Breaking the Attention Trap in Code LLMs: A Rejection Sampling Approach to Enhance Code Execution Prediction

Anonymous ACL submission

Abstract

Code-specific Large Language Models (Code LLMs) have greatly improved performance across code-related tasks, offering substantial benefits in practical applications. However, existing research reveals significant performance bottlenecks in Code Execution tasks, which requires models to predict the execution results of given code snippets. This study identifies that, the *Attention Trap* phenomenon in training data constitutes a key constraint on model performance. To address this phenomenon, we propose the Attention Cracking with Rejection Sampling (AC-RS) method. The method first applies structural optimization to training data to eliminate attention traps. Then, it conducts secondary training on the outputs generated by the fine-tuned model to mitigate potential negative impacts from manual data intervention. Experimental results show that AC-RS significantly enhances the accuracy of Code Execution while preserving models' original capabilities. Notably, the optimized 7B model achieves prediction accuracy comparable to 32B model and GPT-4o.

1 Introduction

With the rapid advancement of large language models (LLMs) (OpenAI, 2022; Ouyang et al., 2022; OpenAI et al., 2024; Touvron et al., 2023a,b; Grattafiori et al., 2024; Bai et al., 2023; Yang et al., 2024), Code LLMs have attracted substantial academic and industrial attention due to their direct applicability and broad potential. From early models like StarCoder (Li et al., 2023) and CodeLlama (Rozière et al., 2024) to recent advancements including Deepseek Coder (Guo et al., 2024; DeepSeek-AI et al., 2024) and Qwen Coder (Qwen-Team, 2024; Hui et al., 2024), Code LLMs have shown remarkable performance across code-related tasks.

However, studies (Austin et al., 2021; Nye et al., 2021; Gu et al., 2024) indicate that current Code LLMs underperform in Code Execution tasks. Austin et al. (2021) reveals that even 137B model struggles to predict execution results of basic Python code, achieving merely 29% accuracy on test case from the proposed MBPP benchmark, while fine-tuning only provides minimal performance gains. Nye et al. (2021) attributes this to the lack of explicit step-by-step reasoning before giving the predicted results. While previous work focuses on reasoning deficiencies, our work reveals that attention traps in widely-used LeetCode[1] training data fundamentally constrain execution prediction capabilities.

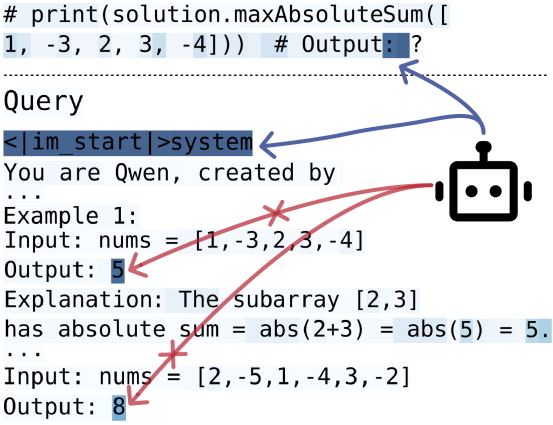

Figure 1: *Attention Trap* in Leetcode data.

When models process training data with lexical similarities, their attention mechanisms become overly focused on surface-level token correlations while neglecting deeper abstract relationships between data components. We term this phenomenon the "*Attention Trap*". In Code Execution tasks using LeetCode data, this issue becomes prominent. Figure 1 demonstrates how trained model distributes attention during Code Execution predictions. The presence of target outputs "5" in Query creates strong attention biases. During learning, models excessively attend to these reference out-

[1] https://leetcode.com/

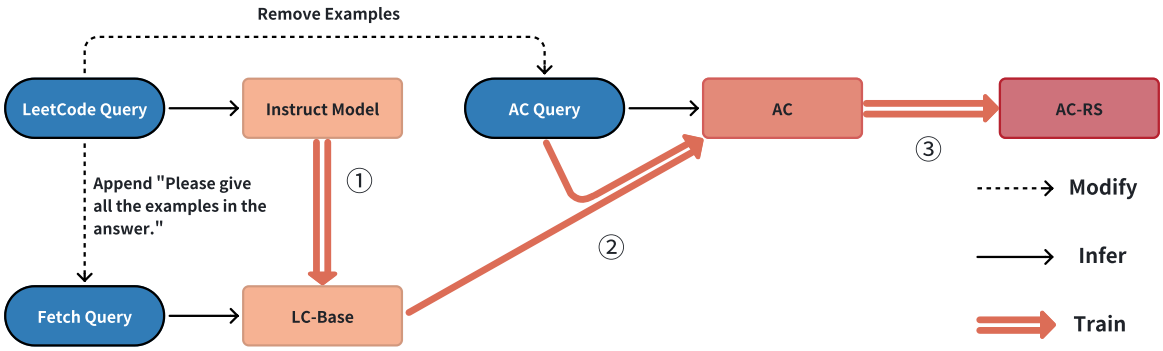

Figure 2: Pipeline of Attention Cracking with Rejection Sampling (AC-RS).

puts in the input queries, sometimes even forming erroneous correlations with unrelated examples("8" in example). This prevents proper modeling of the multi-step reasoning chain connecting problem descriptions, program code, and execution results. Full example and comparations are provided in Appendix A.

To eliminate attention traps in training data, we propose Attention Cracking with Rejection Sampling. Our method contains two stages: (1) Attention Cracking (AC) modifies training data to eliminate attention traps; (2) Rejection Sampling (RS) (Liu et al., 2024b) employs self-generated model outputs for secondary training, preventing performance degradation from manual data modifications. Experimental results demonstrate that AC-RS significantly improves performance with minimal data requirements. Using only 1,000 LeetCode samples, our method achieves 13.57% improvements on the Code Execution tasks of LiveCodeBench (Jain et al., 2024). It also shows 10.96% gains on Test Output Prediction tasks, which require predicting results from problem descriptions rather than code, while maintaining code generation capabilities. Remarkably, the enhanced 7B-Instruct model matches the Code Execution accuracy of 32B-Instruct model and GPT-4o-20240806 (OpenAI, 2024).

2 Related Works

The field of Code LLMs originated from data-centric methodologies and has gradually developed into a thriving research area (Jiang et al., 2024). Early studies in code-related domains adopted data construction methods from general-purpose domains. For instance, Chaudhary (2023) employed the Self-Instruct (Wang et al., 2023) approach to automatically generate code instruction dataset CodeAlpaca. Luo et al. (2023) further enhanced this dataset through Evol-Instruct (Xu et al., 2023), training the WizardCoder model. Additionally, Magicoder (Wei et al., 2024) attempted to generate high-quality instruction tuning data using open-source code. As data-related challenges were progressively addressed, multiple high-performance open-source code models emerged. Representative examples include the Qwen Coder series and DeepSeek Coder series. Concurrently, researchers achieved notable progress in other dimensions of code-related tasks. Frameworks like MFTCoder (Liu et al., 2024a) and models like Phi (Abdin et al., 2024) advanced the field through multi-task training strategies and parameter efficiency improvements, respectively.

3 Method

This section details the implementation of AC-RS method. To ensure fair comparison and better prepare for subsequent training data generation, we first train LC-Base model using Leetcode data through Rejection Sampling (① in Figure 2). AC-RS method then introduces two formal stages: Attention Cracking and Rejection Sampling.

3.1 Attention Cracking

The AC stage aims to eliminate attention traps. Concretely, by removing target outputs from queries, we prevent models from relying on superficial pattern matching. The AC stage modifies LeetCode queries through two operations: (1) **AC Queries**: Remove target outputs from examples in original queries for training. (2) **Fetch Queries**: Append "Please give all the examples in the answer." at query endings, increasing the

Table 1: Accuracy(%) on LiveCodeBench. Qwen2.5-Coder, DeepSeek-Coder, CodeLlama are all Instruct models.

Model	Size	Code Gen	Self Repair	Test Output Prediction	Code Exec w/ COT	Code Exec w/o COT	Avg
GPT-4o-0806	-	49.35%	59.75%	76.02%	96.24%	58.04%	67.88%
Qwen2.5-Coder	32B	52.61%	62.25%	70.81%	89.35%	57.41%	66.49%
CodeLlama	7B	10.29%	10.50%	25.11%	27.97%	20.46%	18.87%
DeepSeek-Coder	6.7B	19.44%	24.25%	26.02%	35.91%	39.67%	29.06%
Qwen2.5-Coder	7B	36.44%	45.75%	49.55%	68.06%	44.68%	48.90%
LC-Base	7B	38.07%	48.50%	54.52%	72.86%	48.23%	52.44%
AC	7B	37.42%	46.75%	57.92%	70.98%	58.04%	54.22%
AC-RS	7B	39.54%	47.75%	60.41%	71.19%	58.25%	55.43%

likelihood of including examples in retrieved results. Fetch Queries collect generation results from the LC-Base model. Generated data is processed by selecting responses with the same examples as queries, prioritizing those passing tests. This filtering criterion applies to both LC-Base and RS stage outputs.

3.2 Rejection Sampling

To prevent performance degradation from AC stage data modifications, we introduce a RS stage. This mechanism directly uses AC queries to obtain outputs from AC-trained models, eliminating attention distortion caused by query-output mismatches. Through quality filtering of model-generated responses, RS substantially reduces training difficulty while mantaining data quality. Notably, we pre-applied Rejection Sampling in both LC-Base model and AC model training stages and incorporated 30 additional samples to ensure instruction following.

In implementation, we encountered output formatting issues when applying RS with LeetCode data(Appendix B). To resolve this, we developed specialized Helper models by combining CodeAlpaca samples (Chaudhary, 2023) with LeetCode/Fetch/AC queries. These Helper models effectively replace direct model generations for training purposes.

4 Experiments

4.1 Datasets & Models

During training, we validate the AC method using LeetCode data from Shen and Zhang (2024). To build helper models, we randomly select 10,000 samples from CodeAlpaca (Chaudhary, 2023) and obtain corresponding outputs via GPT-4o-20240806 (OpenAI, 2024). For evaluation, we employ LiveCodeBench (Jain et al., 2024), HumanEval (HE) (Chen et al., 2021) and MBPP (Austin et al., 2021) benchmarks with the EvalPlus framework (Liu et al., 2023) to assess AC-RS effectiveness.

Table 2: Accuracy(%) on HE and MBPP. Qwen* represents Qwen2.5-Coder-7B-Instruct.

Model	HE	HE+	MBPP	MBPP+
Qwen*	87.19%	82.20%	83.33%	71.67%
LC-Base	86.10%	80.30%	84.92%	74.07%
AC	85.24%	79.63%	77.25%	67.20%
ACnE	84.63%	79.09%	75.66%	65.87%
AC-RS	86.46%	80.67%	83.07%	72.75%

For model selection, Qwen2.5-Coder-7B-Instruct (Hui et al., 2024) serves as baseline model. Comparative experiments include CodeLlama-7B-Instruct (Rozière et al., 2024), DeepSeek-Coder-6.7B-Instruct (Guo et al., 2024), GPT-4o-20240806, and Qwen2.5-Coder-32B-Instruct (Hui et al., 2024). All models are trained using LLaMA Factory (Zheng et al., 2024) and deployed via vLLM (Kwon et al., 2023). Detailed experimental configurations are elaborated in Appendix C.

4.2 Results

Table 1 presents performance comparisons between AC-RS and other models on LiveCodeBench. Experimental results demonstrate that AC-RS outperforms Qwen2.5-Coder-7B-Instruct across all evaluation tasks. On the tasks central to our research objectives, Test Output Prediction and Code Execution, the method improves accuracy from 49.55% to 60.41% and 44.68% to 58.25%. Remarkably, AC-RS slightly outperforms larger models like Qwen2.5-Coder-32B-Instruct and GPT-4o-20240806 in Code Execution results.

We analyze contributions from both AC and RS stages. During AC implementation, models show significant gains in Test Output Prediction and Code Execution by avoiding attention traps

in LeetCode data. However, this comes with a 0.65% decrease in general Code Generation ability comparing to LC-Base. This trade-off stems from using Fetch Query outputs as training data, which introduces misalignment issues between queries and outputs, causing distortion in data probability distributions. The Rejection Sampling (RS) stage addresses two critical challenges: It resolves query-output alignment issues through self-generated training data from AC-trained models, while simultaneously reducing model adaptation complexity. This stage further improves performance in Test Output Prediction and Code Execution, while maintaining Code Generation performance without degradation.

Experimental results from HumanEval (HE) and MBPP benchmarks (Table 2) further validate method robustness. During the AC stage alone, we observe performance declines of 0.86% on HE and 7.67% on MBPP, confirming the risks of data distribution disruption from single-stage optimization. However, the RS stage successfully mitigates these declines, with AC-RS ultimately matching LC-Base performance on both benchmarks.

4.3 Ablations & Discussions

This section systematically analyzes two core questions: (1) the necessity of introducing Fetch Queries, and (2) different implementations of the AC method. Experimental results reveal critical factors in method design.

ACnR vs. AC: How Output Refetch Amplifies Attention Shifting Figure 3 presents experimental results for ACnR (**A**ttention **C**racking with no **R**efetch). This approach modifies queries while retaining original outputs. Results show that ACnR improves Test Output Prediction and Code Execution performance, but achieves weaker gains (2.72% and 0.62% improvements over LC-Base) compared to the Refetch-enhanced AC method. The limited improvement stems from insufficient example coverage in original outputs. Statistical analysis reveals that only 43.1% of LC-Base outputs contain examples. By introducing specially designed Fetch Queries, we increase the example-containing output ratio to 99.9%, significantly improving data collection efficiency. The Fetch Query mechanism enables better data utilization, ultimately unleashing greater model potential.

ACnE vs. AC: Trade-offs Between Difficulty and Generalization The AC method removes answer references from LeetCode problem descrip-

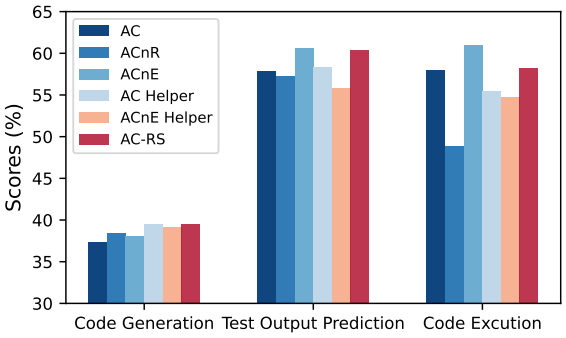

Figure 3: Model performance differences on LiveCodeBench in the ablation study. (ACnR refers to AC with no Refetch, ACnE refers to AC with no Example).

tions to mitigate attention traps. A comparable approach, termed ACnE (**A**ttention **C**racking with **n**o **E**xamples), eliminates entire example sections. Figure 3 demonstrates comparable performance between ACnE and AC-RS across three key tasks. This equivalence arises from ACnE's increased learning demands: Models must not only predict execution results but also autonomously generate test cases, forcing deeper understanding of problem-code-example relationships. However, ACnE incurs two substantial costs: (1) Reduced generalization capability: While ACnE achieves higher code generation accuracy than AC on test sets from May 2023 to March 2024 (closer to train data period), its performance degrades on later datasets (April-August 2024). Table 2 shows ACnE underperforms AC on both HE and MBPP benchmarks. (2) Limited multi-dataset compatibility: When trained with 10,000 CodeAlpaca samples (ACnE_Helper), performance declines significantly due to gradient signal dilution from standard training data. Given our primary objective, eliminate attention traps through minimal data modifications, we select the more adaptable AC method as the preferred implementation.

5 Conclusion

Our study proposes AC-RS method. The AC stage eliminates attention traps in training data through data restructuring. The RS stage addresses performance degradation by training models with self-generated outputs. Experimental results demonstrate that our 7B model trained with AC-RS achieves superior performance on LiveCodeBench. Notably, it matches the Code Execution accuracy of 32B parameter model and performs comparably to GPT-4o.

6 Limitations

While AC-RS effectively eliminate attention traps in Code Execution training data, two limitations persist: First, our validation remains constrained by the scarcity of high-quality open-source code instruction data and computational resource limitations. Second, AC-RS specifically targets Code Execution tasks. Systematically identifying diverse attention traps across massive training data and developing universal solutions remains an unresolved research challenge.

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A Examples for attention trap

Figure 4 and Figure 5 compare attention weight distributions between the LC-Base model and AC-RS model. The LC-Base model demonstrates clear attention trap patterns when processing LeetCode training data. During output learning, the model disproportionately focuses on reference answers in input queries rather than problem descriptions or code logic. Visual analysis reveals two dominant attention patterns in the LC-Base model: (1) Strong focus on sequence-initial tokens (2) Heightened attention to recent colon symbols (:) and space character. Beyond these common high-attention elements, tokens corresponding to example answers in queries receive maximum attention weights, followed by other example answers and their explanatory components. The AC method eliminates this trap through targeted training data modifications. These modifications enable proper attention allocation to critical elements like problem statements, input parameters, and program code. This improvement allows effective capture of abstract reasoning patterns in Code Execution tasks. The approach better utilizes the performance potential inherent in training data.

<|im_start|>system
You are Qwen, created by Alibaba Cloud. You are a helpful assistant.<|im_end|>
<|im_start|>user
You are given an integer array nums. The absolute sum of a subarray [numsl, numsl+1, ..., numsr-1, numsr] is abs(numsl + numsl+1 + ... + numsr-1 + numsr).
Return the maximum absolute sum of any (possibly empty) subarray of nums.
Note that abs(x) is defined as follows:

If x is a negative integer, then abs(x) = -x.
If x is a non-negative integer, then abs(x) = x.

Example 1:

Input: nums = [1,-3,2,3,-4]
Output: 5
Explanation: The subarray [2,3] has absolute sum = abs(2+3) = abs(5) = 5.

Example 2:

Input: nums = [2,-5,1,-4,3,-2]
Output: 8
Explanation: The subarray [-5,1,-4] has absolute sum = abs(-5+1-4) = abs(-8) = 8.

Constraints:

1 <= nums.length <= 10^5
-10^4 <= nums[i] <= 10^4

Please complete the following Python code:
```python
class Solution:
    def maxAbsoluteSum(self, nums: List[int]) -> int:
```<|im_end|>
<|im_start|>assistant
To solve the problem of finding the maximum absolute sum of any subarray, we can utilize a strategy that involves tracking two running computations as we iterate through the array:

1. **Maximum Subarray Sum (Kadane's Algorithm)**: This helps us find the maximum sum of any contiguous subarray. We'll use this to find the maximum positive sum a subarray can achieve.

2. **Minimum Subarray Sum**: Similarly, this helps us find the minimum sum of any contiguous subarray. By negating the array elements and applying Kadane's again, we can find the minimum sum, which helps in calculating the maximum absolute sum when considering negative subarray sums.

The maximum absolute sum of a subarray can be either the maximum subarray sum or the maximum negative of the minimum subarray sum. Additionally, any subarray that happens to sum to zero will also contribute to the maximum absolute sum as zero's absolute value is zero, which might be the maximum if other max sums are negative.

Here's the implementation of the above logic:

```python
from typing import List

class Solution:
    def maxAbsoluteSum(self, nums: List[int]) -> int:
        max_sum = 0
        min_sum = 0
        current_max = 0
        current_min = 0

        for num in nums:
            current_max += num
            current_min += num

            # Update global max and min sums
            max_sum = max(max_sum, current_max)
            min_sum = min(min_sum, current_min)

            # Reset current max and min if they drop below zero
            if current_max < 0:
                current_max = 0
            if current_min > 0:
                current_min = 0

        # The result is the maximum of the maximum positive sum
        # and the absolute value of the minimum negative sum
        return max(max_sum, abs(min_sum))

# Example usage:
# solution = Solution()
# print(solution.maxAbsoluteSum([1, -3, 2, 3, -4]))  # Output: 5
# print(solution.maxAbsoluteSum([2, -5, 1, -4, 3, -2]))  # Output: 8
```

Explanation:

- **current_max** and **current_min** are used to track the sum of the current subarray.
- As we iterate through the array, we update these values by adding the current number.
- We update the global maximum and minimum sums (`max_sum` and `min_sum`) whenever the current values exceed or drop below them, respectively.
- If at any point `current_max` or `current_min` becomes negative or positive, we reset them to zero because starting a new subarray from the next element might yield a higher sum.
- Finally, the result is the maximum of `max_sum` and the absolute value of `min_sum`, ensuring we account for both positive and negative subarray contributions to the maximum absolute sum.

Figure 4: Attention weights of the LC-Base model trapped in attention traps.

<|im_start|>system
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<|im_start|>user
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<|im_start|>assistant
To solve the problem of finding the maximum absolute sum of any subarray, we can utilize a strategy that involves tracking two running computations as we iterate through the array:

1. **Maximum Subarray Sum (Kadane's Algorithm)**: This helps us find the maximum sum of any contiguous subarray. We'll use this to find the maximum positive sum a subarray can achieve.

2. **Minimum Subarray Sum**: Similarly, this helps us find the minimum sum of any contiguous subarray. By negating the array elements and applying Kadane's again, we can find the minimum sum, which helps in calculating the maximum absolute sum when considering negative subarray sums.

The maximum absolute sum of a subarray can be either the maximum subarray sum or the maximum negative of the minimum subarray sum. Additionally, any subarray that happens to sum to zero will also contribute to the maximum absolute sum as zero's absolute value is zero, which might be the maximum if other max sums are negative.

Here's the implementation of the above logic:

```python
from typing import List

class Solution:
    def maxAbsoluteSum(self, nums: List[int]) -> int:
        max_sum = 0
        min_sum = 0
        current_max = 0
        current_min = 0

        for num in nums:
            current_max += num
            current_min += num

            # Update global max and min sums
            max_sum = max(max_sum, current_max)
            min_sum = min(min_sum, current_min)

            # Reset current max and min if they drop below zero
            if current_max < 0:
                current_max = 0
            if current_min > 0:
                current_min = 0

        # The result is the maximum of the maximum positive sum
        # and the absolute value of the minimum negative sum
        return max(max_sum, abs(min_sum))

# Example usage:
# solution = Solution()
# print(solution.maxAbsoluteSum([1, -3, 2, 3, -4])) # Output: 5
# print(solution.maxAbsoluteSum([2, -5, 1, -4, 3, -2]))  # Output: 8
```

Explanation:

- **current_max** and **current_min** are used to track the sum of the current subarray.
- As we iterate through the array, we update these values by adding the current number.
- We update the global maximum and minimum sums (`max_sum` and `min_sum`) whenever the current values exceed or drop below them, respectively.
- If at any point `current_max` or `current_min` becomes negative or positive, we reset them to zero because starting a new subarray from the next element might yield a higher sum.
- Finally, the result is the maximum of `max_sum` and the absolute value of `min_sum`, ensuring we account for both positive and negative subarray contributions to the maximum absolute sum.

Figure 5: Attention weights of AC-RS on training data.

B Qwen2.5-Coder-7B-Instruct Prediction Example

````
```python
class Solution:
    def maxAbsoluteSum(self, nums: List[int]) -> int:
        max_sum = 0
        current_sum = 0
        for num in nums:
            current_sum = max(0, current_sum + num)
            max_sum = max(max_sum, current_sum)
        current_sum = 0
        for num in nums:
            current_sum = max(0, -current_sum - num)
            max_sum = max(max_sum, current_sum)
        return max_sum
```
````

Figure 6: Generation result of Qwen2.5-Coder-7B-Instruct on the example illustrated in Figure 4.

C Experiment Settings

LiveCodeBench Version LiveCodeBench serves as a continuously updated benchmark where each category of tasks contains multiple versions. To ensure clear experimental variables and reproducibility, we specify the exact versions and sample information used. For Code Generation tasks, we employ the latest version v3 available at experiment initiation, containing 612 test samples from May 1, 2023 to September 1, 2024. Self Repair tasks rely on error outputs from Code Generation tasks, but their test sets differ in this study. This occurs because the Self Repair test set only updated to version v1 during our experiments, containing 400 test samples from May 1, 2023 to April 1, 2024. Test Output Prediction uses version v1 with 442 samples from May 1, 2023 to April 1, 2024. Code Execution employs version v2 containing 479 test samples from May 1, 2023 to December 1, 2023. We note that LiveCodeBench leaderboard data changes cause slight sample count mismatches within identical time ranges. For example, the Self Repair tasks actually contain 439 samples (May 1, 2023 to April 1, 2024) on the leaderboard, exceeding our reported 400 samples. This difference stems from subsequent updates adding 39 new samples from March 1, 2024 to April 1, 2024.

Hyperparamter Settings We maintain consistent parameter configurations for both model training and inference. The training process uses full-parameter bf16 precision mode with sequence length 4096 and batch size 32. To optimize memory usage, we enable Deepspeed framework's O2 optimization level. This configuration allows complete training on a server with 4 NVIDIA A800 80G GPUs. Models undergo 5 full training epochs with initial learning rate $1 * 10^{-5}$ using a cosine learning rate scheduler. During inference, we follow LiveCodeBench's standard test script configuration: topp=0.95 and temperature=0.2. For cost control, we request single outputs from GPT-4o during data collection. For local models performing Rejection Sampling, we consistently execute 20 output predictions with topp=0.8 and temperature=0.95 to ensure sampled data quality.