MCTS-Judge: Test-Time Scaling in LLM-as-a-Judge for Code Correctness Evaluation

Anonymous ACL submission

Abstract

001

005

011

015

017

031

034

042

The LLM-as-a-Judge paradigm shows promise for evaluating generative content but lacks reliability in reasoning-intensive scenarios, such as programming. Inspired by recent advances in reasoning models and shifts in scaling laws, we pioneer bringing test-time computation into LLM-as-a-Judge, proposing MCTS-Judge, a resource-efficient, System-2 thinking framework for code correctness evaluation. MCTS-Judge leverages Monte Carlo Tree Search (MCTS) to decompose problems into simpler, multi-perspective evaluations. Through a node-selection strategy that combines selfassessment based on historical actions in the current trajectory and the Upper Confidence Bound for Trees based on prior rollouts, MCTS-Judge balances global optimization and refinement of the current trajectory. We further designed a high-precision, unit-test-level reward mechanism to encourage the Large Language Model (LLM) to perform line-by-line analysis. Extensive experiments on three benchmarks and five LLMs demonstrate the effectiveness of MCTS-Judge, which improves the base model's accuracy from 41.0% to 80.0%, surpassing the o1-series models with $3 \times$ fewer tokens. Further evaluations validate the superiority of its reasoning trajectory in logic, analytics, thoroughness, and overall quality, while revealing the test-time scaling law of the LLMas-a-Judge paradigm.

1 Introduction

LLM-as-a-Judge, wherein Large Language Models (LLMs) serve as the golden rule for evaluation criteria (Gu et al., 2024), has been proposed for applications such as generative content assessment (Li et al., 2024b), and data captioning (Chen et al., 2024), serving as a cost-effective solution compared to human expert evaluators. Among those, LLM-as-a-Judge has revolutionized code evaluation by automating judgment (Yang et al., 2024), repair (Liu et al., 2024), and explanation (Weyssow



Figure 1: With test-time scaling, our MCTS-Judge method doubles the accuracy of *DeepSeek-Coder-V2-16B-Instruct* on the APPS benchmark, surpassing o1-series models and *Qwen-QwQ-32B*, while using $3 \times$ fewer tokens and a smaller model. The circle sizes indicates the relative sizes of the models.

et al., 2024), replacing inaccurate similarity-based execution-free methods (Ren et al., 2020; Tran et al., 2019), and expensive execution-based methods reliant on manually-crafted test cases (Zheng et al., 2023; Zhuo et al., 2024).

043

044

047

051

055

057

059

060

061

062

063

064

065

066

067

Despite its growing adoption, recent studies highlight critical challenges in the LLM-as-a-Judge paradigm, including bias (Gu et al., 2024), misalignment (Ye et al., 2024), and fairness concerns (Li et al., 2024a), questioning its reliability for accurate, human-like judgments. To address these issues, researchers have focused on pretraining (Hui et al., 2024), fine-tuning (Wang et al., 2024a), and in-context learning (Wei et al., 2022) to improve reasoning capabilities, which are highly demanded in programming scenarios. Unfortunately, as LLMs near the upper bounds imposed by scaling laws, further advancements involve increasing costs in training with diminishing returns (Snell et al., 2024).

To address these limitations, inspired by the shift of scaling laws from training to test time (Xu et al., 2025) and recent breakthroughs in *Reasoning LLMs*, such as OpenAI's o-series (Jaech et al., 2024), we introduce the first framework that in-

157

158

159

160

161

162

163

164

165

166

167

168

169

120

tegrates test-time computation into the LLM-as-a-Judge paradigm. We target code correctness evalua-069 tion and propose MCTS-Judge, a resource-efficient 070 LLM-as-a-Judge framework with System-2 thinking, offering human-like reasoning for more reliable evaluations. It achieves State-Of-The-Art (SOTA) performance compared to prior LLM-asa-Judge methods, which rely on rapid and superficial System-1 thinking (Tong and Zhang, 2024; Zhuo, 2023). MCTS-Judge leverages a tailored 077 Monte Carlo Tree Search (MCTS) to decompose problems into simpler, multi-perspective evaluation tasks. In the selection phase of MCTS, we introduce a global-local node selection strategy that combines self-assessment based on historical actions in the current trajectory, and the Upper Confidence Bound for Trees (UCT) algorithm, guided by prior rollouts, to balance the optimization of highvalue regions in the global search space with local reasoning trajectories. We further designed a highprecision simulated execution reward mechanism. This mechanism combines cost-effective automatic test case synthesis with LLM-as-an-interpreter execution, prompting line-by-line analysis for unittest-level reliability.

experiments Extensive on five LLMs benchacross three challenging code 094 marks-BigCodeBench (Zhuo et al., 2024), HumanEval-X (Zheng et al., 2023), and APPS (Hendrycks et al., 2021)—with varying code complexity and languages, highlight the reliability of MCTS-Judge powered by test-time computation. As shown in Fig. 1, our approach elevates the 100 accuracy of DeepSeek-Coder-Lite-16B (Zhu et al., 101 102 2024) from 41.0% to 80.0%, surpassing o1-series models (Jaech et al., 2024) and open-source Qwen-103 QwQ-32B (Qwen, 2024), while using only $3 \times$ 104 fewer tokens and a smaller model. Furthermore, we achieve SOTA performance on all experiments 106 compared to previous System-1 thinking-based LLM-as-a-judge frameworks, with up to 32% 108 improvement on APPS, and demonstrate strong 109 robustness in generalizable scenarios without code 110 references. Case studies on HumanEval-X further 111 showcase MCTS-Judge's superior reasoning 112 across four fine-grained dimensions, such as logic 113 and analytics, achieving a higher win rate over 114 115 o1-series models. Finally, we validated that scaling test-time computation, including tree depth and 116 rollouts, further enhances MCTS-Judge's accuracy, 117 shedding light into the test-time scaling law for 118 LLM-as-a-judge paradigms. 119

2 Related Work

2.1 Code Correctness Evaluation

Code correctness evaluation can be broadly broken down into two paradigms. Execution-free methods, such as BLEU (Papineni et al., 2002), ROUGE-L (Lin, 2004), METEOR (Denkowski and Lavie, 2014), ChrF (Popović, 2015), RUBY (Tran et al., 2019), and CodeBLEU (Ren et al., 2020), assess code based on textual or code-specific feature similarity to reference code. In this paper, we refer to them as similarity-based evaluation methods. However, reference code is often unavailable in practice, and these methods struggle to distinguish semantically equivalent but syntactically different code, leading to low accuracy, as shown in Appendix B. In contrast, execution-based methods, commonly used in code generation benchmarks (Zheng et al., 2023; Zhuo et al., 2024), assess code correctness by executing it against test cases. However, this approach demands comprehensive handcrafted test cases and isolated environments, making it costly and operationally complex (Zhang et al., 2022). To address these limitations, recent efforts have explored LLM-as-a-Judge paradigms with in-context learning. ICE-Score (Zhuo, 2023) integrates evaluation criteria into prompts, while CODEJUDGE (Tong and Zhang, 2024) employs a two-stage prompting approach. However, these methods rely on System-1 thinking (Kahneman, 2011), leading to rapid, superficial decisions that are constrained by the inherent uncertainties of LLMs, resulting in limited reliability.

2.2 Test-time Computation Boost Reasoning

Recent studies highlight a shift in scaling laws from train-time to test-time (Ji et al., 2025; Xu et al., 2025), as pretrained models approach data scale limits (Snell et al., 2024), while reasoning models leverage test-time computation, demonstrating remarkable performance improvements, exemplified by OpenAI's o-series models (Jaech et al., 2024). To advance human-like System-2 thinking, key innovations include chain-of-thought data curation (Wang et al., 2022, 2024b), reinforcement learning (DeepSeek-AI, 2025; Qwen, 2024), and reward models (Guan et al., 2025; Yu et al., 2024). As a core support, search paradigms like beam search and MCTS dynamically select diverse reasoning trajectories, significantly enhancing accuracy in large search spaces. Examples include ReST-MCTS (Zhang et al., 2024a), rStar (Qi et al.,

2024), MCTSr (Zhang et al., 2024b), and (Xie et al., 170 2024), which integrate MCTS with reinforced self-171 training, self-play mutual reasoning, and prefer-172 ence optimization, driving advancements in reason-173 ing tasks such as math and code problem-solving. 174 Building on this remarkable improvement in relia-175 bility, we pioneeringly integrate test-time computa-176 tion into the LLM-as-a-Judge paradigm, proposing 177 a novel framework, MCTS-Judge, which leverages System-2 thinking to generate reliable, human-like 179 reasoning trajectories for comprehensive, multi-180 perspective code correctness evaluation. 181

3 MCTS-Judge

In this section, we first introduce the overview of MCTS-Judge for code evaluation (Sec.3.1), then detail its MCTS architecture (Sec.3.2) and reward mechanism (Sec. 3.3).

3.1 Overview

183

184

185

186

The code correctness evaluation task determines whether a code snippet c correctly implements the functionality described in a problem statement p, 190 expressed as x = (c, p). In MCTS-Judge, we de-191 compose this task into subtasks, each prompting 192 the LLM to verify a specific requirement. The 193 action space of our MCTS consists of these sub-194 tasks and a null action representing no evalua-195 tion. At each node in the search tree, the sub-196 197 action space includes one non-repeating subtask 198 and the null action. Each action in MCTS produces an output $s_i \in S$ with state transitions de-199 fined as $s_i = L(x, s_1, \ldots, s_{i-1})$, where L represents an LLM. This forms a reasoning trajectory $\mathbf{t} = x \oplus s_1 \oplus \cdots \oplus s_k$, where k is the maximum depth of the search tree. The prediction for a tra-203 jectory is computed as $f(\mathbf{t}, \mathbf{g})$, where f aggregates 204 the subtask outcomes in t along with a global evaluation g. A task-specific terminal reward is assigned based on the agreement between $f(\mathbf{t}, \mathbf{g})$ and the simulated execution result. We perform multiple 208 rollouts, yielding a set of reasoning trajectories $\mathbf{T} = {\mathbf{t}^1, \mathbf{t}^2, \dots, \mathbf{t}^n}.$ The cumulative rewards 210 $R(\mathbf{t}^{\mathbf{i}}) = \sum_{s \in \mathbf{t}^{\mathbf{i}}} r(s)$ for these trajectories are used 211 for weighted sampling to select the optimal tra-212 jectory $\mathbf{t}^{\mathbf{b}}$. The final prediction for x is given by 213 $f(\mathbf{t}^{\mathbf{b}}, \mathbf{g}).$ 214

215 **3.2** Architecture Design

We chose MCTS to implement System-2 thinking essential for code evaluation for two reasons: First, MCTS breaks down the overall code evaluation task into simpler subtasks, reducing the task complexity compared to other System-2 methods like Best-of-N (Brown et al., 2024) and selfconsistency (Wang et al., 2022), which require generating complete solutions in a single inference. Second, our MCTS introduces rewards to guide the search and select the optimal trajectory, further improving the reliability of the LLM-as-a-Judge paradigm. As shown in Fig. 2, our tailored MCTS follows four key stages: selection, expansion, simulation, and backpropagation. 218

219

220

221

222

223

224

225

226

227

228

229

230

231

232

233

234

235

236

237

238

239

240

241

242

243

244

245

246

247

240

250

251

252

253

254

255

256

257

258

259

260

261

262

263

265

266

267

268

269

1) Selection. The selection process begins at the root node and progresses hierarchically until it reaches a node that has not been fully expanded yet. We propose a selection strategy that combines global and local information to balance the optimization of high-value regions in the search space with the current trajectory, resulting in a more coherent evaluation. Specifically, we employ a twolevel approach: a global-level UCT algorithm (Kocsis and Szepesvári, 2006), leveraging insights from previous rollouts, and a local-level LLM-driven self-assessment, which evaluates historical actions within the current trajectory. The final selection is obtained through weighted sampling, with the UCT result weighted by w_u and the self-assessment result weighted by w_l . The UCT algorithm selects the node with the highest UCT value, computed as:

$$UCT(s) = \frac{Q(s)}{N(s)} + \alpha \cdot \sqrt{\frac{\ln N_{parent}(s)}{N(s)}}, \qquad (1)$$

where Q(s) represents the cumulative reward of node s, N(s) is the visit count of s, $N_{parent}(s)$ the visit count of s's parent node, and α is a constant that helps balance exploration and exploitation. The LLM self-assessment result is obtained by prompting the LLM whether including this subtask enhances code evaluation completeness based on the completed subtasks in the current trajectory.

2) Expansion. If the maximum depth has not been reached, a new child node is added to the selected node by randomly sampling an unused action and executing it. If the action is not null, a subtask outcome is obtained by prompting the LLM to carefully analyze c and p (optionally with reference code) from a specific perspective and then summarize the analysis into a binary decision.

3) Simulation. During the simulation process, MCTS-Judge consistently selects non-null actions to execute until the maximum depth is reached. At this point, a complete reasoning trajectory $\mathbf{t} = x \oplus s_1 \oplus \cdots \oplus s_k$ that evaluates the code across



Figure 2: MCTS-Judge generates reasoning trajectories with multi-dimensional evaluations using Monte-Carlo Tree Search (MCTS). Each trajectory is iteratively constructed through selection, expansion, simulation, and backpropagation. Our node selection strategy combines LLM-driven self-assessment, based on historical actions in the current trajectory, with the Upper Confidence Bound for Tree (UCT) algorithm based on prior rollouts. This strategy effectively integrates global and local information, balancing the optimization of high-value regions in the search space with the refinement of the current trajectory. Moreover, we introduce a high-precision, unit-test-level reward mechanism, encouraging the LLM to perform line-by-line analysis. This simulated execution reward guides the search process and selects the final answer from candidate trajectories.

multiple dimensions is generated. The prediction of this trajectory (i.e. $f(\mathbf{t}, \mathbf{g})$) is determined by a consistency check using the majority vote across all binary subtask outcomes, combined with an additional global evaluation g.

4) Backpropagation. Once the maximum depth is reached, a terminal reward is calculated for the trajectory and propagated upward through the search tree. Each node in the trajectory updates its Q(s) by adding the terminal reward and incrementing its N(s) by one.

3.3 Reward Mechanism

Reward is crucial in MCTS to guide the search toward promising paths while minimizing suboptimal exploration. Moreover, cumulative rewards directly determine the final answer in MCTS-Judge, further underscoring the importance of reward accuracy. However, verifying the correctness of predictions without ground truth labels is challenging. Approaches like M* (Kang et al., 2024) and LLaMA-Berry (Zhang et al., 2024c) attempted to address this issue by training a reward model, but these methods often struggle with data collection and risk overfitting. RAP (Hao et al., 2023) introduced a self-evaluation mechanism where rewards are derived by asking the LLM to identify errors in its reasoning within a single completion. However, this mechanism may perform close to random if the LLM's capabilities are limited (Qi et al., 2024).

Therefore, inspired by execution-based evaluation methods (Liu et al., 2024; Xia et al., 2024; Zhang et al., 2024d) and the recently established



Figure 3: Flowchart of the fully LLM-driven Simulated Execution Reward Mechanism. $f(\mathbf{t}, \mathbf{g})$ represents the prediction of the trajectory, and $h(\mathbf{x})$ represents the simulated execution result.

302

303

304

305

306

307

308

310

311

312

313

314

315

316

317

319

322

success of commercial models, represented by GPT-40, in code-related tasks and applications (Ma et al., 2025; Liu et al., 2025; Anysphere, 2024), we propose a fully LLM-powered simulated execution reward mechanism that requires no training and improves reliability through cross-checking and stepby-step, in-depth analysis. As illustrated in Fig.3, the mechanism comprises two key phases: test case generation and execution simulation. The test case generation phase occurs prior to the MCTS process and requires only the problem statement p. GPT-40(OpenAI, 2024) is used to construct, validate, and store diverse test cases. The execution simulation phase is invoked once MCTS reaches its maximum depth and is carried out using the same LLM as in the search phase. Each test case is represented as an input-output pair, where the evaluated code must produce the correct output corresponding to a given input.

1) **Recipe for Test Case Generation.** In the test case generation phase, we instruct GPT-40 to

301

271

analyze the problem statement thoroughly, identifying key requirements, constraints, boundary conditions, and special cases. Based on this analysis, the model generates low-complexity test cases that span a range of scenarios, each with a brief explanation. These cases are organized into structured input-output pairs. To ensure correctness, each pair undergoes a validation process in which the LLM is prompted β times to self-evaluate whether the output aligns with the input and the intended behavior. Test cases that consistently pass this validation are retained, while those that do not are discarded.

324

328

329

332

334

336

337

338

340

341

342

354

357

361

367

372

2) LLM-driven Execution Simulation. When the MCTS search reaches its maximum depth, the test case execution simulation phase begins. We randomly select γ stored test cases, mask their outputs, and provide the inputs to the LLM one by one. We instruct the LLM to simulate a code interpreter, executing the code line by line while tracking variable changes, and then determining the expected output for the given input based on this execution trace. This process repeats δ times per test case, and the generated outputs are compared with the originally stored outputs. The majority vote from the δ repetitions finally determines whether a test case passes. The reward mechanism predicts that the code is correct only if all sampled test cases pass, and the result is expressed by $h(\mathbf{x})$. This design mirrors practical test case evaluation: if a code passes all test cases, it may be correct; however, if it fails any test case, it is definitively incorrect. Finally, if the trajectory's prediction $f(\mathbf{t}, \mathbf{g})$ matches $h(\mathbf{x})$, the trajectory receives a terminal reward ϵ .

In doing so, our reward mechanism is both cautious and reliable, leveraging the characteristics of the code evaluation task to establish a systematic, cross-checking evaluation process that effectively minimizes errors. Additionally, by simulating an interpreter that executes the code line by line, our approach encourages LLMs to perform fine-grained deductive reasoning, considering code flow, variable updates, and logical branches. This detailed analysis helps uncover potential errors that might otherwise go unnoticed with a superficial "general impression", ensuring that final conclusions are grounded in concrete and verifiable evidence.

4 Experiments

4.1 Setup

Following previous work (Tong and Zhang, 2024), we evaluated MCTS-Judge on three challenging benchmarks: HumanEval-X (Zheng et al., 2023), APPS (Hendrycks et al., 2021), and Big-CodeBench (Zhuo et al., 2024). HumanEval-X includes 164 introductory coding tasks across five programming languages. APPS consists of Python coding tasks of three different difficulty levels, from which we randomly selected 100 competitionlevel tasks. BigCodeBench contains 1,140 practical and challenging Python programming tasks, covering 723 function calls from 139 libraries. For tasks in BigCodeBench that lack meaningful inputoutput pairs, such as drawing or compressing, we shift the reward mechanism from simulated execution to simulated discussions, granting rewards only when all reasoning steps yield positive signals that enhance generalizability.

373

374

375

376

377

378

379

380

381

384

385

390

391

392

393

395

396

397

398

399

400

401

402

403

404

405

406

407

408

409

410

411

412

413

414

415

416

417

418

419

420

MCTS-Judge is a general framework compatible with various LLMs. To assess its effectiveness and generalizability, we employed five different LLMs as base models, including code-specialized LLMs: Qwen2.5-Coder-14B (Hui et al., 2024), DeepSeek-Coder-V2-16B-Instruct (Zhu et al., 2024) and Mistralai-Codestral-22B (team, 2024), as well as general LLMs: Llama-3.1-8B-Instruct (Touvron et al., 2023) and GPT-4o-mini (Achiam et al., 2023). We compare MCTS-Judge with three System 2 thinking LLMs, including OpenAI o1-preview (Jaech et al., 2024), o1-mini (Jaech et al., 2024), and Qwen-QwQ-32B (Qwen, 2024), as well as two LLM-as-a-Judge paradigms designed for code evaluation with System 1 thinking: CodeJudge (Tong and Zhang, 2024) and ICE-Score (Zhuo, 2023).¹ We further introduce a Vanilla baseline, which prompts the LLM directly for code correctness, reflecting its native evaluation capability. Additionally, we also include a test-case-only verification baseline using GPT-40, demonstrating that the MCTS-Judge's effectiveness derives from its architecture rather than modelspecific advantages. BigCodeBench is excluded here as it's evaluated with non-test-case-based approach. More details such as hyperparameters and prompts are included in Appendix A.

4.2 Main Results

Table 1 presents the comparison results between MCTS-Judge and baselines. We highlight three key observations: (1) MCTS-Judge significantly enhances the code evaluation capabilities of all

¹ICE-Score produces ratings ranging from 0 to 4. Following the approach in (Tong and Zhang, 2024), only a rating of 4 is considered correct.

Table 1: Accuracy (%) of MCTS-Judge and baselines on BigCodeBench, APPS, and HumanEval-X. MCTS-Judge significantly improves the accuracy of base models and achieves the highest accuracy among existing LLM-as-a-Judge methods across all benchmarks and five LLMs (highlighted in bold). It also surpasses larger reasoning model, *Qwen-QwQ-32B* in most tasks and outperforms o1-series models in certain tasks (highlighted with underlines).

Method	Approach	BigCodeBench	APPS	HumanEval-X					
Method	rippiodeli	Digeodebenen	1115	Python	Java	C++	JavaScript	Go	Average
Test-case Verification									
GPT-40	System-1	-	55.00	59.09	53.79	60.61	62.12	65.91	60.30
Commercial Reasonin	g LLMs								
GPT-o1-preview	System-2	82.02	75.00	82.58	89.39	87.12	86.36	83.33	85.76
GPT-o1-mini	System-2	75.70	78.00	95.45	92.42	94.70	90.91	88.64	92.42
Open-sourced Reason	ing LLMs								
Qwen-QwQ-32B	System-2	50.96	60.00	72.73	75.00	75.00	64.39	78.03	73.03
	Code-Specialized Base Model: Owen2.5-Coder-14B-Instruct								
Vanilla	System-1	63.33	62.00	62.12	64.39	68.94	64.39	73.48	66.66
ICE-Score	System-1	70.44	65.00	72.73	74.24	71.97	72.73	78.79	74.09
CodeJudge	System-1	63.33	68.00	86.36	81.06	79.55	82.58	75.75	81.06
MCTS-Judge (Ours)	System-2	71.23	<u>79.00</u>	<u>90.15</u>	85.61	84.09	84.85	81.06	85.15
	Code-S _l	pecialized Base M	odel: De	epSeek-Co	oder-V2-	16B-Inst	truct		
Vanilla	System-1	51.75	41.00	73.48	64.39	63.64	66.67	60.61	65.76
ICE-Score	System-1	57.89	48.00	71.21	76.52	69.70	70.45	74.24	72.42
CodeJudge	System-1	52.45	62.00	73.48	69.70	67.42	69.70	66.67	69.39
MCTS-Judge (Ours)	System-2	62.46	<u>80.00</u>	80.30	77.27	80.30	78.79	82.58	79.85
	Co	de-Specialized Bas	se Model.	: Mistrala	i-Codest	tral-22B			
Vanilla	System-1	42.81	62.00	82.58	68.18	70.45	62.88	66.67	70.15
ICE-Score	System-1	51.93	56.00	82.58	68.18	60.61	63.64	61.36	67.27
CodeJudge	System-1	49.04	54.00	85.61	69.70	68.94	71.21	66.67	72.43
MCTS-Judge (Ours)	System-2	68.77	72.00	<u>87.78</u>	75.76	77.27	73.48	75.76	78.01
		General Base M	lodel: Ll	ama-3.1-8	8B-Instri	ıct			
Vanilla	System-1	43.16	56.00	65.91	63.64	64.39	62.12	70.45	65.30
ICE-Score	System-1	45.88	42.00	72.73	64.39	62.88	56.82	54.55	62.27
CodeJudge	System-1	63.86	53.00	73.48	73.48	75.76	70.45	67.42	72.12
MCTS-Judge (Ours)	System-2	71.84	62.00	74.24	79.55	77.27	70.45	71.97	74.70
		Commercial Gen	eral Base	e Model: (GPT-40-i	mini			
Vanilla	System-1	72.37	65.00	86.36	82.58	85.61	86.36	84.85	85.15
ICE-Score	System-1	77.37	72.00	84.85	78.79	86.36	83.33	85.61	83.79
CodeJudge	System-1	70.70	72.00	87.12	83.33	87.88	86.36	84.09	85.76
MCTS-Judge (Ours)	System-2	<u>79.12</u>	<u>76.00</u>	<u>87.88</u>	86.36	<u>88.64</u>	<u>88.64</u>	<u>85.61</u>	<u>87.43</u>

436

421

base models. When using open-source LLMs with substantially smaller model sizes, its performance can match or even surpass o1-series models. This phenomenon is illustrated more clearly in Fig. 4. On average, MCTS-Judge achieves a 14.34% accuracy improvement across five different base models on three benchmarks. In particular, DeepSeek-Coder-V2-16B-Instruct, originally at 41% accuracy on the APPS benchmark, improved dramatically to 80% with MCTS-Judge, surpassing both olpreview and o1-mini. (2) Any base model we evaluated, when powered by MCTS-Judge, outperforms the open-source reasoning model Qwen-QwQ-32B on most tasks. For instance, MCTS-Judge based on Llama-3.1-8B-Instruct, with a model size only a quarter of Qwen-QwQ-32B, outperforms it in all

tasks except those using the Go language, achieving up to a 20.88% higher accuracy. (3) Compared to previous LLM-as-a-Judge paradigms with System 1 thinking, MCTS-Judge demonstrates significantly superior performance in all tasks. For example, MCTS-Judge with *DeepSeek-Coder-V2-16B-Instruct* achieved 18% higher accuracy than CodeJudge and 32% higher than ICE-Score on the APPS benchmark. 437

438

439

440

441

442

443

444

445

446

447

448

449

450

451

4.3 Inference Efficiency

To evaluate the test-time computational efficiency of MCTS-Judge, we analyzed the average number of reasoning tokens generated on the APPS benchmark. As presented in Table 2, when using *DeepSeek-Coder-V2-16B-Instruct* as the base

478

479

480

481

482

483

484

485

486

487

488

489



Figure 4: MCTS-Judge (darker colors) significantly enhances LLMs' inherent code evaluation capabilities (lighter colors) across three benchmarks.

model, MCTS-Judge outperforms *o1-preview* in accuracy, while only consuming one third as many reasoning tokens, with an additional 20% equivalent token consumption for simulation in parallelization indicated by the superscript, and maintaining a model size that is 19 times smaller².

Methods	Model Size	# Reasoning Tokens	Acc
o1-preview	~300B	5631	75.0
o1-mini	~100B	3755	78.0
Qwen-QwQ-32B	32B	2559	60.0
Ours w/ Deepseek	16B	2065 ₊₄₁₂	80.0

Table 2: Compared to advanced reasoning LLMs, MCTS-Judge is cost-effective. With *DeepSeek-Coder-V2-16B-Instruct* on the APPS benchmark, it achieves the highest accuracy using the fewest tokens and the smallest model size.

4.4 Fine-grained Quality Assessment

MCTS-Judge demonstrated superior code correctness evaluation ability, while simultaneously generating multi-perspective analyses during reasoning trajectory construction. We believe that this may offer developers deeper insights into the code, providing a distinct advantage over both similaritybased and execution-based evaluation methods. To evaluate the quality of meta-analysis and reasoning capabilities, we compared the reasoning trajectories generated by MCTS-Judge with three reasoning models—*o1-preview*, *o1-mini*, and *Qwen-QwQ-32B* across four critical dimensions: thoroughness, logic, analysis, and overall reasoning quality, with GPT-40 assessing the win rate. As shown in Table 3, MCTS-Judge with *Deepseek-Coder-V2-16B-Instruct* and *Qwen2.5-Coder-14B-Instruct* consistently achieves higher win rates, particularly excelling at thoroughness and depth of analysis.

Dimensions	Deepseek- V2-16B-In	Coder- nstruct	Qwen2.5-Coder- 14B-Instruct		
	o1-preview	Ours	o1-preview	Ours	
Thoroughness	35.6%	64.4%	28.8%	71.2%	
Logic	51.5%	48.5%	49.2%	50.8%	
Analysis	33.3%	66.7%	34.8%	65.2%	
Overall	54.5%	45.5%	52.3%	47.7%	
	o1-mini	Ours	o1-mini	Ours	
Thoroughness	25.8%	74.2%	14.4%	85.6%	
Logic	40.9%	59.1%	22.7%	77.3%	
Analysis	16.7%	83.3%	15.9%	84.1%	
Overall	46.2%	53.8%	47.0%	53.0%	
	QwQ	Ours	QwQ	Ours	
Thoroughness	28.0%	72.0%	31.1%	68.9%	
Logic	25.8%	74.2%	43.2%	56.8%	
Analysis	38.6%	61.4%	40.1%	59.9%	
Overall	49.2%	50.8%	43.9%	56.1%	

Table 3: Comparison of MCTS-Judge's reasoning trajectories with advanced reasoning LLMs across thoroughness, logic, analysis, and overall reasoning quality, with GPT-40 assessing the win rate.

4.5 Extensions to General Scenarios

Reference code is crucial for similarity-based evaluation but is often unavailable in practice. While it aids LLMs in understanding problems, LLM-as-a-Judge methods should adapt to more generalizable settings without it. We evaluated MCTS-Judge and baselines on three benchmarks without reference code (full results in Appendix C). As shown in Table 4, the absence of reference code significantly degrades the performance of existing LLMas-a-Judge frameworks. In contrast, our MCTS-Judge demonstrates exceptional robustness, with only minimal performance drop, highlighting its promising generalization capabilities.

Method	BigCode- Bench	APPS	Human Eval-X
ICE-Score	45.9	42.0	62.3
w/o reference	34.5 (- <u>11.4%</u>)	46.0 (+4%)	52.3 (-10.0%)
CodeJudge	63.9	53.0	72.1
w/o reference	41.4 (-22.5%)	47.0 (-6.0%)	57.4 (-14.7%)
Ours w/o reference	71.8 65.8 (-6%)	62.0 62.0 (+0.0%)	74.7 69.5 (-5.2%)

Table 4: In the absence of reference code, MCTS-Judge with *Llama-3.1-8B-Instruct* demonstrates robustness with minimal performance drop, while other baselines degrade significantly.

457



458

459

466 467

468 469 470

471

 $^{^{2}}$ The model sizes of o1-preview, o1-mini, and GPT-4omini are referenced from this paper (Abacha et al., 2024).



Figure 5: Increasing test cases (α), executions per case (δ) , tree depth, and rollouts improves MCTS-Judge's accuracy on APPS, revealing a test-time scaling law.

Scaling Test-time Computation 4.6

491

501

514

515

516

517

518

519

521

522

523

We explore the relationship between test-time com-492 putational scale and performance gains under our 493 LLM-as-a-Judge framework. MCTS-Judge relies 494 on simulated execution of test cases to determine 495 the terminal reward, thereby providing more accu-496 rate guidance for MCTS and final prediction selec-497 tion. Intuitively, increasing the number of test cases 498 (α) reduces the likelihood of misjudging incorrect 499 code as correct, while increasing the execution times per test case (δ) further enhances accuracy. Furthermore, extending the maximum tree depth provides a more comprehensive evaluation, and more rollouts enable broader exploration. Fig. 5 504 demonstrates the impact of these key hyperparameters on the APPS benchmark using DeepSeek-506 Coder-V2-16B-Instruct and Qwen2.5-Coder-14B-Instruct as base models. MCTS-Judge bene-508 fits from increased test-time computation, though the gains vary with specific hyperparameters and models. These results align with OpenAI's find-511 ings (Openai, 2024), highlighting the potential of 512 test-time scaling for LLM-as-a-Judge frameworks. 513

Ablation Studies 4.7

Table 5 presents ablation results evaluating the key components of MCTS-Judge. Under System-1 thinking, the Vanilla baseline reflects the base model's intrinsic evaluation capability, while Majority Vote executes all subtasks and selects the most frequent answer. Majority Vote improves accuracy by 13% over Vanilla, highlighting the value of incorporating multi-perspective evaluation.

Under System-2 thinking, driven by MCTS, re-

ward mechanisms are further analyzed. RM_{SC} assigns rewards based on self-consistency majority voting (Qi et al., 2024), while RM_{SE} incorporates self-evaluation rewards (Hao et al., 2023). Our proposed simulated execution reward, closely aligned with ground truth, surpasses RM_{SC} and RM_{SE} by 13% in accuracy. Moreover, a variant using pure UCT-based node selection is outperformed by the full MCTS-Judge, highlighting the benefit of our global-local-aware node selection strategy.

Method	Reward Model	Node Selection	Acc				
System-1 Think	ting						
Vanilla	-	-	41.0				
Majority Vote	-	-	54.0				
System-2 Thinking							
	RM_{SC}	UCT	65.0				
Monte Carlo	RM_{SE}	UCT	65.0				
Tree Search	RM _{Ours}	UCT	78.0				
	RM _{Ours}	UCT+LLM	80.0				

Table 5: Ablation of System-2 thinking, reward mechanism, and node selection strategy on APPS with DeepSeek-Coder-V2-16B-Instruct highlights the effectiveness of our designed components. The grey line represents the complete MCTS-Judge, improving from 41.0% to 80.0% over Vanilla.

5 Conclusion

In this work, we propose MCTS-Judge, a novel resource-efficient, test-time computation LLM-asa-Judge framework with System-2 thinking for code correctness evaluation. Powered by a fully LLM-driven MCTS, MCTS-Judge decomposes problems into simpler, multi-perspective evaluations. Through our global-local node selection strategy, along with guidance from a simulated execution reward mechanism, MCTS-Judge performs line-by-line deep analysis. Experiments on five LLMs and three benchmarks show that MCTS-Judge significantly improves base model accuracy, surpassing o1-series models and Qwen-QwQ-32B with one-third of the tokens and a smaller model size. Compared to existing LLM-as-a-Judge frameworks with System-1 thinking, MCTS-Judge achieves SOTA performance while reducing dependence on reference code. Moreover, its reasoning trajectory shows superiority in logic, analytics, thoroughness, and overall quality. We further reveal the test-time scaling law of MCTS-Judge, marking an important first step in integrating test-time computation with the LLM-as-a-Judge paradigm.

534

535

536

537

538

539

540

541

542

543

544

545

546

547

548

549

550

551

552

553

554

555

556

557

524

525

526

527

528

529

530

531

6 Limitation

558

579

584

589

590

591

595

596

598

599

602

In this work, we propose a System-2 thinking approach with a carefully designed architecture 560 for code correctness evaluation. Our current reward mechanism leverages GPT-40, one of the few models capable of producing reliable and 564 well-formatted reward signals. In contrast, existing open-source LLMs often struggle with accurate, line-by-line code execution using only pretrained capabilities and frequently fail to generate structured, precise outputs for programming tasks. 568 Looking forward, we aim to integrate future advancements in open-source models to develop a 570 more cost-effective and broadly deployable solution. To ensure full and reliable reproducibility, we will release the complete codebase, data flywheel pipeline for test case generation, and comprehensive documentation upon acceptance. For review 575 purposes, we have also included our source code in the Supplementary Materials. 577

References

- Asma Ben Abacha, Wen-wai Yim, Yujuan Fu, Zhaoyi Sun, Meliha Yetisgen, Fei Xia, and Thomas Lin. 2024. Medec: A benchmark for medical error detection and correction in clinical notes. *arXiv preprint arXiv:2412.19260*.
- Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. 2023. Gpt-4 technical report. *arXiv preprint arXiv:2303.08774*.
- Anysphere. 2024. Cursor: The ai-first code editor. https://www.cursor.so.
- Bradley Brown, Jordan Juravsky, Ryan Ehrlich, Ronald Clark, Quoc V Le, Christopher Ré, and Azalia Mirhoseini. 2024. Large language monkeys: Scaling inference compute with repeated sampling. *arXiv preprint arXiv:2407.21787*.
- Dongping Chen, Ruoxi Chen, Shilin Zhang, Yinuo Liu, Yaochen Wang, Huichi Zhou, Qihui Zhang, Yao Wan, Pan Zhou, and Lichao Sun. 2024. Mllmas-a-judge: Assessing multimodal llm-as-a-judge with vision-language benchmark. *arXiv preprint arXiv:2402.04788*.
- DeepSeek-AI. 2025. Deepseek-r1: Advancing reasoning in ai models. Technical report, DeepSeek-AI.
- Michael Denkowski and Alon Lavie. 2014. Meteor universal: Language specific translation evaluation for any target language. In *Proceedings of the ninth workshop on statistical machine translation*.

Jiawei Gu, Xuhui Jiang, Zhichao Shi, Hexiang Tan, Xuehao Zhai, Chengjin Xu, Wei Li, Yinghan Shen, Shengjie Ma, Honghao Liu, et al. 2024. A survey on Ilm-as-a-judge. *arXiv preprint arXiv:2411.15594*. 608

609

610

611

612

613

614

615

616

617

618

619

620

621

622

623

624

625

626

627

628

629

630

631

632

633

634

635

636

637

638

639

640

641

642

643

644

645

646

647

648

649

650

651

652

653

654

655

656

657

658

659

660

661

- Xinyu Guan, Li Lyna Zhang, Yifei Liu, Ning Shang, Youran Sun, Yi Zhu, Fan Yang, and Mao Yang. 2025. rstar-math: Small llms can master math reasoning with self-evolved deep thinking. *arXiv preprint arXiv:2501.04519*.
- Shibo Hao, Yi Gu, Haodi Ma, Joshua Jiahua Hong, Zhen Wang, Daisy Zhe Wang, and Zhiting Hu. 2023. Reasoning with language model is planning with world model. *arXiv preprint arXiv:2305.14992*.
- Dan Hendrycks, Steven Basart, Saurav Kadavath, Mantas Mazeika, Akul Arora, Ethan Guo, Collin Burns, Samir Puranik, Horace He, Dawn Song, et al. 2021. Measuring coding challenge competence with apps. *arXiv preprint arXiv:2105.09938*.
- Binyuan Hui, Jian Yang, Zeyu Cui, Jiaxi Yang, Dayiheng Liu, Lei Zhang, Tianyu Liu, Jiajun Zhang, Bowen Yu, Keming Lu, et al. 2024. Qwen2. 5-coder technical report. *arXiv preprint arXiv:2409.12186*.
- Aaron Jaech, Adam Kalai, Adam Lerer, Adam Richardson, Ahmed El-Kishky, Aiden Low, Alec Helyar, Aleksander Madry, Alex Beutel, Alex Carney, et al. 2024. Openai o1 system card. arXiv preprint arXiv:2412.16720.
- Yixin Ji, Juntao Li, Hai Ye, Kaixin Wu, Jia Xu, Linjian Mo, and Min Zhang. 2025. Test-time computing: from system-1 thinking to system-2 thinking. *arXiv* preprint arXiv:2501.02497.
- Daniel Kahneman. 2011. Thinking, fast and slow. Farrar, Straus and Giroux.
- Jikun Kang, Xin Zhe Li, Xi Chen, Amirreza Kazemi, Qianyi Sun, Boxing Chen, Dong Li, Xu He, Quan He, Feng Wen, et al. 2024. Mindstar: Enhancing math reasoning in pre-trained llms at inference time. *arXiv preprint arXiv:2405.16265*.
- Levente Kocsis and Csaba Szepesvári. 2006. Bandit based monte-carlo planning. In *Proceedings of the* 17th European Conference on Machine Learning (ECML).
- Haitao Li, Qian Dong, Junjie Chen, Huixue Su, Yujia Zhou, Qingyao Ai, Ziyi Ye, and Yiqun Liu. 2024a. Llms-as-judges: A comprehensive survey on llm-based evaluation methods. *arXiv preprint arXiv:2412.05579*.
- Lijun Li, Bowen Dong, Ruohui Wang, Xuhao Hu, Wangmeng Zuo, Dahua Lin, Yu Qiao, and Jing Shao. 2024b. Salad-bench: A hierarchical and comprehensive safety benchmark for large language models. *arXiv preprint arXiv:2402.05044*.
- Chin-Yew Lin. 2004. Rouge: A package for automatic evaluation of summaries. In *Text summarization branches out*.

Rundong Liu, Andre Frade, Amal Vaidya, Maxime

Labonne, Marcus Kaiser, Bismayan Chakrabarti,

Jonathan Budd, and Sean Moran. 2025. On iterative

evaluation and enhancement of code quality using

Yizhou Liu, Pengfei Gao, Xinchen Wang, Jie Liu,

Zeyao Ma, Xiaokang Zhang, Jing Zhang, Jifan Yu, Si-

jia Luo, and Jie Tang. 2025. Dynamic scaling of

unit tests for code reward modeling. arXiv preprint

Kishore Papineni, Salim Roukos, Todd Ward, and Wei-

Jing Zhu. 2002. Bleu: a method for automatic evalu-

ation of machine translation. In Proceedings of the

40th annual meeting of the Association for Computa-

Maja Popović. 2015. chrf: character n-gram f-score for

Zhenting Qi, Mingyuan Ma, Jiahang Xu, Li Lyna Zhang,

Qwen. 2024. Qwen2.5 technical report. arXiv preprint

Shuo Ren, Daya Guo, Shuai Lu, Long Zhou, Shujie Liu,

Charlie Snell, Jaehoon Lee, Kelvin Xu, and Aviral Ku-

Weixi Tong and Tianyi Zhang. 2024. Codejudge: Eval-

Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier

Martinet, Marie-Anne Lachaux, Timothée Lacroix,

Baptiste Rozière, Naman Goyal, Eric Hambro,

Faisal Azhar, et al. 2023. Llama: Open and effi-

cient foundation language models. arXiv preprint

Ngoc Tran, Hieu Tran, Son Nguyen, Hoan Nguyen, and

Tien Nguyen. 2019. Does bleu score work for code

migration? In 2019 IEEE/ACM 27th International

uating code generation with large language models.

mar. 2024. Scaling llm test-time compute optimally

can be more effective than scaling model parameters.

Duyu Tang, Neel Sundaresan, Ming Zhou, Ambrosio

Blanco, and Shuai Ma. 2020. Codebleu: a method for automatic evaluation of code synthesis. arXiv

Fan Yang, and Mao Yang. 2024. Mutual reasoning

makes smaller llms stronger problem-solvers. arXiv

workshop on statistical machine translation.

automatic mt evaluation. In Proceedings of the tenth

Yexuan Shi, Zhao Zhang, and Chao Peng. 2024.

Marscode agent: Ai-native automated bug fixing.

gpt-40. arXiv preprint arXiv:2502.07399.

arXiv preprint arXiv:2409.00899.

OpenAI. 2024. Gpt-4o system card. OpenAI.

Openai. 2024. Learning to reason with llms.

arXiv:2501.01054.

tional Linguistics.

preprint arXiv:2408.06195.

preprint arXiv:2009.10297.

arXiv preprint arXiv:2408.03314.

arXiv preprint arXiv:2410.02184.

arXiv:2302.13971.

Mistral AI team. 2024. Codestral: Hello, world!

arXiv:2412.15115.

- 672 673
- 676

- 681
- 682

- 703
- 705
- 707

711

712 713

710

Conference on Program Comprehension (ICPC). 714

Weiyun Wang, Zhe Chen, Wenhai Wang, Yue Cao, Yangzhou Liu, Zhangwei Gao, Jinguo Zhu, Xizhou Zhu, Lewei Lu, Yu Qiao, et al. 2024a. Enhancing the reasoning ability of multimodal large language models via mixed preference optimization. arXiv *preprint arXiv:2411.10442.*

715

716

717

719

721

724

725

726

727

728

729

730

731

732

733

734

735

736

737

738

739

740

741

742

743

744

745

746

747

748

749

750

751

752

754

755

756

757

758

759

760

761

762

763

764

765

766

767

768

769

- Xuezhi Wang, Jason Wei, Dale Schuurmans, Quoc Le, Ed Chi, Sharan Narang, Aakanksha Chowdhery, and Denny Zhou. 2022. Self-consistency improves chain of thought reasoning in language models. arXiv preprint arXiv:2203.11171.
- Yu Wang, Shiwan Zhao, Zhihu Wang, Heyuan Huang, Ming Fan, Yubo Zhang, Zhixing Wang, Haijun Wang, and Ting Liu. 2024b. Strategic chain-of-thought: Guiding accurate reasoning in llms through strategy elicitation. arXiv preprint arXiv:2409.03271.
- Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, Fei Xia, Ed Chi, Quoc V Le, Denny Zhou, et al. 2022. Chain-of-thought prompting elicits reasoning in large language models. Advances in neural information processing systems.
- Martin Weyssow, Aton Kamanda, and Houari Sahraoui. 2024. Codeultrafeedback: An llm-as-a-judge dataset for aligning large language models to coding preferences. arXiv preprint arXiv:2403.09032.
- Chunqiu Steven Xia, Yinlin Deng, Soren Dunn, and Lingming Zhang. 2024. Agentless: Demystifying llm-based software engineering agents. arXiv preprint arXiv:2407.01489.
- Yuxi Xie, Anirudh Goyal, Wenyue Zheng, Min-Yen Kan, Timothy P Lillicrap, Kenji Kawaguchi, and Michael Shieh. 2024. Monte carlo tree search boosts reasoning via iterative preference learning. arXiv preprint arXiv:2405.00451.
- Fengli Xu, Qianyue Hao, Zefang Zong, Jingwei Wang, Yunke Zhang, Jingyi Wang, Xiaochong Lan, Jiahui Gong, Tianjian Ouyang, Fanjin Meng, et al. 2025. Towards large reasoning models: A survey of reinforced reasoning with large language models. arXiv preprint arXiv:2501.09686.
- Jian Yang, Jiaxi Yang, Ke Jin, Yibo Miao, Lei Zhang, Liqun Yang, Zeyu Cui, Yichang Zhang, Binyuan Hui, and Junyang Lin. 2024. Evaluating and aligning codellms on human preference. arXiv preprint arXiv:2412.05210.
- Jiayi Ye, Yanbo Wang, Yue Huang, Dongping Chen, Qihui Zhang, Nuno Moniz, Tian Gao, Werner Geyer, Chao Huang, Pin-Yu Chen, et al. 2024. Justice or prejudice? quantifying biases in llm-as-a-judge. arXiv preprint arXiv:2410.02736.
- Yue Yu, Zhengxing Chen, Aston Zhang, Liang Tan, Chenguang Zhu, Richard Yuanzhe Pang, Yundi Qian, Xuewei Wang, Suchin Gururangan, Chao Zhang, et al. 2024. Self-generated critiques boost reward modeling for language models. arXiv preprint arXiv:2411.16646.

Dan Zhang, Sining Zhoubian, Ziniu Hu, Yisong Yue, Yuxiao Dong, and Jie Tang. 2024a. Rest-mcts*: Llm self-training via process reward guided tree search. *arXiv preprint arXiv:2406.03816*.

771

775

785

788

790

791

793

794

797

807 808

809

810

811

- Di Zhang, Xiaoshui Huang, Dongzhan Zhou, Yuqiang Li, and Wanli Ouyang. 2024b. Accessing gpt-4 level mathematical olympiad solutions via monte carlo tree self-refine with llama-3 8b. *arXiv preprint arXiv:2406.07394*.
- Di Zhang, Jianbo Wu, Jingdi Lei, Tong Che, Jiatong Li, Tong Xie, Xiaoshui Huang, Shufei Zhang, Marco Pavone, Yuqiang Li, et al. 2024c. Llama-berry: Pairwise optimization for o1-like olympiad-level mathematical reasoning. *arXiv preprint arXiv:2410.02884*.
- Yue Zhang, Shuoyang Wang, and Xinyun Zhang. 2022. Codet: Code generation with generated tests. *arXiv* preprint arXiv:2207.10397.
- Yuntong Zhang, Haifeng Ruan, Zhiyu Fan, and Abhik Roychoudhury. 2024d. Autocoderover: Autonomous program improvement. In *Proceedings of the 33rd* ACM SIGSOFT International Symposium on Software Testing and Analysis.
- Qinkai Zheng, Xiao Xia, Xu Zou, Yuxiao Dong, Shan Wang, Yufei Xue, Zihan Wang, Lei Shen, Andi Wang, Yang Li, et al. 2023. Codegeex: A pre-trained model for code generation with multilingual evaluations on humaneval-x. *arXiv preprint arXiv:2303.17568*.
- Qihao Zhu, Daya Guo, Zhihong Shao, Dejian Yang, Peiyi Wang, Runxin Xu, Y Wu, Yukun Li, Huazuo Gao, Shirong Ma, et al. 2024. Deepseek-coder-v2: Breaking the barrier of closed-source models in code intelligence. *arXiv preprint arXiv:2406.11931*.
- Terry Yue Zhuo. 2023. Ice-score: Instructing large language models to evaluate code. *arXiv preprint arXiv:2304.14317*.
- Terry Yue Zhuo, Minh Chien Vu, Jenny Chim, Han Hu, Wenhao Yu, Ratnadira Widyasari, Imam Nur Bani Yusuf, Haolan Zhan, Junda He, Indraneil Paul, et al. 2024. Bigcodebench: Benchmarking code generation with diverse function calls and complex instructions. arXiv preprint arXiv:2406.15877.

A Experiment Settings

Table 6 details the hyperparameter settings of MCTS-Judge employed to generate the results presented in this paper. These settings encompass various aspects of the MCTS architecture, including maximum tree depth, number of rollouts, exploration constant α , LLM sample weight w_l , and UCT sample weight w_u . Additionally, the reward mechanism parameters include the number of test case validations β , number of test cases used γ , number of test case simulations δ , and reward scaling factor ϵ . Hyperparameters related to the LLM configuration, such as temperature, top_p, top_k, and maximum output tokens, are also specified. All experiments were executed on a single H100 GPU with 80GB of memory, ensuring consistency and reproducibility in computational performance.

812

813

814

815

816

817

818

819

820

821

822

823

824

825

826

827

828

829

830

831

832

833

834

835

836

837

838

839

840

841

842

843

Hyperparameter	Value
Maximum tree depth	9
Number of rollouts	8
Constant α	3
LLM sample weight w_l	0.1
UCT sample weight w_{ij}	0.9
Number of test case validations β	5
Number of test cases used γ	3
Number of test case simulations δ	7
Reward ϵ	1.1
Temperature	0.4
Top_p	0.95
Top_k	40
Maximum tokens	2048

Table 6: Hyperparameters of MCTS-Judge.

B Limitations of Execution-Free Methods

In this experiment, we evaluate whether similaritybased execution-free metrics, which do not require test cases and isolated environments, can be used to accurately assess code correctness. We evaluated six representative metrics on the APPS benchmark: BLEU, ROUGE-L, METEOR, ChrF, CodeBLEU, and RUBY. Fig. 6 shows that the score distributions for incorrect and correct code differ only slightly for these metrics. This further highlights the importance of developing high-precision execution-free methods for assessing code correctness.

C Evaluation without References

As discussed in Sec.4.5, we present the complete results for extending to more general scenarios,



Figure 6: Score distributions of six execution-free metrics on the APPS benchmark show negligible distinction between correct and incorrect code, indicating a lack of reliability.

specifically in the absence of reference data. Table7 compares the performance of MCTS-Judge with baselines across three benchmarks and five LLMs. The results highlight MCTS-Judge's greater robustness and generalization ability, as evidenced by reduced performance decay compared to other LLM-as-a-Judge methods, aligning with the conclusions drawn in the main paper's analysis.

D Case Study

844

845

851

852

855

857

864

We demonstrated the superiority of analysis metadata from reasoning chains generated by MCTS-Judge across four key dimensions in Section 4.4. To further highlight MCTS-Judge's advantages over the System-1 thinking approach in terms of accuracy and comprehensive analysis, we present a case study comparing the vanilla *Deepseek-Coder-V2-16B-Instruct* model with the one integrated with MCTS-Judge.

As shown in Fig. 7, at each step, MCTS-Judge provides evaluations from diverse perspectives, such as verifying whether requirements are met (Step 2) and assessing the correctness of the code logic (Step 5). In contrast, the vanilla model generates an incorrect answer with only superficial analysis, demonstrating a lack of deeper understanding.

Problem Statement: Check if two words have the same characters

Code Snippet: def same_chars(s0: str, s1: str): return sorted(s0) == sorted(s1)

Ground Truth: False

Answer from Vanilla:

This method efficiently checks for anagrams, which are words or phrases created by rearranging the letters of another word or phrase, utilizing all original letters exactly once. It's a concise and effective approach for comparing the characters between two strings. Final Answer: **True**

Reasoning trajectory of MCTS-Judge: Step 1:

Analysis: Objectively, we're determining if two strings share the same characters. The given code sorts both strings and compares them. This is effective if the goal is to check whether the two strings are anagrams (i.e., identical characters with identical frequencies). However, for checking only the presence of the same unique characters, frequency doesn't matter, so this code may not align with the exact requirement.

Step 2:

Decision (s_1) : True

Analysis: The formal requirement states: 'Check if two words have the same UNIQUE characters, ignoring frequency and order.' The sortingbased code compares frequency and order. Thus, it does not satisfy the exact requirement of ignoring frequency. A set-based comparison would do that correctly

Decision (s₂): False

Step 3:

Analysis: According to the specification, we need to identify unique characters in each string and compare those sets. Sorting compares ordered characters, including duplicates. Hence, it goes beyond just checking presence of characters. The specification is not fully met by the provided code.

Decision (s₃): False

Step 4:

Analysis: We can declare the code as correct for an anagram check, since sorting ensures that same-frequency characters appear in identical positions. But for the stated requirement—comparing only unique characters—it falls short. Decision (s_4): True

Step 5:

Analysis: Logically, sorting each string and comparing them is a sound approach for determining if they have the same characters AND the same counts. But since the problem only requires checking for unique-character presence, there's a logical mismatch between the solution and the stated requirement.

Decision (s_5) : False

Step 6:

Analysis: Functionality demands ignoring frequency and order. The sorting solution goes beyond that by implicitly matching frequencies. Hence, for THIS functionality (unique characters only), the code is not correct. But for an anagram check, it would be correct. Decision (s_{α}): False

Step 7:

Analysis: From an algorithmic standpoint, sorting is $O(n \log n)$, set comparison is typically O(n). For ignoring frequency, sets are both more appropriate and more efficient. Still, sorting is a valid algorithm for verifying anagrams, but not for simply checking shared unique characters. Decision (s_7): True

Step 8:

Analysis: Revalidating the initial problem: it asks to see if two words share the same set of unique characters. Sorting inevitably measures frequency as well. Therefore, for the EXACT requirement, the sorting solution is inadequate. Decision (s_o): False

Summary

Some of the 8 agents evaluated the problem and concluded that the provided sorting-based code does not meet the problem's requirements. Final consensus from all agents: False

Figure 7: Case Study: System-2 Thinking vs. System-1 Thinking. MCTS-Judge leads with comprehensive evaluations, while vanilla fails with superficial analysis.

Method	Approach	Approach BigCodeBench		HumanEval-X					
Wiethou	rippiouen	Digeodebenen	1110	Python	Java	C++	JavaScript	Go	Average
Commercial Reasoning LLMs									
GPT-o1-mini	System-2	71.14	78.00	93.18	86.36	86.36	89.39	87.88	88.63
Open-sourced Reason	ing LLMs								
Qwen-QwQ-32B	System-2	51.05	69.00	61.36	68.18	66.67	67.42	77.27	68.18
	Code	-Specialized Base	Model: (2wen2.5-0	Coder-14	B-Instru	ıct		
Base Model	System-1	46.84	61.00	60.61	62.88	68.94	65.91	76.52	66.97
ICE-Score	System-1	66.23	69.00	75.00	66.67	71.21	72.73	75.00	72.12
CodeJudge	System-1	47.02	62.00	87.12	75.76	79.55	81.06	73.48	79.40
MCTS-Judge (Ours)	System-2	70.35	74.00	86.36	<u>87.12</u>	80.30	82.58	82.58	83.79
	Code-S	vecialized Base M	odel: De	epSeek-Co	oder-V2-	16B-Inst	truct		
Base Model	System-1	35.09	49.00	69.70	58.33	53.79	53.79	56.06	58.33
ICE-Score	System-1	47.19	56.00	74.24	69.70	71.21	66.67	69.70	70.30
CodeJudge	System-1	35.44	62.00	75.76	66.67	63.64	66.67	66.67	67.89
MCTS-Judge (Ours)	System-2	51.58	71.00	82.58	72.73	84.85	75.00	81.82	79.40
	Co	de-Specialized Ba	se Model	: Mistrala	i-Codes	tral-22B			
Base Model	System-1	32.63	43.00	75.76	58.33	58.33	57.58	58.33	61.67
ICE-Score	System-1	31.05	41.00	76.52	57.58	53.03	59.09	53.79	60.00
CodeJudge	System-1	35.44	48.00	78.79	59.09	59.09	60.61	63.64	64.24
MCTS-Judge (Ours)	System-2	52.37	74.00	79.55	72.73	75.76	65.91	77.27	74.24
		General Base M	10del: Ll	ama-3.1-8	8B-Instri	ıct			
Base Model	System-1	33.95	58.00	59.85	60.61	62.88	64.39	67.42	63.30
ICE-Score	System-1	34.47	46.00	62.12	51.52	50.76	54.55	42.42	52.27
CodeJudge	System-1	41.40	47.00	61.36	60.61	58.33	54.55	52.27	57.42
MCTS-Judge (Ours)	System-2	65.79	62.00	71.21	69.70	65.15	68.18	73.48	69.54
Commercial General Base Model: GPT-4o-mini									
Base Model	System-1	71.05	61.00	81.82	80.30	83.33	83.33	83.33	82.42
ICE-Score	System-1	58.60	62.00	78.03	75.00	75.76	81.06	82.58	78.49
CodeJudge	System-1	57.46	70.00	81.06	82.58	85.61	84.85	83.33	83.49
MCTS-Judge (Ours)	System-2	<u>73.68</u>	72.00	82.58	83.33	<u>87.12</u>	87.12	85.61	85.15

Table 7: Accuracy (%) of MCTS-Judge and baselines **without reference code** on BigCodeBench, APPS, and HumanEval-X. Compared to existing LLM-as-a-Judge methods, MCTS-Judge without reference code still achieves the highest accuracy across all benchmarks and five LLMs (highlighted in bold). MCTS-Judge without reference code maintains its advantage over advanced reasoning LLMs, with superior accuracy compared to the o1-series models highlighted with underlines.

E Prompts

We present the key prompt designs utilized in MCTS-Judge, including the vanilla baseline (Fig. 8), the test-case verification baseline (Fig. 9), the LLM-driven self-assessment (Fig. 10), the logic assessment action (Fig. 11), the test case generation and validation (Fig. 12), and the simulated execution (Fig. 13).

873

874

875

876

Vanilla

systeml>:Determine the correctness of the code snippet. Output Yes or No.
<luserl>: Problem Statement: {problem}
Example: {example}
Reference Solution ({language}): {reference code}
Code Snippet ({language}): {code}
<lassistantl>:Answer (Yes or No only):

Table 8: Prompt of the baseline named Vanilla.

Test Cases Generation

You are an AI assistant specialized in analyzing Python functions and generating test cases. You will be provided with a problem statement and its solution to evaluate the correctness of the code.<luserl>: Full Code: {language} {code}

Public Test Case for the Main

Function:{example}

Instructions: Please analyze how the {function name} function is used within the main function and how it contributes to the expected outputs in the gold test case. For each test case, you should analyze step-by-step based on both the input and the expected output of the main function, and then provide the corresponding input and expected output for the {function name} function. Ensure that the generated test cases are consistent with the behavior expected in the public test cases.

<lassistantl>:Let's break down the code and give the input and expected output of the {function name} function step-by-step for each given gold test case ignoring any discrepancie between the function's logic and the expected outputs of public test case:

Test Case Validation

systeml>: You are an AI assistant specializing in test case validation. Your task is to assess the correctness of a given test case based on the problem description, which consists of four parts: the problem statement, input description, output description, and several input-output pair examples.
eluserl>: Problem:{problem}

Test Cases: {test_cases}

Instructions: Validate the correctness of the test case and determine if it aligns with the expected behavior outlined in the problem description. Do not provide a corrected version. Return PASS or FAIL to indicate the accuracy of the given test case.

<lassistantl>: Let's validate the correctness of the test case step-by-step:

Simulated Execution

<lsysteml>: You are an AI assistant skilled in executing {language} scripts.

<luserl>:Execute the following {language} script. Analyze the code and run each subfunction in the test case step-by-step.

Code: {code}

Test Case: {test case}

Instruction: Act as a {language} interpreter to execute the code line-by-line, tracking changes in each variable throughout the process. Based on this execution trace, determine the output of the unit test case. <lassistantl>:Let's execute the code step-by-step, analyzing the input test case:

Table 9: Prompt for the test-case verification baseline.

LLM-drive Self-Assessment for Node Selection

You are a code evaluation planning expert. Your task is to assess whether the suggested evaluator agent should proceed based on the provided problem statement, code snippet, and evaluation history. Determine if this evaluator will enhance coverage or completeness of the assessment.
<luserl>: Problem Statement: {problem}
Code Snippet: {language} {code}
Proposed Next Evaluator: {agent}
Evaluation History: Agents previously used: {history}
Instruction: Skip the evaluation only if it very negatively affect the assessment. Otherwise, please
respond 'Yes' to include the evaluator.

<lassistantl>: Decision: (Yes or No only)

Table 10: Prompt for LLM-driven self-assessment in MCTS node selection.

Code Logic Evaluation

Evaluation Steps:1. Read the problem statement carefully and identify the required functionalities of the implementation. You can refer to the example and reference answer to understand the problem better.2. Read the code snippet and analyze its logic. Check if the code snippet covers all the required functionalities of the problem. 3. Finally, conclude your evaluation.

<luserl>:Problem Statement:{problem}

Example:{example}

Reference Solution ({language}):{reference code}

Code Snippet ({language}):{code}

<lassistantl>:Evaluation (Code Logic Analysis):

Analysis Summarization

systeml>: You will be provided with an analysis result of a code snippet. If the analysis believes that the code snippet is correct, output: "Yes". Otherwise, output: "No".

<luserl>: Analysis Result: { analysis }

sistantl>: Final Answer (Yes or No only):

Table 11: Example of subtasks: prompt focused on logic assessment

Initial Test Cases Generation

systeml>: You are an AI assistant specializing in problem analysis and test case generation, with particular expertise in {difficulty} test cases. Your task is to generate comprehensive test cases based on the given problem description.

<luserl>: Problem: {problem}

Instructions: Please analyze the problem statement carefully and create five well-rounded test cases. The test cases should be at {difficulty} difficulty level. Your test cases should: 1. Cover a variety of scenarios to thoroughly validate code correctness 2. Avoid excessively large computations 3. Avoid extreme edge cases unless specifically required 4. Include common use cases and reasonable boundary conditions 5. Focus on practical, real-world scenarios

For each test case, please provide:- Input values - Expected output- Brief explanation of what the test case verifies.

<lassistantl>:I'll analyze the problem systematically and create carefully curated test cases.
Analysis Approach:1. First, I'll identify the key requirements and constraints 2. Then, I'll determine important edge cases and boundary conditions 3. Finally, I'll design test cases that progressively increase in complexity

Let's examine each test case:

JSON Reformation

<**lsystem**|>: You are an AI assistant specializing in test case reformatting. Your task is to extract and reformat the test cases based on the examples provided.

<luserl>: Problem:{problem}

Test Cases: {test_cases}

Instructions:Reformat the test cases and return them in a list of JSON format, where each test case is structured as follows:

{{"<root_function_name>": {{ "input": "<input>" (as a string), "expected_output": "<expected_ output>" (as a string)}}}

Use the main function name identified in each test case as the key. Retain the original input and output formats, ensuring that all provided test cases are included.

<lassistant|>: Reformatted Test Cases only, without explanation:

Test Case Validation

systeml>: You are an AI assistant specializing in test case validation. Your task is to assess the correctness of a given test case based on the problem description.

<luserl>: Problem:{problem}

Test Case:{test_case}

Instructions: Validate the correctness of the test case and determine if it aligns with the expected behavior outlined in the problem description. Do not provide a corrected version. Return PASS or FAIL to indicate the accuracy of the given test case.

lassistantl>: Let's validate the correctness of the test case step-by-step:

Table 12: Prompt for test case generation and validation.

Simulated Execution

<|system|>: You are an AI assistant skilled in executing {language} scripts.

Execute the following {language} script. Analyze the code and run each subfunction in the test case step-by-step.

Code:{code}

Test Case: {test_case}

Instruction: Act as a {language} interpreter to execute the code line-by-line, tracking changes in each variable throughout the process. Based on this execution trace, determine the output of the unit test case. <lassistantl>: Let's execute the code step-by-step, analyzing the input test case:

Compare Execution Results with Expected Outputs of Test Cases

systeml>: You are an expert in code validation with a focus on comparing code execution outputs. Your goal is to determine if the actual output matches the expected behavior, being flexible about formatting and minor differences that don't affect correctness.

<luserl>: Problem: {problem}

Test Case:{test_case}

Actual Output: {answer}

Instruction: 1. Extract the final execution result from the actual output. Compare this result with the expected answer, focusing on correctness rather than specific formatting. Note: Do not judge the code; simply validate whether the results match.

<lassistantl>: Let's check the results, and conclude with **MATCH** or **NOT MATCH** after the comparison.

Table 13: Prompt for simulated execution and verify whether the execution results match the expected answers.