]) == []
def f(str):
   return str and ''.join(sorted(str))
assert f("h e l l o") == '
                           ehllo'
def f(t):
   return t.replace('or', t.center(len(t), 'o'))
assert f("pomodoro") == 'pomodpomodoroo'
```

F.6.2 FAILING GEMS, INPUT PREDICTION

```
def f(dimension):
    dinline = str(dimension)[1:].zfill(2)
    return dinline[0] * int(dinline[1])
assert f(??) == 'kkkkk'
def f(text):
    for elem in text:
        if elem.isupper():
            try:
                text.remove(elem)
                except ValueError:
                     pass
    return text
assert f(??) == ''
def f(text):
    ls = list(text)
```

```
for i in range(0, len(ls)):
        if ls[i]!='+':
            ls.insert(i, '+')
            ls.insert(i, '*')
            break
return '+'.join(ls)
assert f('nzoh') == '*+++n+z+o+h'
def f(text):
   new_text = list(text)
    dict = {}
    for char in new_text:
       dict[char] = new_text.count(char)
    return dict
assert f('aaabbbccdddzz') == {'a': 3, 'b': 3, 'c': 2, 'd': 3, 'z': 2}
def f(text):
   odd = ''
    even = ''
    for i, c in enumerate(text):
        if i % 2 == 0:
           even += c
        else:
           odd += c
   return even + odd.lower()
assert f('Mammoth') == 'Mmohamt'
def f(nums, i):
   nums.append(nums.pop(i % len(nums)))
nums[i % len(nums)] = '?'
    split = nums[::2]
    split.remove('?')
    return split + nums[1::2]
assert f([4, 2, 4, 2], 0) == [2, 4, 4]
def f(prefix, s):
    return str.removeprefix(prefix, s)
assert f('hymi', 'hymifulhxhzpnyihyf') == 'hymi'
def f(text):
   if ',' in text:
    before, _, after = text.partition(',')
return after + ' ' + before
return ',' + text.partition(' ')[-1] + ' 0'
assert f('244, 105, -90') == ' 105, -90 244'
def f(s):
    return '{}{}{}'.format(s[3:], s[2], s[5:8])
assert f('jbucwc') == 'cwcuc'
def f(nums):
    for i in range(len(nums)):
       nums.insert(i, nums[i]**2)
    return nums
assert f([1, 2, 4]) == [1, 1, 1, 1, 2, 4]
def f(c, text):
    t = c
    for c in reversed(text):
       t = c + t * 2
        t = c + t
   return t + text
assert f(';?', 'i') == 'ii;?;?i'
def f(nums, location, item):
   if len(nums) >= location and 0 <= location:
       return nums.insert(location, item)
    return nums
assert f([1, 2, 3, 4, 5, 6], -5, -5) == [1, 2, 3, 4, 5, 6]
def f(text):
   return max(text.find(ch) for ch in 'aeiou')
assert f("qsqgijwmmhbchoj") == 13
```