Unleashing the Power of Tree Search for Superior Performance in Competitive Coding Tasks

Anonymous ACL submission

Abstract

Competition-level code generation tasks pose significant challenges for current state-of-the-art large language models (LLMs). For example, on the LiveCodeBench-Hard dataset, models such as O1-Mini and O1-Preview achieve pass@1 rates of only 0.366 and 0.143, respectively. While tree search techniques have proven effective in domains like mathematics and general coding, their potential in competition-level code generation remains under-explored. In this work, we propose a novel token-level tree search method specifically designed for code generation. Leveraging Qwen2.5-Coder-32B-Instruct, our approach achieves a pass rate of **0.305** on LiveCodeBench-Hard, surpassing the pass@100 performance of GPT4o-0513 (0.245). Furthermore, by integrating Chain-of-Thought (CoT) prompting, we improve our method's performance to **0.351**, approaching O1-Mini's pass@1 rate. To ensure reproducibility, we report the average number of generations required per problem by our tree search method on the test set. Our findings underscore the potential of tree search to significantly enhance performance on competition-level code generation tasks. This opens up new possibilities for large-scale synthesis of challenging code problems supervised fine-tuning (SFT) data, advancing competition-level code generation tasks.

1 Introduction

Competition-level code generation tasks present a unique set of challenges for large language models (LLMs). These tasks require models to not only comprehend complex problem statements but also generate executable code that adheres to logical and syntactical constraints. While existing state-of-the-art LLMs have achieved remarkable success in general-purpose programming benchmarks, their performance on competitive programming datasets, such as LiveCodeBench-Hard (Naman Jain et al., 2024), remains far from satisfactory. For example, recent models like O1-Mini and O1-Preview exhibit pass@1 rates of only 0.366 and 0.143, respectively. This performance gap highlights the need for novel methodologies to enhance model capabilities in solving these challenging tasks.

Recent research has demonstrated the potential of tree search techniques in reasoning tasks like mathematics and general programming. However, their application to competition-level code generation remains under-explored. Existing approaches primarily rely on large-scale proprietary LLMs within tree search frameworks, overlooking the possibility that smaller, open-source models—when paired with an effective search strategy—could achieve superior results. Moreover, while data augmentation through techniques such as distillation from stronger LLMs has been widely used, generating solutions directly from the target model itself offers the potential for higher-quality supervised fine-tuning (SFT) data, as these solutions are directly generated by the target model, ensuring consistency with its inherent capabilities and output characteristics.

In this work, we propose a novel token-level Monte Carlo Tree Search (MCTS) method tailored specifically for competition-level code generation. Leveraging the open-source Qwen2.5-Coder-32B-Instruct model, as shown in Figure 1, our approach achieves a pass rate of **0.305** on LiveCodeBench-Hard, surpassing the pass@100 performance of GPT4o-0513 (0.245). By incorporating Chain-of-Thought (CoT) prompting, our method further improves to **0.351**, approaching O1-Mini's pass@1 rate. These results demonstrate that our method not only enhances the ability of models to solve previously unsolvable problems but also provides high-quality outputs that can be directly used to synthesize new SFT data. Compared to distillation-based approaches that rely on external models, our framework allows for a more intrinsic and effec-

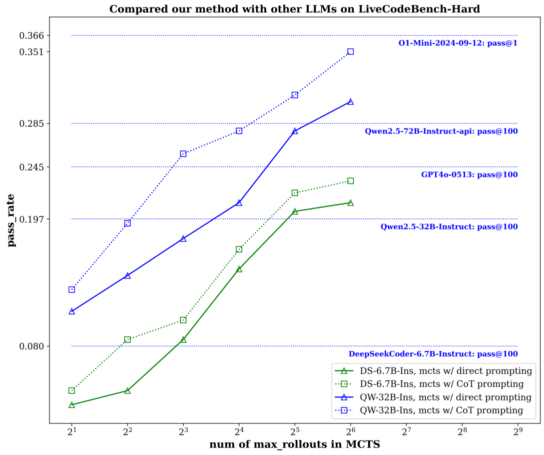


Figure 1: Pass rates of MCTS with DeepSeekCoder-6.7B-Instruct and Qwen2.5-32B-Instruct on LiveCodeBench-Hard: each model surpasses it's own pass@100 rates at max_rollouts = 8. Notably, MCTS with Qwen2.5-32B-Instruct and max_rollouts = 16 outperforms pass@100 of both Qwen2.5-72B-Instruct and GPT4o-0513. In addition, when combined with CoT prompting, MCTS with Qwen2.5-32B-Instruct achieves a pass rate of 0.351 nearing O1-Mini's pass@1 rate of 0.366.

tive alignment of the data with the target model's capabilities.

Experiment results revealed that when combined with MCTS search, CoT prompting significantly outperforms its non-CoT counterpart. In the MCTS framework, CoT prompting helps guide the search process by providing structured intermediate reasoning, and this structured guidance, in turn, enables the model to find higher-quality solutions, as MCTS can evaluate multiple reasoning paths and select the most promising ones. This finding suggests that for CoT prompting to achieve optimal performance in competition-level code generation, it must be integrated with an effective search strategy, highlighting the need for a combination of reasoning and search approaches to fully leverage LLM's potential.

We summarize our contributions as follows:

- **A novel token-level MCTS framework with Cot Prompting:** We propose a token-level tree search framework that combines MCTS with CoT prompting, enabling iterative refinement of both reasoning and code generation for competition-level tasks.

- **Enhancing open-source models for competitive programming tasks:** We demonstrate that open-source models like Qwen2.5-Coder-32B-Instruct can achieve substantial performance improvements on competitive programming datasets when paired with our method. This showcases the potential to elevate the capabilities of open-source models to rival or surpass proprietary counterparts in challenging domains.

- **Comprehensive experimental analysis:** We demonstrate the efficacy of the proposed framework while reporting efficiency metrics such as average generations per problem to ensure reproducibility and fairness.

2 Related Work

2.1 LLMs for Code Generation

Large language models (LLMs), with their powerful reasoning capabilities, have been widely adopted in code-related research and applications. The primary approach to building code LLMs involves pre-training or fine-tuning them on large code datasets, such as CodeX (Chen et al., 2021), AlphaCode (Li et al., 2022), WizardCoder (Luo et al., 2023), CodeGeeX (Zheng et al., 2023), Starcoder (Li et al., 2023) and Code LLama (Roziere et al., 2023). Foundation models, like GPT-4 (Achiam et al., 2023) and Claude[1], exhibit remarkable code generation capabilities despite lacking additional fine-tuning on code-specific data. Additionally, building upon the robust planning capabilities (Yao et al., 2022) and reflection mechanisms (Shinn et al., 2024) of LLMs, LLM-powered autonomous agents have shown significant potential in advancing automated code generation (Huang et al., 2023b; Hong et al., 2023; Wang et al., 2024c; Zhang et al., 2024b). For example, Agentcoder (Huang et al., 2023b) proposes a multi-agent framework that includes programmer agents, test designer agents, and test execution agents to collaboratively generate and test code, MetaGPT (Hong et al., 2023) imitates the main roles in software companies in the real world, using different AI agents to play and ultimately produce a project.

2.2 Prompt Engineering

Designing effective prompts to seamlessly communicate with LLMs to fully harness their full potential can significantly improve LLMs performance without additional training. Some representative technologies of prompt engineering include

[1] https://claude.ai/

Chain-of-Thought (CoT) (Wei et al., 2022), Self-Consistency (Wang et al., 2022), Tree-of-Thought (ToT) (Yao et al., 2024), Reasoning via Planning (RAP) (Hao et al., 2023) and Self-Refine (Madaan et al., 2024). This technique can be directly applied in LLM for iterative and self improving (refining) code generation. For instance, CodeCoT (Huang et al., 2023a) integrates chain-of-thought reasoning with a self-examination process, iteratively refining code based on execution feedback to ensure both logical correctness and syntactic validity. Self-planning (Jiang et al., 2024) enhances code generation by using LLMs to first plan solution steps from intent and then generate code step-by-step. Self-debugging (Chen et al., 2023), an LLM is prompted to iteratively refine code predictions by utilizing feedback from explanations and execution results to identify and fix errors.

2.3 Monte Carlo Tree Search (MCTS) for Reasoning

Chen et al. (2021) showed that repeated sampling can produce correct code solutions, suggesting the answer lies within the LLMs' output space with notable probability, motivating the use of tree search for efficient exploration (Li et al., 2024; Qi et al., 2024; Wang et al., 2024a; Hui et al., 2024). PG-TD (Zhang et al., 2023) introduces a planning-guided Transformer decoding algorithm that uses MCTS and test-case evaluation to iteratively refine code generation, Zhang et al. (2024a) proposed ReST-MCTS*, a method that integrates process reward guidance with tree search to infer high-quality reasoning traces and per-step rewards, enabling more effective self-training of policy. Another common method is LATS (Zhou et al., 2023), which leverages LLMs as agents, value functions, and optimizers, incorporating MCTS to enhance decision-making through external feedback and experience. PlanSearch (Wang et al., 2024b) improves code generation by searching over diverse natural language plans instead of directly over code.

3 Method

3.1 Preliminary

Neural code generation aims to automatically transform natural language descriptions into executable source code through large language models (LLMs). Here we provide a formal definition of the code generation task.

Let D represent a natural language description of a programming task, which may include problem statements, requirements, and additional programming context such as function signatures or assertions. The code generation task can be formalized as learning a model π_θ parameterized by θ that generates code solution C given description D:

$$C \sim \pi_\theta(\cdot \mid D). \tag{1}$$

To evaluate the correctness of generated code, we define a test suite $T = \{(x_i, y_i)\}_{i=1}^n$ where each test case consists of an input x_i and its expected output y_i. The test suite is typically divided into two subsets

$$T = T_{\text{pub}} \cup T_{\text{priv}}, \tag{2}$$

where T_{pub} represents public test cases visible during development, and T_{priv} represents private test cases held out for evaluation.

Given a code solution C, we define an execution function $\text{Exec}(C, x)$ that returns the output of running C on input x. The correctness of C can then be measured by comparing its outputs against the expected outputs across all test cases:

$$\text{Correct}(C \mid D, T) = \frac{1}{|T|} \sum_{(x,y)\in T} \mathbb{1}(\text{Exec}(C, x) = y), \tag{3}$$

where $\mathbb{1}(\cdot)$ is the indicator function.

The objective of code generation is to find model parameters θ^* that maximize the expected correctness across a distribution of programming tasks:

$$\theta^* = \arg\max_\theta \mathbb{E}_{D,T}[\text{Correct}(\pi_\theta(D))]. \tag{4}$$

3.2 MCTS with CoT Prompting

The proposed method is motivated by the desire to integrate Chain-of-Thought (CoT) reasoning with Monte Carlo Tree Search (MCTS). Specifically, the approach enables LLMs to first generate intermediate reasoning steps, followed by code generation. Through iterative refinement and optimization of both the reasoning and code components via MCTS, the method aims to enhance the model's performance on challenging competition-level code generation tasks. Next, we will provide a detailed description of our methods in each key component of MCTS.

CoT Prompting. To improve the performance of LLMs on challenging competition-level code generation tasks, we introduce a structured CoT prompting methodology, which guides the model through a two-step reasoning process **planning** and **coding** to ensure logical and syntactically correct outputs. MCTS iteratively refines and optimizes both the planning and coding stages, improving performance in complex code generation tasks. The prompt explicitly instructs the model to:

- **Solution Planning:** Analyze the problem specification and create a detailed step-by-step plan. This step includes outlining the problem-solving logic, choosing appropriate data structures, and determining the functions required for implementation.
- **Code Generation:** Based on the detailed plan, write Python code adhering to coding standards and ensuring proper syntax.

Here is an example in AppendixC.

Selection. The selection phase in MCTS strives to balance exploration and exploitation by selecting actions that are most likely to yield beneficial results. At the selection stage, the algorithm starts from the root node s_0 and traverses the tree until it reaches a leaf node. Our method use a token-level MCTS so that each state s represents a candidate token. At each node s, the action $a \in \mathcal{A}(s)$, where $\mathcal{A}(s)$ denotes the set of available actions in state s taken by the LLM π, is chosen by maximizing the P-UCB score:

$$\text{P-UCB}(s,a) = Q(s,a) + \beta(s) \cdot p(a \mid s) \cdot \frac{\sqrt{\ln N(s)}}{1+N(s,a)}, \tag{5}$$

$$\beta(s) = \log\left(\frac{N(s)+c_{\text{base}}+1}{c_{\text{base}}}\right) + c. \tag{6}$$

Here:

- $Q(s,a)$ represents the average reward (defined in **Simulation**) of action a at state s.
- $N(s)$ is the total number of visits to state s.
- $N(s,a)$ is the number of times action a has been taken from state s.
- $p(a \mid s)$ is the prior probability of action a at s, proposed by the LLM π.
- c_{base} and c are hyperparameters that balance exploration and exploitation.

This formula combines three essential components: exploitation through $Q(s,a)$, exploration driven by $\sqrt{\ln N(s)/(1+N(s,a))}$, and prior guidance from $P(s,a)$. The algorithm iteratively applies this criterion until it encounters a leaf node s_L, defined as a state either not fully expanded or terminal.

Expansion. When the selection process reaches a node s in the search tree, the expansion phase creates new child nodes by considering potential next tokens. Unlike standard MCTS which might randomly sample actions, we leverage the LLM's predictions to guide expansion:

Given the current state s, we obtain the k most probable next tokens using the TOP-K function:

$$\mathcal{T}_k(s) = \text{TOP\_K}(s,k), \tag{7}$$

where k is a hyperparameter that limits the maximum number of children per node, and $\mathcal{T}_k(s)$ returns the set of k most likely next tokens according to the LLM's probability distribution.

For the new child node s', the visit count $N(s',a')$ and the average reward $Q(s',a')$ for all $a' \in \mathcal{A}(s')$ are initialized to zero:

$$N(s',a') = 0, \quad Q(s',a') = 0, \quad \forall a' \in \mathcal{A}(s'). \tag{8}$$

The use of priors $p(s' \mid a')$ derived from the policy π enables the tree to bias future expansions toward promising regions of the search space.

Simulation. Once a new node s' is added to the tree, the algorithm estimates its value through a simulation, also called a rollout. Starting from s', actions are sampled according to the policy π until a terminal state s_T is reached or a predefined depth limit d_{max} is exceeded. In this paper, we use two methods to estimate the quality for the state s', we call it as hard reward (HR) and partial reward (PR). Normally, we use all public test cases to validate the generated code. HR supposes that if everything passes, the code is considered correct, and if there exist errors, it is incorrect. Assume that T is the set of all test cases, the HR can be formalized as:

$$R^{\text{HR}}_{s'} = \begin{cases} 1, & \text{if } \mathbb{1}(\text{Exec}(C,x)=y) = 1, \forall (x,y) \in T; \\ 0, & \text{otherwise.} \end{cases} \tag{9}$$

However, when addressing challenging coding problems, the distinction between partial success and complete failure is critical. Accordingly, our method leverages the pass rate on the test set as the reward signal, denoted as PR:

$$R^{\text{PR}}_{s'} = \frac{1}{|T|} \sum_{(x,y)\in T} \mathbb{1}(\text{Exec}(C,x)=y). \tag{10}$$

Backpropagation. The backpropagation stage updates the statistics of all nodes along the path from the newly expanded node s' back to the root s_0. For each node-action pair (s, a) on the path, the visit count $N(s, a)$ and the average reward $Q(s, a)$ are updated as follows:

$$N(s, a) \leftarrow N(s, a) + 1, \tag{11}$$

$$Q(s, a) \leftarrow \frac{(N(s, a) - 1) \cdot Q(s, a) + R(s')}{N(s, a)}. \tag{12}$$

These updates propagate the simulation result $R(s')$ upward, refining the action-value estimates $Q(s, a)$ and balancing the contributions of exploration and exploitation.

4 Experiment

We use LiveCodeBench (Naman Jain et al., 2024) as the test dataset, which comprises 659 problems collected between May 1, 2023, and September 1, 2024. The dataset categorizes problems into three difficulty levels: easy, medium, and hard, with 245 medium-level problems and 151 hard-level problems. We expand 5 child nodes in the expansion phase. In the simulation phase, we set the temperature = 0.7, top_p = 0.8 and repetition_penalty = 1.05 to balance randomness, diversity, and coherence. Given that state-of-the-art models, such as Claude-3.5-Sonnet-20240620, have achieved a pass@1 rate of 0.869 on the easy subset, evaluating the impact of alternative inference techniques on these problems would likely be uninformative. Therefore, our study focuses on the medium and hard subsets, where there is greater scope for improvement and more meaningful differences in inference performance.

To validate the model-agnostic nature of the proposed MCTS approach, we employ four generative models, DeepSeekCoder-6.7B-Instruct, Qwen2.5-7B-Instruct, Qwen2.5-14B-Instruct, and Qwen2.5-32B-Instruct, in our experiment.

4.1 MCTS on LiveCodeBench

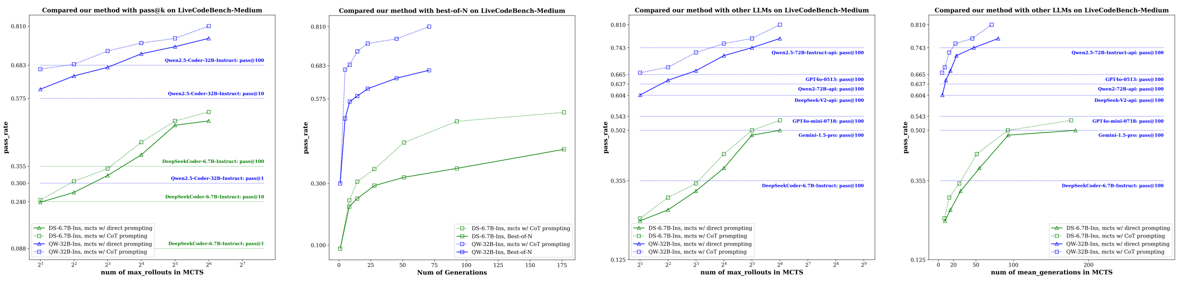
In this section, we evaluate the performance of MCTS across several different generating models on LiveCodeBench-Medium and LiveCodeBench-Hard. For better readability, we present plots in what follows and defer detailed tables to Appendix A.

Medium Level. We begin by comparing the performance of MCTS against the pass@k rates for the same generating models. Figure 2(a) illustrates the performance of MCTS with DeepSeekCoder-6.7B-Instruct and Qwen2.5-32B-Instruct as generating models, compared against their pass@k rates on LiveCodeBench-Medium. In addition, Figure 2(b) illustrates the performance variation of MCTS and Best-of-N (or pass@k) as the number of number of generations increases. Across all tested configurations, MCTS consistently outperforms the Best-of-N baselines, which demonstrates its effectiveness in leveraging the same underlying model to achieve superior results.

In the second part of our analysis, Figure 2(c) compares the performance of MCTS with smaller models (DeepSeekCoder-6.7B-Instruct and Qwen2.5-32B-Instruct) against the pass@100 rates of much larger and more capable models. Key results include: when max_rollouts $=$ 32, the pass@100 rate of MCTS with DeepSeekCoder-6.7B-Instruct reaches 0.488, comparable to the pass@100 rate of Gemini-1.5-pro at 0.502. With max_rollouts $=$ 64, MCTS with Qwen2.5-32B-Instruct achieves a pass rate of 0.770, surpassing the pass@100 rates of much larger models such as Qwen2.5-72B-Instruct-api and GPT4o-0513. Further insights are provided in Figure 2(d), where the x-axis represents the mean number of generations. The results demonstrate that the proposed MCTS approach achieves higher pass rates with fewer sampling attempts, emphasizing its efficiency and effectiveness.

Hard Level. The LiveCodeBench-Hard subset poses significantly greater challenges compared to LiveCodeBench-Medium. Notably, Qwen2.5-72B-Instruct-api achieves the highest pass@1 rate of only 0.087, with a pass@100 rate of 0.285. Both DeepSeekCoder-6.7B-Instruct and Qwen2.5-7B-Instruct exhibit pass@100 rates below 10, underscoring the difficulty of this subset. For detailed pass@k rates of state-of-the-art models on LiveCodeBench-Hard, we refer readers to Table 3 in Appendix A.

Figure 6(a) illustrates the pass@100 rates of various models on LiveCodeBench-Hard, along with the performance variation of MCTS using DeepSeekCoder-6.7B-Instruct and Qwen2.5-32B-Instruct as generating models as the number of max_rollouts increases. Notably, as shown in Figure 6(b), MCTS with DeepSeekCoder-6.7B-Instruct begins to surpass the Best-of-N performance of Qwen2.5-32B-Instruct when max_rollouts $\geq$ 16. These advantages of MCTS



(a) (b) (c) (d)

Figure 2: Results on LiveCodeBench-Medium: (a) Comparison of the pass rates of MCTS with different max_rollouts against the pass@1, pass@10, and pass@100 rates of Qwen2.5-72B-Instruct-api. (b) Comparison of pass rates of MCTS against pass@k with k selected as the mean number of generations in the corresponding MCTS run. (c)-(d) Comparison of the pass rates of MCTS under different max_rollouts against the pass@100 rates of sota models.

become even more compelling as the difficulty of the test dataset increases.

Furthermore, Figure 6(c) presents a comparison of MCTS with smaller models against the pass@100 rates of state-of-the-art models. Key findings include:

- When max_rollouts = 32, MCTS with DeepSeekCoder-6.7B-Instruct achieves a pass rate of 0.205, which is close to Qwen2.5-72B-Instruct-api's pass rate of 0.212, representing a significant relative improvement of 156.25% compared to the standalone pass@100 rate of DeepSeekCoder-6.7B-Instruct at 0.080.

- Similarly, when max_rollouts = 32, MCTS with Qwen2.5-32B-Instruct achieves a pass rate of 0.278, approaching the performance of Qwen2.5-72B-Instruct-api at 0.285.

For a comparison under the same number of generations, Figure 6(d) provides insights into the efficiency of MCTS, with the x-axis representing the mean number of generations. These results highlight that even on this challenging subset, MCTS achieves significantly improved pass rates with fewer sampling attempts. In summary, MCTS demonstrates robust performance on the LiveCodeBench-Hard subset, achieving competitive results against larger models and maintaining efficiency despite the increased difficulty.

The observed improvement of MCTS on LiveCodeBench-Hard is notably greater than that on LiveCodeBench-Medium, indicating that MCTS retains its effectiveness even under increased task difficulty without experiencing performance degradation.

Model-Agnostic. To evaluate the model-agnostic nature of the MCTS method, we compare its performance on LiveCodeBench-Hard subset using four different generating models: DeepSeekCoder-6.7B-Instruct, Qwen2.5-7B-Instruct, Qwen2.5-14B-Instruct, and Qwen2.5-32B-Instruct. For experimental efficiency, we fix max_rollouts = 16.

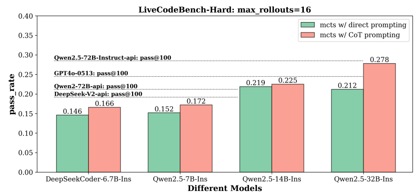


Figure 3: When different models are used as the generating model for MCTS, the pass rates of MCTS tend to increase correspondingly with the enhancement of model capabilities. The pass@100 rates of DeepSeekCoder-6.7B-Instruct, Qwen2.5-7B-Instruct, Qwen2.5-14B-Instruct, and Qwen2.5-32B-Instruct are 0.080, 0.099, 0.189, and 0.197, respectively. It can be observed that after employing MCTS, even with max_rollouts set to only 16, the performance of each model on LiveCodeBench-Hard significantly exceeds its own pass@100 rate.

Figure 3 illustrates that the performance of MCTS improves consistently with the capabilities of the generating models. Notably, when using Qwen2.5-14B-Instruct, MCTS achieves a pass@100 rate of 0.219, surpassing the pass rate of the larger Qwen2.5-72B-api at 0.212.

Additionally, as shown in Figure 4, the average number of generations for MCTS remains below 81 across all generating models when max_rollouts = 16. These results indicate that the MCTS method is

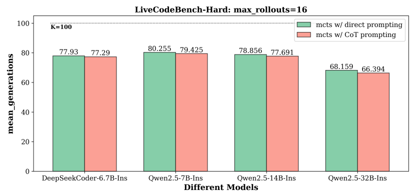


Figure 4: To ensure fairness in comparison with the pass@100 rates, we also recorded the average number of generations produced by MCTS when max_rollouts is set to 16 across different models. It can be observed that for DeepSeekCoder-6.7B-Instruct, Qwen2.5-7B-Instruct, and Qwen2.5-14B-Instruct, the average number of generations is approximately 80, which is significantly lower than 100. For Qwen2.5-32B-Instruct, the average number of generations is even lower.

both model-agnostic and efficient, achieving competitive performance across a variety of generating models while maintaining low sampling overhead. It is also important to note that we plan to optimize pruning techniques for MCTS in the future, which may further reduce the average number of generations.

4.2 Direct Prompting vs CoT Prompting

Chain-of-Thought (CoT) prompting has proven to be an effective technique for enhancing model performance in reasoning tasks. Throughout our experiments, we also explore whether integrating CoT prompting with MCTS can further improve overall performance.

On LiveCodeBench-Medium, Figure 2 demonstrates that MCTS with CoT prompting consistently outperforms the baseline. For example, with max_rollouts $= 64$ and Qwen2.5-Coder-32B-Instruct, MCTS with CoT prompting achieves a pass rate of 0.810, compared to 0.770 with direct prompting. A similar trend is observed on LiveCodeBench-Hard, as shown in Figure 6: with max_rollouts $= 64$ and Qwen2.5-32B-Instruct, MCTS with CoT prompting achieves a pass rate of 0.351, outperforming the pass rate of 0.305 from direct prompting.

Figure 4 further highlights the efficiency of CoT prompting, requiring fewer generations on both datasets when combined with MCTS. Additionally, Figure 3 demonstrates consistent performance improvements across different models when CoT prompting is applied. As model capabilities increase, the combined approach of MCTS with CoT prompting becomes even more effective. To sum up, CoT prompting outperforms pure MCTS across all four tested models, which highlights its robustness and versatility.

4.3 Deep Insight into MCTS's Selection Phase

In the context of MCTS, the final generated response can be decomposed into three key components: (1) the path identified during the selection phase via P-UCB search, (2) the actions sampled by the model during the expansion phase, and (3) the content generated through autoregressive decoding in the simulation phase. Since the sampling methods used in the simulation phase are indistinguishable from techniques like Best-of-N, we are particularly interested in the specific effects of the paths identified during the selection and expansion phases. To explore this, we present an interpretive experiment in the sequel.

Using the LiveCodeBench-Hard dataset with Qwen2.5-14B-Instruct, we fix max_rollouts $= 16$ and record the best paths discovered by MCTS. We the modify the prompt for each problem to include the format prompt + best path and employ standard autoregressive decoding methods to sample and compute pass@k rates. Figure 5 compares the pass@k rates of Qwen2.5-14B-Instruct on LiveCodeBench-Hard when using the original prompt versus the modified prompt.

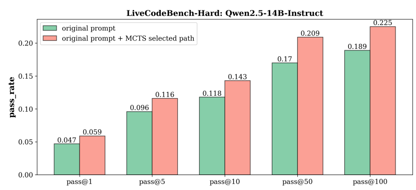
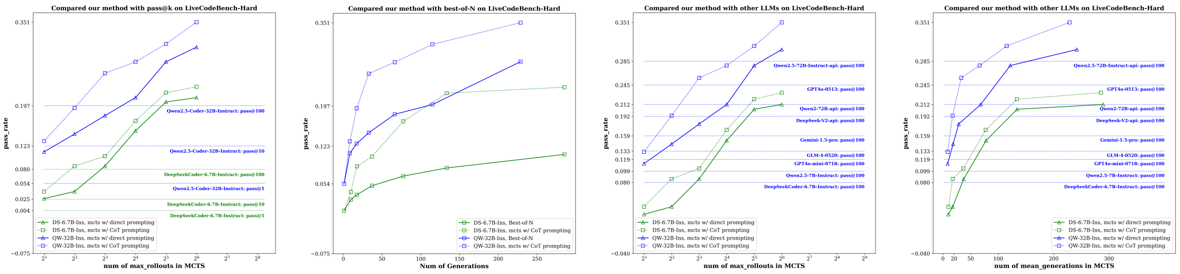


Figure 5: A comparison between the original prompts from LiveCodeBench-Hard and the modified prompts using the optimal paths identified through MCTS. The results show substantial contribution of the paths identified during the selection and expansion phases to the overall performance of MCTS.

The results demonstrate significant improvements with the modified prompt across all evaluated k-values ($K = 1, 5, 10, 50,$ and 100). For instance, at $K = 1$, the pass rate increases by 25.5% compared to the baseline, while at K=100, the relative improvement is 19%. These findings highlight the substantial contribution of the paths identified during the selection and expansion phases to the overall performance of MCTS.



(a) (b) (c) (d)

Figure 6: Results on LiveCodeBench-Hard: (a) Comparison of the pass rates of MCTS with different max_rollouts against the pass@1, pass@10, and pass@100 rates of Qwen2.5-72B-Instruct-api. (b) Comparison of pass rates of MCTS against pass@k with k selected as the mean number of generations in the corresponding MCTS run. (c)-(d) Comparison of the pass rates of MCTS under different max_rollouts against the pass@100 rates of sota models.

4.4 CodeContest-Test

CodeContest-Test is a widely used benchmark set for code competition tasks, complementing LiveCodeBench. To evaluate the generalizability and effectiveness of the methods proposed in this paper across multiple code competition benchmark sets, we also compare our methods against several baseline models on CodeContest-Test.

To control experimental costs, we utilize the Qwen2.5-Coder-32B-Instruct model and fix the MCTS max_rollouts at 32. As shown in Figure 7, when using direct prompting, MCTS achieves a pass rate of 0.582, surpassing the performance of Claude-3.5-Sonnet. Notably, the average number of generations for MCTS in this setup is only 79.055.

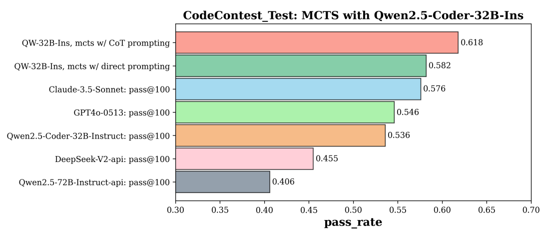


Figure 7: Evaluation results on CodeContest_Test. MCTS with max_rollouts = 16 and Qwen2.5B-Coder-32B-Instruct, which involves less than 80 number of generations, outperforms pass@100 of Claude-3.5-Sonnet.

When employing Chain-of-Thought (CoT) prompting, the performance of MCTS improves further, achieving a pass@100 rate of 0.618, while reducing the average number of generations to 75.962. These results demonstrate the effectiveness of combining MCTS with CoT prompting, achieving better performance with fewer sampling attempts.

5 Conclusions

In this paper, we proposed a novel token-level Monte Carlo Tree Search (MCTS) framework combined with Chain-of-Thought (CoT) prompting, tailored for competition-level code generation tasks. Using the open-source Qwen2.5-Coder-32B-Instruct model, our approach demonstrates its effectiveness by achieving a pass rate of **0.351** on LiveCodeBench-Hard, nearing the pass@1 performance of O1-Mini. The results highlight the capability of our framework to significantly improve the problem-solving efficiency and accuracy of open-source models, thereby reducing the reliance on large-scale proprietary black-box LLMs. Moreover, our method's ability to generate consistent and high-quality solutions making it possible to synthesize supervised fine-tuning (SFT) data for large-scale competition level code problems from open-source LLMs. By synthesizing robust datasets directly from the target model, our approach paves the way for more effective and intrinsically aligned post-training strategies.

In the future, our framework can be further enhanced by integrating with techniques like rejection sampling and self-consistent reasoning. These techniques could complement our MCTS framework, further enhancing the LLMs' reasoning capabilities and improving their performance on competition-level code generation tasks. By enabling more robust and diverse exploration of potential solutions, and minimizing the generation of incorrect or incomplete code, these enhancements have the potential to advance the state of the art in solving complex coding problems.

6 limitation

While the proposed token-level Monte Carlo Tree Search (MCTS) framework combined with Chain-of-Thought (CoT) prompting demonstrates significant improvements in competition-level code generation tasks, several limitations should be acknowledged. First, the method's computational overhead is non-trivial, as MCTS requires multiple rollouts and simulations to explore the search space effectively. This can lead to increased inference time and resource consumption, particularly when applied to larger models or more complex problems. Second, the framework's performance is highly dependent on the quality of the underlying generative model. Although the method enhances the capabilities of open-source models, it may still fall short when compared to state-of-the-art proprietary models in terms of absolute performance. Third, the current implementation of MCTS does not incorporate advanced pruning techniques, which could further optimize the search process and reduce the average number of generations required. Additionally, our method requires a sandbox environment to execute the currently generated code for validation, which may limit its applicability in real-world scenarios where such execution environments are not readily available or where security concerns restrict the execution of untrusted code.

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A Extra Tables of MCTS and Pass@k on LiveCodeBench

A.1 LiveCodeBench-Medium

Table 1: Evaluation results on LiveCodeBench-Medium: pass@k

Model	pass@1	pass@5	pass@10	pass@50	pass@100
Qwen2.5-72B-Instruct-api	0.477	0.611	0.646	0.716	0.743
Qwen2.5-Coder-32B-Instruct	0.300	0.511	0.575	0.657	0.683
GPT4o-0513	0.387	0.528	0.567	0.638	0.665
Qwen2-72B-api	0.214	0.394	0.461	0.589	0.637
Qwen2.5-Coder-7B-Instruct	0.275	0.444	0.506	0.602	0.625
DeepSeek-V2-api	0.432	0.521	0.550	0.592	0.604
GLM-4-0520	0.190	0.336	0.398	0.510	0.551
GPT4o-mini-0718	0.292	0.427	0.468	0.524	0.543
Gemini-1.5-pro	0.210	0.314	0.359	0.462	0.502
DeepSeekCoder-6.7B-Instruct	0.088	0.194	0.240	0.319	0.355

Table 2: Evaluation results on LiveCodeBench-Medium: MCTS Results

Metric \Rollouts	4	8	16	32	64
DeepSeekCoder-6.7B-Instruct					
pass rate w/direct prompting	0.270	0.325	0.392	0.488	0.502
pass rate w/CoT prompting	0.306	0.347	0.433	0.502	0.531
mean generations w/direct prompting	15.990	29.547	54.824	93.024	182.572
mean generations w/CoT prompting	14.384	27.871	51.063	92.519	176.505
Qwen2.5-Coder-32B-Instruct					
pass rate w/direct prompting	0.648	0.676	0.720	0.743	0.770
pass rate w/CoT prompting	0.686	0.729	0.755	0.770	0.810
mean generations w/direct prompting	9.871	15.943	24.053	47.089	79.751
mean generations w/CoT prompting	8.455	14.360	22.579	45.163	70.767

A.2 LiveCodeBench-Hard

Table 3: Evaluation results on LiveCodeBench-Hard: pass@k Results

Model	pass@1	pass@5	pass@10	pass@50	pass@100
Qwen2.5-72B-Instruct-api	0.087	0.150	0.182	0.256	0.285
GPT4o-0513	0.068	0.133	0.161	0.223	0.245
Qwen2-72B-api	0.025	0.070	0.094	0.168	0.212
Qwen2.5-Coder-32B-Instruct	0.054	0.102	0.123	0.174	0.197
DeepSeek-V2-api	0.090	0.138	0.156	0.187	0.192
Gemini-1.5-pro	0.035	0.068	0.088	0.136	0.159
GLM-4-0520	0.013	0.035	0.053	0.105	0.133
GPT4o-mini-0718	0.043	0.068	0.078	0.107	0.119
Qwen2.5-Coder-7B-Instruct	0.025	0.050	0.061	0.083	0.099
DeepSeekCoder-6.7B-Instruct	0.004	0.016	0.025	0.062	0.080

Table 4: Evaluation results on LiveCodeBench-Hard: MCTS Results

Model \Metric	**4**	**8**	**16**	**32**	**64**
DeepSeekCoder-6.7B-Instruct					
pass rate w/direct prompting	0.040	0.086	0.146	0.205	0.212
pass rate w/CoT prompting	0.083	0.102	0.166	0.217	0.232
mean generations w/direct prompting	17.721	37.513	77.932	133.946	289.51
mean generations w/CoT prompting	17.635	36.933	77.297	133.471	285.396
Qwen2.5-Coder-32B-Instruct					
pass rate w/direct prompting	0.145	0.179	0.212	0.278	0.305
pass rate w/CoT prompting	0.193	0.257	0.278	0.311	0.351
mean generations w/direct prompting	18.359	28.519	68.159	121.616	241.927
mean generations w/CoT prompting	17.303	32.912	66.394	115.072	228.696

B Case Comparison on Best-of-100 and our method

Here is an example where our method passes all the test cases, but the Best-of-100 method does not:

Problem Description of Leetcode/2839

You are given two 0-indexed integer arrays `nums1` and `nums2`, each of length `n`, and a 1-indexed 2D array `queries` where `queries[i] = [x_i, y_i]`. For the i^{th} query, find the maximum value of `nums1[j] + nums2[j]` among all indices `j` ($0 \leq j < n$), where `nums1[j] >= x_i` and `nums2[j] >= y_i`, or -1 if there is no `j` satisfying the constraints.

Return an array `answer` where `answer[i]` is the answer to the i^{th} query.

Constraints

- `nums1.length == nums2.length`
- `1 <= n <=` 10^5
- `1 <= nums1[i], nums2[i] <=` 10^9
- `1 <= queries.length <=` 10^5
- `1 <= x_i, y_i <=` 10^9

Examples

- **Example 1:**
  Input: nums1 = [4,3,1,2], nums2 = [2,4,9,5], queries = [[4,1],[1,3],[2,5]]
  Output: [6,10,7]

- **Example 2:**
  Input: nums1 = [3,2,5], nums2 = [2,3,4], queries = [[4,4],[3,2],[1,1]]
  Output: [9,9,9]

- **Example 3:**
  Input: nums1 = [2,1], nums2 = [2,3], queries = [[3,3]]
  Output: [-1]

Best-of-100 on Leetcode/2839

```
class Solution:
    def maximumSumQueries(self, nums1: List[int], nums2: List[int], queries: List[
        List[int]]) -> List[int]:
        from sortedcontainers import SortedList

        # Combine nums1 and nums2 into pairs and sort them by nums1 in descending
            order
        combined = sorted(zip(nums1, nums2), reverse=True)
        query_with_index = [(x, y, i) for i, (x, y) in enumerate(queries)]
        query_with_index.sort(reverse=True)

        # Initialize a sorted list to keep track of the maximum sums
        max_sums = SortedList()
        result = [-1] * len(queries)
        j = 0

        for x, y, i in query_with_index:
            # Add valid pairs to max_sums
            while j < len(combined) and combined[j][0] >= x:
                num1, num2 = combined[j]
                # Maintain the sorted list with only the maximum sums for each
                    unique num2
                if not max_sums or max_sums[-1][1] < num1 + num2:
                    max_sums.add((num2, num1 + num2))
                j += 1

            # Find the maximum sum for the current query
            idx = max_sums.bisect_left((y, float('inf')))
            if idx > 0:
                result[i] = max_sums[idx-1][1]

        return result
```

Our method on Leetcode/2839

```
from typing import List

class Solution:
    def maximumSumQueries(self, nums1: List[int], nums2: List[int], queries: List[
        List[int]]) -> List[int]:
        combined = sorted(zip(nums1, nums2), reverse=True)
        queries = sorted([(x, y, i) for i, (x, y) in enumerate(queries)], reverse=
            True)
        result = [-1] * len(queries)
        stack = []

        for x, y, i in queries:
            while combined and combined[0][0] >= x:
                a, b = combined.pop(0)
                while stack and stack[-1][0] <= a + b:
                    stack.pop()
                stack.append((a + b, b))
            for val, min_b in stack:
                if min_b >= y:
                    result[i] = val
                    break

        return result
```

Problem Description of atcoder/abc322_e

AtCoder Inc. is planning to develop a product. The product has K parameters, whose values are currently all zero. The company aims to raise all parameter values to at least P.

There are N development plans. Executing the i^{th} development plan $(1 \leq i \leq N)$ increases the value of the j^{th} parameter by $A_{i,j}$ for every integer j such that $1 \leq j \leq K$, at the cost of C_i. A development plan cannot be executed more than once.

Determine whether the company can achieve its goal, and if it can, find the minimum total cost required to achieve the goal.

Constraints

- $1 \leq N \leq 100$
- $1 \leq K, P \leq 5$
- $0 \leq A_{i,j} \leq P \quad (1 \leq i \leq N, 1 \leq j \leq K)$
- $1 \leq C_i \leq 10^9 \quad (1 \leq i \leq N)$
- All input values are integers.

Examples

- **Example 1:**
  Input:

  ```
  4 3 5
  5 3 0 2
  3 1 2 3
  3 2 4 0
  1 0 1 4
  ```

  Output:

  ```
  9
  ```

  Explanation: If you execute the first, third, and fourth development plans, each parameter will be $3 + 2 + 0 = 5$, $0 + 4 + 1 = 5$, $2 + 0 + 4 = 6$, all of which are at least 5, so the goal is achieved. The total cost in this case is $5 + 3 + 1 = 9$. It is impossible to achieve the goal at a total cost of 8 or less. Thus, the answer is 9.

- **Example 2:**
  Input:

  ```
  7 3 5
  85 1 0 1
  37 1 1 0
  38 2 0 0
  45 0 2 2
  67 1 1 0
  12 2 2 0
  94 2 2 1
  ```

  Output:

  ```
  -1
  ```

  Explanation: You cannot achieve the goal no matter what you do. Thus, print -1.

Best-of-100 on Atcoder/abc322_e

```
import sys
import itertools

def main():
    import sys
    import itertools

    def readints():
        return list(map(int, sys.stdin.readline().split()))

    N, K, P = readints()
    plans = [readints() for _ in range(N)]

    # Generate all possible combinations of plans
    min_cost = float('inf')
    for r in range(1, N + 1):
        for combination in itertools.combinations(range(N), r):
            total_cost = sum(plans[i][0] for i in combination)
            total_increase = [sum(plans[i][j + 1] for i in combination) for j in
                range(K)]
            if all(increase >= P for increase in total_increase):
                min_cost = min(min_cost, total_cost)

    if min_cost == float('inf'):
        print(-1)
    else:
        print(min_cost)

if __name__ == "__main__":
    main()
```

Our method on Atcoder/abc322_e

```
# YOUR CODE HERE
import sys
input = sys.stdin.read
data = input().split()

N = int(data[0])
K = int(data[1])
P = int(data[2])

plans = []
index = 3
for _ in range(N):
    C = int(data[index])
    A = list(map(int, data[index + 1:index + 1 + K]))
    plans.append((C, A))
    index += 1 + K

min_cost = float('inf')

def dfs(current_params, current_cost, plan_index):
    global min_cost
    if current_cost >= min_cost:
        return
    if all(param >= P for param in current_params):
        min_cost = current_cost
        return
    if plan_index == N:
        return
    # Include the current plan
    new_params = [a + b for a, b in zip(current_params, plans[plan_index][1])]
    dfs(new_params, current_cost + plans[plan_index][0], plan_index + 1)
    # Exclude the current plan
    dfs(current_params, current_cost, plan_index + 1)

```

```
dfs([0] * K, 0, 0)

if min_cost == float('inf'):
    print(-1)
else:
    print(min_cost)
```

C Example of Cot prompting

Cot Prompting Example

Instruction: As an AI language model, you are tasked with generating Python code based on given problem specifications. To accomplish this, you need to follow a two-step process:
1. **Planning**: Analyze the problem and create a detailed plan that outlines the steps needed to solve the problem. This plan should include the logic, data structures, and Python functions you'll use.
2. **Coding**: Based on the plan, write the Python code that solves the problem. Make sure your code adheres to the Python coding standards and uses the correct syntax.
Problem: You are given a 0-indexed integer array `nums`. The teacher wants to form a group of students with maximal strength. The strength of a group is defined as the product of all the elements in the group. Return the maximum strength of a group the teacher can create.
Plan:
<startofplan>
Step 1: Import the combinations function from itertools module.
Step 2: Define a class Solution with a method maxStrength that takes a list of integers as input.
......
Step 8: After all combinations are processed, return max_strength.
<endofplan>
Python Code:

```python
from itertools import combinations

class Solution:
    def maxStrength(self, nums: List[int]) -> int:
        if len(nums) == 1:
            return nums[0]
        max_strength = float('-inf')
        for i in range(1, len(nums)+1):
            for comb in combinations(nums, i):
                strength = 1
                for num in comb:
                    strength *= num
                max_strength = max(max_strength, strength)
        return max_strength
```