# LLAMA-BERRY: PAIRWISE OPTIMIZATION FOR O1-LIKE OLYMPIAD-LEVEL MATHEMATICAL REASONING

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#### ABSTRACT

This paper presents an advanced mathematical problem-solving framework, LLaMA-Berry, for enhancing the mathematical reasoning ability of Large Language Models (LLMs). The framework combines Monte Carlo Tree Search (MCTS) with iterative Self-Refine to optimize the reasoning path and utilizes a pairwise reward model to evaluate different paths globally. By leveraging the self-critic and rewriting capabilities of LLMs, Self-Refine applied to MCTS (SR-MCTS) overcomes the inefficiencies and limitations of conventional stepwise and greedy search algorithms by fostering a more efficient exploration of solution spaces. Pairwise Preference Reward Model (PPRM), inspired by Reinforcement Learning from Human Feedback (RLHF), is then used to model pairwise preferences between solutions, utilizing an Enhanced Borda Count (EBC) method to synthesize these preferences into a global ranking score to find better answers. This approach addresses the challenges of scoring variability and nonindependent distributions in mathematical reasoning tasks. The framework has been tested on general and advanced benchmarks, showing superior performance in terms of search efficiency and problem-solving capability compared to existing methods like ToT and rStar, particularly in complex Olympiad-level benchmarks, including AIME24 and AMC23.

#### 1 Introduction

Mathematical reasoning represents a great challenge in artificial intelligence, with broad applications across automated theorem proving, mathematical problem solving, and scientific discovery (Ahn et al., 2024). Recently, significant strides have been made by Large Language Models (LLMs) like GPT-4 (Achiam et al., 2023) in general mathematical tasks involving arithmetic or geometric problem-solving (Cobbe et al., 2021; Sun et al., 2024; Ying et al., 2024). However, complex mathematical reasoning remains challenging, especially at the Olympiad-level benchmarks such as AIME (MMA). One intuitive way is to break the complex problem-solving solutions into step-bystep thoughts, known as reasoning paths, as shown in Chain-of-Thought (CoT) (Wei et al., 2022). Although prompt-based methods can directly construct such reasoning paths, they remain limited in efficiency and accuracy. As a result, researchers have begun exploring search-based optimization algorithms to enhance the generation of effective reasoning paths.

One line of research focuses on generating solutions based on complete reasoning paths. Tree search techniques with backtracking capabilities are proposed to address the inefficiencies of naive methods, such as Tree-of-Thought (ToT) (Yao et al., 2024) and Breadth-First Search (BFS) based on greedy strategies (Zhang et al., 2024). Heuristic tree search methods like RAP (Hao et al., 2023) and Q\* (Wang et al., 2024) treat each step in a reasoning path as a state and the generation of steps as actions, framing the search for reasoning paths as a Markov Decision Process (MDP) problem.

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Monte Carlo Tree Search (MCTS) methods have further improved the efficiency of path searches in reasoning paths. Yet, the generation of steps in reasoning paths faces challenges due to the infinite action space of thought steps, particularly under limited search conditions, which constrains the performance of step-wise search methods. Unlike methods that generate a single step simultaneously, another approach considers the entire CoT solution as an independent state with iterative optimization actions. This method, known as rewriting, includes techniques such as reflection and self-refine, where optimization of a solution depends on its previous contents and typically involves only local corrections, ensuring that the new solution remains within the "trust region" of the original. This strategy offers the iterative optimization methods a proximal optimization characteristic, making the action space more compact. However, this continuous and greedy iterative approach also suffers from low search efficiency and the risk of local optima, limiting the performance ceiling of rewriting methods.

Another line of research focuses on evaluating the quality of reasoning paths, which includes outcome and process reward models (Uesato et al., 2022). The former focuses on whether the final answer of a reasoning path is correct, while the latter emphasizes the correctness of each step and the logical connections between steps. Although both approaches enable models to score using a scalar, labelled data for training these reward models are scarce. Furthermore, the scoring standards in mathematical reasoning tasks are highly variable, and the reward distribution for different problems is typically not i.i.d. (independently and identically distributed), with each problem presenting unique scoring characteristics. This non-independence complicates the scaling up of single-scalar score-based reward models and their abilities to detail local preference relations between answers.

To address the above challenges, we design the LLaMA-Berry framework (in Figure 1) based on LLaMA-3.1-8B Instruct (Meta, 2024b), which includes two novel methods called Self-Refine applied to Monte Carlo Tree Search (SR-MCTS) and Pairwise Preference Reward Model (PPRM). Specifically, SR-MCTS is a novel Markov Decision Process (MDP) framework focusing on a pathwise problem-solving search where a complete solution is defined as an independent state, and self-refine is considered an optimization action. Then, Monte Carlo Tree Search (MCTS) is leveraged for the exploration of optimal solutions with guiding of PPRM evaluations. PPRM is inspired by Reinforcement Learning from Human Feedback (RLHF) (Christiano et al., 2017) techniques; we have transformed the task of reward models into an RL problem that models preferences between solutions, then aggregating local preferences into a global ranking score with an Enhanced Borda Count (EBC) method.

Finally, evaluations on general benchmarks such as GSM8K (Cobbe et al., 2021) and MATH (Hendrycks et al., 2021) have demonstrated that our method outperforms baseline approaches like ToT (Yao et al., 2024) and rStar (Qi et al., 2024) in both search efficiency and performance. Moreover, in challenging Olympiad-level benchmarks such as AIME24 and AMC23 and in the Graduate-level GPQA Diamond (Rein et al., 2023) benchmark, our approach has elevated the performance of LLaMA-3.1-8B without any further training to a level comparable to proprietary solutions including GPT-4 Turbo. These encouraging results suggest that our method can effectively improve the LLM's reasoning ability with only a small amount of data, and this capability can be generalized to other fields, such as physics and chemistry. Furthermore, it can enable multimodal reasoning, allowing the model to achieve even greater reasoning power.

To summarize, our contributions in LLaMA-Berry framework integrate three essential components:

- SR-MCTS establishes a novel MDP framework that treats complete path-wise solutions as independent states and utilizes Self-Refine as an optimization action, balancing efficiency and performance in search.
- Inspired by Reinforcement Learning from Human Feedback (RLHF), PPRM leverages the preference relationship between solutions to evaluate their quality, which avoids the volatility of absolute scores while providing a more guided exploration of optimal paths.
- Finally, EBC method aggregates the local preferences into a global ranking score, allowing the model to identify the overall patterns and enhance the decision-making process.

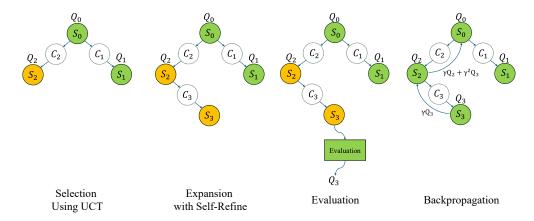


Figure 1: The main pipeline of LLaMA-Berry, where  $S_i$  stand for problem-solving solutions and  $C_i$  stands for critiques. This Pipeline consists of four phases detailed in 2.2, including Selection, Expansion, Evaluation and Backpropagation.

#### 2 METHODOLOGY

#### 2.1 PRELIMINARY

In the realm of mathematical problem-solving, we face significant challenges that require systematic approaches to derive accurate and efficient solutions. A core issue in this field is generating and optimizing reasoning paths, which can be formalized as a path-wise Markov Decision Process (MDP) framework. This framework allows us to define the state space S, where each state s represents a complete solution to a given problem, and the action space S consists of all feasible rewriting actions S that make transitions between states.

The central issues we aim to address include the development of the value function Q(s, a), which quantifies the expected rewards from executing action a at state s, defined as:

$$Q(s,a) = \mathbb{E}[R(s')|s' = T(s,a)] \tag{1}$$

Where T(s,a) indicates the transition to another solution s' from solution s with rewriting operation denoted as a. Our primary objective is to identify the optimal state  $s^*$ , which represents the best solution to the problem. This optimal state can be achieved through the selection of actions that maximize the value function, guiding us toward the most desirable outcomes:

$$s^* = \arg\max_{s' \in S} \mathbb{E}[Q(s)] \tag{2}$$

#### 2.2 Self-refine applied to Monte Carlo Tree Search

Monte Carlo Tree Search (MCTS) is an effective reinforcement learning method within the Markov Decision Processes (MDP) framework, employing states, actions, and cost functions through sampling. The algorithm follows four key steps: selection, expansion, simulation/evaluation, and backpropagation. In the selection phase, the root node is expanded using the Upper Confidence Bound applied to Trees (UCT) algorithm, which selects a node *s* by balancing exploration and exploitation, that is,

$$a = \arg\max_{a \in A(s)} \left( Q(s, a) + c \cdot \sqrt{\frac{\ln N(s)}{N(s, a)}} \right), \tag{3}$$

where N(s) is the visitation count of node s, N(s,a) is the action frequency, and c is a parameter controlling exploration. In the expansion phase, node s generates subsequent states s', added as

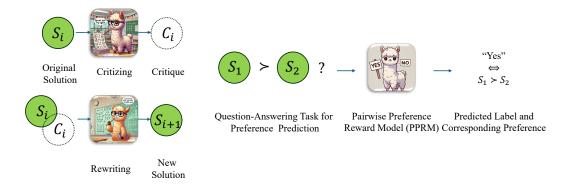


Figure 2: (Left) Self-Refine Process and (Right) Preference Prediction process of PPRM

new nodes in tree  $\mathcal{T}$ . The evaluation phase typically uses simulations or heuristics to estimate the Q-values for these nodes. Finally, during backpropagation, the estimated Q-values are updated retroactively from the leaf nodes to the root. This iterative process allows MCTS to explore and exploit the state space effectively, refining decision-making by balancing the exploration of new options with the exploitation of known high-value paths.

As shown in Figure 1, the SR-MCTS method combines Monte Carlo Tree Search (MCTS) with Self-Refine, which optimizes the solution search via a structured tree. This method continuously evaluates and improves solutions by combining the iterative nature of MCTS with the self-critique and rewriting capabilities of LLMs as following sections:

**Selection Phase:** The selection phase identifies a node  $s_i$  from the search tree  $\mathcal{T}$  for expansion, where each node represents a complete solution state. The Upper Confidence Bound applied to Trees (UCT) algorithm is employed to select the optimal node, with dynamic pruning used to avoid local optima. A node  $s_i$  is considered fully explored when its child nodes reach a predefined limit, and at least one child node's Q value exceeds the Q value of  $s_i$ .

**Expansion Phase:** In the expansion phase, as shown in Figure 2, the selected answer  $s_i$  is expanded by generating successor answers through a Self-Refine process, which includes a **Critizing** and **Rewriting** process. The **Critizing** generates a critique  $c_i = C(s_i)$  that identifies drawbacks (e.g., mathematical wrongs or logical fault) in the current chosen answer  $S_i$ , and then **Rewriting** process generates a new answer  $s_{i+1} = R(s_i, c_i)$ . In practice, to simplify the problem, we assume this process is deterministic, ensuring that the same original state of solutions  $s_i$  consistently produces the same successor state of solution  $s_{i+1}$ . The new state of solution s' is then added to the search tree  $\mathcal T$  as a new node.

**Evaluation Phase:** The evaluation phase calculates the value Q(s') of the newly generated node s' using the Pairwise Preference Reward Model (PPRM). The evaluation involves two steps: global and local value assessments. The global value  $Q_g(s')$  is determined by the quantile of s' in a winloss matrix M, which reflects the win-loss relationships between nodes. The local value  $Q_l(s')$  is derived from comparisons with adjacent nodes in the search tree  $\mathcal{T}$ . The total value Q(s') is then computed as a weighted combination of global and local values:  $Q(s') = \alpha Q_g(s') + (1-\alpha)Q_l(s')$ , where  $\alpha$  controls the relative influence of each component.

**Backpropagation Phase:** In the backpropagation phase, the value Q(s') of the new node is propagated back to its parent node  $s_i$ , updating Q value of  $s_i$  as a discounted sum of its child nodes' Q values:  $Q(s_i) = (1 - \gamma)Q(s_i) + \gamma Q(s')$ . The discount factor  $\gamma$  represents the importance of future rewards. This iterative update mechanism ensures that the values of parent nodes are progressively refined, enhancing the guidance for future selections.

Additionally, to control the growth of the search tree, the SR-MCTS method restricts the maximum number of rollouts  $N_{max}$ . The search process terminates when the restriction is reached, imposing limits on the unbounded expansion of the tree. The overarching objective of SR-MCTS is to maximize the expected highest Q value of all existing nodes S, guiding us towards the most desirable outcomes  $S^*$ , ensuring that the search method efficiently converges to high-quality solutions.

#### 2.3 Pairwise Preference Reward Model

In mathematical problem-solving tasks, reliable evaluation of solutions is crucial, as it leads to better estimation of Q-values, thereby offering improved guidance. Existing reward models typically evaluate solutions by giving absolute scores, such as (PRM) (Lightman et al., 2023) and outcome reward mode (ORM) (Yu et al., 2023a). However, the score-based reward models may fall short in leveraging the instruction following capability of LLMs or effectively handling the variations in data distributions and exhibit volatility, especially when the differences between different solutions are subtle. To address this issue, we propose the Pairwise Preference Reward Model (PPRM), which leverages a comprehensive preference dataset incorporating substantial samples from both approaches to learn preference relationships among mathematical solutions. Please refer to Appendix for details about training and inference of PPRM.

For two answers to a given mathematical problem, denoted as  $a_1 > a_2 | \phi$  where  $a_1$  and  $a_2$  denote the preferred and dispreferred completion, PPRM predicts their relative quality using a pairwise partial ordering, represented by the following probability formula:

$$P(a_1 \succ a_2 \mid \phi) = \frac{e^{\phi(a_1)}}{e^{\phi(a_1)} + e^{\phi(a_2)}} \tag{4}$$

Where  $\phi(a_1 \succ a_2)$  denotes the feature representation of a partial ordering relation between solution  $a_1$  and  $a_2$ , with  $\phi$  representing the parameters of the model. In our method,  $a_1 \succ a_2$  are represented by tokens of the LLM, and  $P(a_1 \succ a_2 \mid \phi)$  is estimated using the logits value of tokens calculated by the LLM.

Then, inspired by advancements in Language Interface Fine-Tuning (LIFT) (Dinh et al., 2022), we frame the training process of PPRM as a question-answering task. The model is tasked with answering the question, "For Question Q, is solution  $a_1$  better than solution  $a_2$ ?" as shown in Figure 2. To form a robust training objective, the predicted token labels  $\hat{y}$  ('Yes' or 'No') are evaluated using the indicator function I:

$$\mathbf{I}(\hat{y}, y) = \begin{cases} 1, & \text{if } \hat{y} = y \\ 0, & \text{if } \hat{y} \neq y \end{cases}$$
 (5)

Finally, a pairwise preference dataset  $\mathcal{D}$  that contains millions of mathematical problem-solving solution pairs is converted into a dataset  $\mathcal{D}'$  suitable for a question-answering task. We employ RLHF techniques to train the model to improve its performance in the partial-order prediction question-answering task. Subsequently, the Direct Preference Optimization (DPO) (Rafailov et al., 2024) method is utilized to find the optimal  $P_{\phi}$  by maximizing the objective  $\arg\max_{\phi}\mathbb{E}_{P}[\mathbf{I}(\hat{y},y)]$ .

#### 2.4 ENHANCED BORDA COUNT METHOD

Although PPRM allows us to directly compare the quality of two answers, we still need to convert these local partial order relations into a cohesive global ranking to gain a comprehensive evaluation for the answers. This conversion process can be formalized as the global optimal ranking aggregation (GORA) problem. To address this problem, we propose the Enhanced Borda Count (EBC) method based on a transitivity assumption of mathematical problem-solving solutions (detailed in Figure 3), which integrates the naive Borda Count Algorithm with a transitive closure of partial order relations calculated by the Floyd-Warshall (Cormen et al., 2009) Algorithm. For formalized proof, please refer to Appendix E.

**Local Preference Calculation:** First, as shown in Figure 3 (1), the PPRM generates a win-loss matrix  $M \in \mathbb{R}^{n \times n}$  for all n problem-solving solutions, where M[i,j] = 1 indicates that solution  $a_i$  is superior to solution  $a_j$ , and M[i,j] = 0 otherwise. This process can be represented as:

$$M[i,j] = \begin{cases} 1, & \text{if } P(a_i \succ a_j) \ge 0.5\\ 0, & \text{if } P(a_i \succ a_j) < 0.5 \end{cases}$$
 (6)

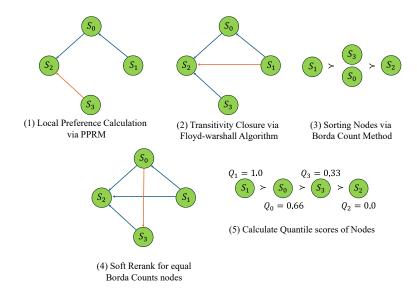


Figure 3: The Pipeline of Enhanced Borda Count (EBC) Method

This matrix can be viewed as an adjacency matrix of a directed graph G = (V, E), where each solution  $a_i$  corresponds to a vertex  $v_i$ , and an edge  $e = (v_i, v_j)$  exists if M[i, j] = 1, indicating that solution  $a_i$  is preferred over  $a_j$ .

**Transitive Closure:** As shown in Figure 3 (2), to simplify the problem, we adopt the assumption of transitivity for mathematical solutions, that is, if  $v_i \succ v_k$  and  $v_k \succ v_j$ , then  $v_i \succ v_j$ . Under this assumption, the transitive closure C of a preference matrix can be computed. Specifically, if M[i,k]=1 and M[k,j]=1, then M[i,j]=1. This is achieved by updating the transitive closure matrix C using Floyd-Warshall algorithm with dynamic programming rule:

$$C[i,j] = \bigvee_{k=1}^{n} (C[i,k] \wedge C[k,j])$$
 (7)

where  $\bigvee$  denotes the logical OR operator and  $\wedge$  denotes the logical AND operator.

**Borda Count-Based Global Ranking:** Next, based on the transitive closure matrix C, we apply the Borda Count method for global ranking. The Borda Count determines the ranking of each node by calculating its out-degree, which corresponds to the number of nodes it defeats. For each node  $v_i$ , the Borda Count Borda $(v_i)$  is defined as  $\sum_{j=1}^n C[i,j]$ , like the ranked node list in Figure 3 (3).

Nodes with higher Borda counts are ranked higher. However, in practice, cyclic preferences can cause efficiency issues with the naive Borda Count method. To further refine the ranking, as shown in Figure 3 (4), a re-ranking stage is introduced, where the logits generated by the PPRM are used for soft comparison among nodes with equal Borda counts. Specifically, for two nodes  $v_i$  and  $v_j$  with equal Borda counts, the soft comparison rule can be denoted as  $v_i \succ v_j \iff P(a_i \succ a_j) > P(a_j \succ a_i)$ . This process ensures that even in the presence of cycles or local ambiguities, the ranking remains consistent and reasonable.

Global Quantile Score of Solutions: Finally, as shown in Figure 3 (5), the ranking is converted into a global quantile quality score  $Q_g$  for each solution v is  $Q_g[v] = 1 - \frac{\operatorname{rank}(v) - 1}{|V| - 1}$ , where  $\operatorname{rank}(v)$  is the position of v in the ranking based on Borda counts, and |V| is the total number of nodes. To reflect local advantages in the search tree structure, the local win rate  $Q_l(x)$  for a node v is calculated with its children nodes Children v as follows:

$$Q_{l}[v] = \frac{\sum_{u \in \text{Children}[v]} C[u, v]}{|\text{Children}[v]|}$$
(8)

Table 1. Benefithark Comparison of Different Math Woodels						
Benchmark Model	GSM8K	MATH	GaoKao 2023 En	OlympiadBench	College Math	MMLU STEM
DeepSeekMath-7B-RL (Shao et al., 2024)	88.2	52.4	43.6	19.0	37.5	64.8
DeepSeek-Coder-V2-Lite-Instruct (Zhu et al., 2024)	87.6	61.0	56.1	26.4	39.8	68.6
Internlm2-math-plus-7b (Ying et al., 2024)	84.0	54.4	50.1	18.8	36.2	55.2
Internlm2-math-plus-20b (Ying et al., 2024)	87.9	56.5	51.9	23.1	37.5	63.5
Internlm2-math-plus-mixtral8x7b (Ying et al., 2024)	92.1	59.4	49.6	25.0	37.5	71.9
Mathstral-7B-v0.1 (Mistral AI, 2024)	84.9	56.6	46.0	21.5	33.7	64.0
NuminaMath-7B-CoT (Beeching et al., 2024b)	75.4	55.2	47.5	19.9	36.9	60.8
NuminaMath-72B-CoT (Beeching et al., 2024a)	90.8	66.7	58.4	32.6	39.7	64.5
Qwen2-7B-Instruct (Yang et al., 2024)	85.7	52.9	36.4	21.3	24.5	68.2
Qwen2-Math-7B-Instruct (Yang et al., 2024)	89.9	75.1	62.1	38.2	45.9	63.8
Qwen2-72B-Instruct (Yang et al., 2024)	93.2	69.0	58.7	33.2	43.2	84.4
Qwen2-Math-72B-Instruct (Yang et al., 2024)	96.7	84.0	68.3	43.0	47.9	79.9
Meta-Llama-3.1-8B-Instruct (Meta, 2024b)	76.6	47.2	30.1	15.4	33.8	60.5
Meta-Llama-3.1-70B-Instruct (Meta, 2024a)	94.1	65.7	54.0	27.7	42.5	80.4
LLaMA 3.1-8B-Instruct (Meta, 2024b)	89.8@major8	54.8@major8	36.4@major8	24.8@major8	36.4@major8	68.3@major8
+ SR-MCTS (Ours)	94.9@rm8	69.4@rm8	61.6@rm8	47.2@rm8	63.7@rm8	82.9@rm8
+ SK-WC15 (Ours)	96.1@rm16	75.3@rm16	68.6@rm16	55.1@rm16	68.9@rm16	88.3@rm16

Table 1: Benchmark Comparison of Different Math Models

The final score Q(x) for a solution is a weighted sum of local win rate  $Q_l(x)$  and global ranking quantification  $Q_g$ , computed as:

$$Q(x) = \alpha \cdot Q_l(x) + (1 - \alpha) \cdot Q_g(x) \tag{9}$$

where  $\alpha$  controls the balance between local win probabilities and global ranking. The softened re-ranking process ensures that even in cyclic preferences, the local win probabilities and global ranking results are consistent, ultimately producing a reasonable and reliable ranking.

# 3 EVALUATION

#### 3.1 Experiment Settings

**Settings:** To better evaluate the effectiveness of our approach, we select LLaMA-3.1-8B-Instruct model (Meta, 2024b) as the base model for SR-MCTS search, **without any additional training**. We train a Gemma2-2B-Instruct model (Google, 2024) as PPRM to provide reward signals during the search process. To ensure robust and efficient inference, we contribute the Berry-Tree inference framework to the community, which supports advanced features such as fault tolerance, checkpoint recovery, multi-query concurrency, and automatic multi-server load balancing (hyperparameter settings detailed in Appendix A).

**Grading:** We assess algorithm-generated answers using the correctness evaluation method from PRM800K (Lightman et al., 2023), focusing on format adherence and content accuracy. The model receives a prompt detailing the expected answer format. We score answers as consistent if they exactly match the ground truth, closely approximate it numerically, or are equivalent in symbolic form. Then, to provide a comprehensive and robust evaluation metric, we adopt **major@k** and pass@k based on our reward-ranked sorting which is denoted as **rm@k**, as the evaluation metrics. Details on the evaluation method and metrics are further outlined in the Appendix B.

#### 3.2 Benchmark

General Mathematical Reasoning Benchmarks We summarize the results on general mathematical reasoning benchmarks in Table 1, which indicates that our method significantly boosts the base model's performance. The results also illustrate that the improvements are consistent across various difficulty levels. Specifically, the capability of Meta-Llama-3.1-8B-Instruct has improved by more than 35% on 4 benchmarks at rm@16. Qwen2-Math-72B-Instruct has demonstrated the strongest mathematical capability among the competing methods, while our LLaMA-Berry exceeds it on four benchmarks. In particular, LLaMA-Berry reaches 55.1% on OlympiadBench and 68.9% on College Math, surpassing the 70B model by 11.9% and 21%, respectively.

Additionally, we observe that majority voting results are often lower than rm@k under the same number of simulations. For benchmarks like GSM8K and MATH, The performance of majority voting is not significantly inferior to that of rm@k. However, for those more challenging (e.g., GaoKao 2023 En, OlympiadBench and College Math shown in Table 1), the performance gap between their result become wider. We suspect the reason is that, on benchmarks with lower question difficulty, the

performance of LLM primarily relies on its inherent reasoning capabilities, whereas on more complex benchmarks, it's performance is largely dependent on its Self-Refine abilities. As shown in Table 2, in both the AMC2023 and GPQA Diamond benchmarks, we again observe this phenomenon, which becomes increasingly evident as benchmark difficulty scales when comparing MATH and other benchmarks. This indicates the potential of our method on solving more complex reasoning problems

A comparison between MATH and OlympiadBench shows that the latter is much more difficult and challenging, with less dataset leakage and higher inference costs, making Self-Refine harder to apply. The increased variance in answer sequences means the model does not hit the diminishing returns ceiling of Self-Refine as quickly as it does with GSM8K.

AIME2024 AMC2023 Math Odyssey GPQA Diamond TheoremQA DeepMind Mathematics AIME1983-2023 Claude 3 Opus 42.0 (5-shot) 50.4 GPT 4 Turbo 73.4 3.3 47.0 38.8 48.4 60.3 85.5 GPT 4o 13.4 56.1 OpenAI of Preview 78.3 56.7 OpenAI o1 94.8 833 78.0 Gemini 1.5 Pro 67.7 46.2 Gemini Math-Specialized 1.5 Pro Meta-LLaMA-3.1-8B-Instruct 80.6 23.3 55.8 15.7 41.7 30.4 25.7 49.3 15.5 Owen2-Math-7B-Instruct 75.1 13.3 62.5 naMath-72B CoT Owen2-Math-72B-Instruc 20.0 84.0 60.0 13.3@major8 44.2@major 8@major 22.9@major 39.4@major8 29.7@major 56.4@major 18.0@major8 LLaMA-3.1-8B-Instruct+ SR-MCTS 69.4@rm8 16.7@rm8 48.2@rm8 60.4@rm8 77.3@rm8 39.9@rm8 60.1@rm8 28.6@rm8 75.3@rm16 26.7@rm16

Table 2: Performance Comparison across Multiple Olympiad Benchmarks

Cutting-edge Mathematical Olympiad Benchmarks: We evaluate the performance of our model on the cutting-edge mathematical olympiad benchmarks, as shown in Table 2. The results demonstrate that LLaMA-Berry remains highly competitive on Olympic-level problems, demonstrating its capability in complex reasoning. Notably, on the most challenging AIME2024 benchmark, the success rate increases from 2/30 (LLaMA-3.1-8B-Instruct) to 8/30 (ours), which not only surpasses typical open-source models but also exceeds all commercial closed-source solutions, except the OpenAI o1 series. On the GPQA Diamond benchmark, which includes advanced graduate-level questions across physics, biology, and chemistry—representing the highest reasoning difficulty. Our algorithm achieves accuracy comparable to GPT-4 Turbo on this benchmark.

Our approach demonstrates remarkable performance not only on mathematical reasoning problems but also across a variety of science and engineering problems. For instance, it excels in benchmarks such as GPQA diamond in Table 1 and MMLU STEM in Table 2. This highlights the generalizability and robustness of our method, which can effectively tackle a wide range of challenges in technical domains, thereby showcasing its potential for broader applications in both research and practical scenarios.

Table 3: Performance of Different Tree-Based Methods in LLaMA-3-8B-Instruct on GSM8K, GSMHARD, and MATH500 Benchmarks

Benchmark Method	GSM8K (%)	GSMHARD (%)	MATH500 (%)
Zero-Shot CoT	68.4	14.9	5.8
Few-shot CoT	74.5	25.6	17.8
One-turn Self-Refine	75.7	26.5	25.0
Self-Consistency with 8 Samplings	78.4	28.5	30.0
Self-Consistency with 64 Samplings	83.2	30.3	33.0
Self-Consistency with 128 Samplings	84.7	31.2	33.8
Tree of Thoughts	69.1	19.6	13.6
Reasoning via Planning	80.6	29.6	18.8
rStar with 32 Rollouts	88.7@major32	33.4@major32	38.3@major32
rStar with mutual reasoning and 32 Rollouts	91.7@rm32	37.5@rm32	42.9@rm32
CD MCTC 14 OD II 4	86.4@major8	30.2@major8	35.2@major8
SR-MCTS with 8 Rollouts	94.1@rm8	37.1@rm8	56.4@rm8
CD MCTC	88.1@major16	31.5@major16	39.6@major16
SR-MCTS with 16 Rollouts	96.4@rm16	41.1@rm16	63.8@rm16

**Comparison with Other Tree-Based or CoT Methods:** We also compare our algorithm with other tree-based reasoning methods and CoT on GSM8K, GSMHard (Gao et al., 2022), and MATH500 (Lightman et al., 2023), a representative and highly challenging 10% subset of MATH.

The results are depicted in Table 3. Shown in Table 3, as the benchmark difficulty increases (from GSM8K to GSMHard), performances of the RAP and ToT methods tend to degrade relative to simpler methods like Few-shot CoT and One-turn Self-Refine. We suspect the reason could be the weak self-evaluation capability of LLMs, which may guide reasoning step to wrong side. Moreover, tree search-based methods can incur a more computational overheads compared to these simpler methods. In contrast, rStar and our method maintain a positive trend in output performance, highlighting the superior energy efficiency of both approaches.

By analyzing the result from rStar, Self-consistency, and our algorithm, it becomes evident that our method achieves the highest efficiency in rollouts. Specifically, when observing majority voting metrics, our method achieves an accuracy of 86.4% which is among the same level on GSM8K as others, with only 1/4 of the exploration cost of rStar and 1/16 of Self-consistency. This provides compelling validation of the efficacy of the global evaluation mechanism within PPRM, as well as the aggressive exploration fostered by the dynamic pruning strategy.

#### 3.3 ABLATION STUDY

Table 4: Performance Breakdown of LLaMA-3.1-8B-Instruct with SR-MCTS

	GSM8K		MATH500		AIME2024	
Zero-shot CoT	76.6		46.2		6.7	
One-turn Self-Refine	84.4		55.4		10.0	
Rollouts or Samples	8	16	8	16	8	16
Major Voting with Random Repeated Sampling	88.3	88.9	46.8	48.2	10.0	10.0
Self-Consistency	88.5	88.6	43.8	43.0	10.0	10.0
Tree of Thoughts	83.2	82.5	40.2	35.0	6.7	10.0
Multi-turn Self-Refine with Self-Evaluation	78.9	78.2	40.2	40.4	6.7	6.7
CoT based MCTS with Process Self-Reward	68.5	70.7	33.2	33.8	6.7	3.3
Self-Refine based MCTS with Outcome Self-Reward	82.0@rm8	81.4@rm16	37.2@rm8	36.4@rm16	6.7@rm8	6.7@rm16
SR-MCTS (Self-Refine applied to MCTS with PPRM)	95.0@rm8	96.1@rm16	69.0@rm8	76.6@rm16	16.7@rm8	26.7@rm16

In our research, we design a series of ablation experiments based on the concept of a contrast matrix, systematically evaluating the key components of our methods across three benchmarks of increasing difficulty: GSM8K, MATH500, and AIME2024. We incorporate three baseline methods as control groups: Zero-shot CoT, One-turn Self-Refine, and Major Voting with Random Repeated Sampling. By comparing the performance of our experimental groups with these baselines, we assess the necessity of adopting more sophisticated mechanisms.

**Self-Refine based Search vs. CoT based Search:** In the GSM8K and MATH500 benchmarks, the Self-Refine method demonstrates significant advantages over Zero-shot CoT. Specifically, in the GSM8K task, Self-Refine achieves accuracy rates of 95.0% and 96.1% for 8 and 16 rollouts, respectively, substantially surpassing the 76.6% achieved by CoT. In the MATH500 task, the difference is even more pronounced, with Self-Refine achieving accuracies of 69.0% and 76.6% for 8 and 16 rollouts, compared to CoT's 46.2%.

**Self-Reward vs. PPRM:** Comparing the self-reward mechanism with PPRM, the latter exhibit particularly strong performance in the GSM8K benchmark. The SR-MCTS using PPRM achieves a high accuracy of 96.1% with 16 rollouts, significantly better than the process and outcome self-reward approaches, which only reach 81.4% and 70.7%. PPRM, by considering both the process and performance comprehensively, more effectively motivates the model to explore optimal solutions, thereby significantly enhancing performance.

These findings underscore the efficacy of combining the Self-Refine method with PPRM when addressing complex problems. Lastly, the contrast between self-reward mechanisms and PPRM emphasizes the importance of designing reward mechanisms that consider both process and outcome comprehensively. PPRM provides a more holistic incentive to the model, thus fostering more effective problem-solving strategies.

#### 3.4 SCALING STUDY

**Scaling of Test-time Rollouts:** To explore the potential and trends of the scaling with rollouts in test-time, we depict the pass rate with rollouts in three benchmarks with different difficulty levels. Analyzing the performance alongside the Figure 4, the increment in the number of rollouts consis-

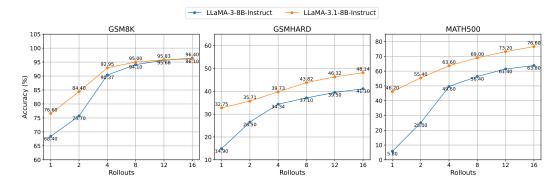


Figure 4: Scaling of Test-time Rollouts

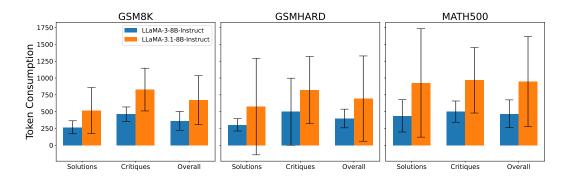


Figure 5: Average Token Consumption Comparison Across Datasets

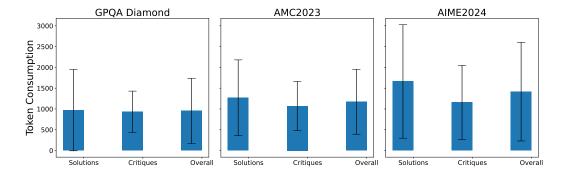


Figure 6: Average Token Consumption for LLaMA-3.1-8B-Instruct Across Olympiad-level Datasets

tently enhances model performance across various benchmarks, and the extent of these improvements differs depending on the benchmark's complexity and the base model's reasoning capability. The LLaMA-3-8b-Instruct model displays a steady progression in performance with each increase in rollouts but faces more pronounced challenges in the complex MATH500 benchmark, suggesting a limitation in handling intricate mathematical reasoning without substantial computational support. In contrast, the LLaMA-3.1-8b-Instruct model begins with a higher baseline performance across all benchmarks. This indicates that its self-refine capabilities better utilize the additional computational resources provided by more extensive rollouts. This is particularly evident in the MATH500 benchmark, where the performance disparity between the two models significantly expands, highlighting the critical role of foundational model capabilities in managing sophisticated tasks.

**Scaling of Test-time Token Overheads:** Comparing LLaMA-3-8B-Instruct and LLaMA-3.1-8B-Instruct across GSM8K, GSMHARD, and MATH500, LLaMA-3.1-8B-Instruct consistently consumes more tokens across all categories—Solutions, Critiques, and Overall. This 3.4 result reflects

LLaMA-3.1-8B-Instruct's tendency to generate more detailed and comprehensive outputs with increased overhead. While this likely improves solution quality, it also introduces greater resource demands and variability in token usage, highlighting a trade-off between accuracy and computational resources. LLaMA-3.1-8B-Instruct is thus better suited for tasks prioritizing precision over speed. As shown in 3.4, Token overheads during inference also scale with task difficulty across different olympiad-level benchmarks with LLaMA-3.1-8B-Instruct. AIME2024 exhibits the highest token consumption with significant variability, reflecting the complexity of its solution paths. In contrast, GPQA Diamond shows lower overall overhead, while AMC2023 falls in between, with moderate token consumption and less variability than AIME2024 but still notable.

# 4 RELATED WORK

#### 4.1 PRM&ORM

The mathematical reasoning capabilities of LLMs exhibit continuous enhancement. OpenAI o1 (OpenAI, 2024) even achieves ability comparable to graduate students on challenging GPQA benchmarks. Recent studies mainly focus on collecting high quality data or domain-specific knowledge (Liao et al., 2024; Huang et al., 2024; Toshniwal et al., 2024; Lu et al., 2024; Yu et al., 2023b; Zhao et al., 2024) or training external reward models (Kang et al., 2024; Wang et al., 2023; Havrilla et al., 2024; Lightman et al., 2023; Ma et al., 2023). There are primarily two types of reward models. The first one is Outcome-supervised Reward Models (ORMs), which are trained from the final CoT answer of the model, while ORMs assign a reward to a complete answer. This kind of feedback is not precise enough, and it is challenging to align the reward. The second one is process-supervised reward models (PRMs), which receive feedback at each step in CoT. PRMs are considered to be more effective (Lightman et al., 2023). However, PRMs face significant challenges such as the need for extensive manually annotated data (Luo et al., 2024a; Havrilla et al., 2024), and the inefficiency in guiding LLMs to generate answers (Feng et al., 2023; Ding et al., 2023). To address these issues, we propose the Pairwise Preference Reward Model (PPRM), which uses the following instructions and the learning ability of LLMs in context. Our approach effectively improves the efficiency and accuracy of answer search by directly comparing the quality of two answers and globally ranking all generated answers. The whole process saves the cost of collecting much human-annotated data.

#### 4.2 TREE SEARCH REASONING

Sampling diverse reasoning paths (Brown et al., 2024) can significantly enhance the probability of finding the correct answers. Self-Consistency (Wang et al., 2022) sample a complete path each time while tree search methods like Tree-of-Thought (ToT) (Yao et al., 2023) and MCTS (Chen et al., 2024a;b; Luo et al., 2024b; Feng et al., 2023; Xie et al., 2024; Xu, 2023; Liu et al., 2023; Tian et al., 2024; Ding et al., 2023) extend numerous steps to optimize step answers and ultimately obtain the optimal solution. Additionally, Self-refine (Madaan et al., 2023b) method has become a recent focus. Self-verification (Gero et al., 2023; Weng et al., 2022) and rStar (Qi et al., 2024) utilize the inherent capabilities of the model to iteratively explore and refine answers. However, the performance of self-refine is typically constrained by the inherent capabilities of the model, especially for small language models (SLMs) with significantly weaker self-refine abilities (Madaan et al., 2023a). Our approach explores the answers by combining MCTS with self-refine. Ultimately, we construct a global win-loss matrix of answers following a directed graph process.

# 5 CONCLUSION

The research aims to address the challenges in complex mathematical reasoning, especially at the Olympiad level, where generating accurate and efficient reasoning paths for problem-solving. By combining iterative optimization methods Self-Refine applied to Monte Carlo Tree Search (SR-MCTS), the LLaMA-Berry framework improves the efficiency of solution generation. The Pairwise Preference Reward Model (PPRM) further enhances performance by modeling preferences between solutions rather than just scoring outcomes. Experimental results demonstrate that LLaMA-Berry outperforms baseline approaches on benchmarks like GSM8K and MATH, and demonstrates a competitive level with GPT-4 Turbo on difficult benchmarks without additional training.

In practice, the LLaMA-Berry framework still faces several limitations. The potential high computational cost of Monte Carlo Tree Search (MCTS) and Self-Refine methods may limit their practicality in resource-constrained environments. Additionally, the framework's assessment has been still narrow, focusing primarily on mathematical reasoning benchmarks, and its effectiveness on larger parameter or close-source models remains unexplored, warranting future experiments to assess its scalability and broader applicability.

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Table 5: Hyper-parameter settings

Hyper-parameter	Description	Value
$\alpha$	Balance coefficient between local and global	0.9
$\overline{}$	Exploration coefficient in UCT function	1.4
$\gamma$	Discount factor for backpropagation	0.1
$max\_child$	Dynamic pruning hyper-parameter in search	2

#### A HYPER-PARAMERER SETTINGS

All hyper-parameter settings for Section 3 are listed in Table 5.

# B DETAILS OF GRADING AND METRICS

**Grading:** We follow the correctness evaluation method proposed in PRM800K (Lightman et al., 2023) to score the answers generated by the algorithm. For the mathematical solutions proposed by the algorithm and their corresponding ground truth, we inform the model of the expected response format in a prompt. The answer's formula or value is extracted by matching the response format with predefined rules. If the model fails to follow the expected format in the prompt and the rule-based extraction fails, the answer is directly judged as inconsistent.

For the extracted label, we score the answer based on the following criteria. The answer is considered consistent with the ground truth label and passes the evaluation if at least one of the criteria is met:

- 1. The answer label string is exactly equal to the ground truth label string in terms of literal value.
- 2. Both the answer label and the ground truth label can be converted to floating-point numbers, and the difference between the two values is less than  $1 \times 10^{-6}$ .
- 3. Following the criterion proposed in PRM800K. (Lightman et al., 2023), we use the Sympy library to simplify the difference between the expression corresponding to the answer label, denoted as a, and the expression corresponding to the ground truth label, denoted as b. If the simplification yields  $a b \iff 0$ , the criterion is satisfied.

**Metrics:** To provide a comprehensive and robust evaluation metric, we adopt **major@k** and **pass@k** based on reward-ranked sorting (denoted as **rm@k**) as the evaluation metrics.

• pass@k represents the fraction of tasks that pass evaluation for at least one of the top k samples generated. This is calculated using the unbiased estimator:

$$\operatorname{pass@k} := \mathbb{E}_{\operatorname{Problems}} \left[ 1 - \frac{\binom{n-c}{k}}{\binom{n}{k}} \right]$$

where  $n \geq k$  is the number of samples generated per task,  $c \leq n$  is the number of correct samples that pass the unit tests, and  $\binom{n}{k}$  represents the binomial coefficient. The reward-ranked metric,  $\mathbf{rm}@\mathbf{k}$ , follows the same definition but sorts the samples by their reward values before evaluation.

• major@k is defined as the fraction of tasks where a majority of the top k samples generated return the same correct solution. This metric focuses on consistency across multiple generated answers. Majority weight is calculated on answer's extracted labels.

For results without a subscript, the score represents the greedy evaluation using the default prompt of the base model. Result with a notation indicate the use of the corresponding prompt engineering technique, and those marked with **self-consistency** use the self-consistency aggregation method.

For closed-source models, we report the scores from existing official technical reports (Anthropic, 2024; Reid et al., 2024; OpenAI, 2024) or dataset-provided results, with no modifications.

# C DETAILS OF PPRM TRAINGING

#### C.1 OVERVIEW

The design goal of the PPRM is to integrate the properties of both PRM and ORM, providing a more nuanced ordinal response between any two solution answers. We attempt to utilize reinforcement learning methods for training, leveraging the model's instruction-following capability to predict the relative merits of pairs of problem-solving answers. This will further enable the use of the EBC method to evaluate the global quantile scores of mathematical solutions.

#### C.2 DATA COLLECTION

Our data synthesis is derived from two datasets: PRM800K and OpenMathInstruct-1. The PRM800K dataset, collected from the MATH dataset, comprises a substantial number of step-divided problem-solving answers, with manual quality annotations for each step. We primarily utilize this dataset to generate pairs of answers for comparative analysis based on step-wise process quality. The OpenMathInstruct-1 dataset incorporates data from the GSM8K and MATH datasets, which have been manually annotated for outcome correctness. We use this dataset to synthesize pairs for comparative analysis based on outcome quality.

In processing PRM800K, for a given problem, we first sample steps of varying quality annotations from the step-wise dataset to construct a complete reasoning path. For pairs with the same final step annotation, paths composed of higher-quality steps are considered superior to those with lower-quality steps. In cases where the final step annotations are identical, the reasoning path with the superior final step annotation is regarded as better.

During the processing of OpenMathInstruct-1, we exclusively utilize samples without Python interpreter calls. For the same problem, we sample pairs composed of outcomes with higher and lower quality annotations.

Notably, we filtered out any data samples from PRM800K and OpenMathInstruct-1 that may overlap with the GSM8K and MATH test sets. Ultimately, we formed a dataset of 7,780,951 entries for training the PPRM model.

#### C.3 DIRECT PREFERENCE PAIR CONSTRUCTION

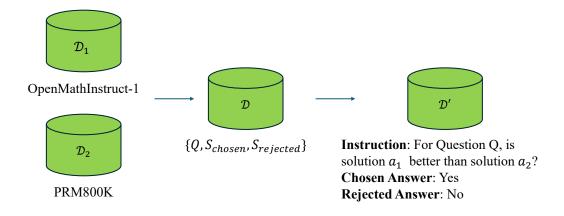


Figure 7: Dataset Construction of PPRM

For all pairs, we frame the inquiry as "For Question Q, is solution  $a_1$  better than solution  $a_2$ ?" If solution  $a_1$  is deemed superior to solution  $a_2$ , we label it as 'Yes'; otherwise, it is labeled as 'No'.

In this manner, we transform the ordinal relationship prediction task into a question-answer format, employing the Direct Preference Optimization (DPO) method for model training through reinforce-

ment learning from human feedback (RLHF). This approach aims to enhance the model's capability to follow instructions in predicting the relative merits of pairs of problem-solving answers.

#### C.4 RLHF TRAINING

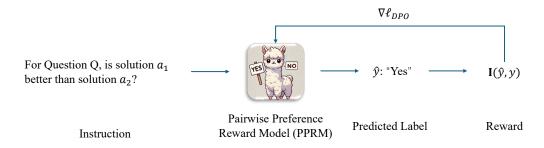


Figure 8: RLHF Training of PPRM

We subsequently apply the DPO method to train the Gemma2-2B-it model using RLHF. The loss function for DPO is structured as follows:

$$\mathcal{L}_{\text{DPO}}(\pi_{\theta}; \pi_{\text{ref}}) = -\mathbb{E}_{(x, y_w, y_l) \sim \mathcal{D}} \left[ \log \sigma \left( \beta \log \frac{\pi_{\theta}(y_w \mid x)}{\pi_{\text{ref}}(y_w \mid x)} - \beta \log \frac{\pi_{\theta}(y_l \mid x)}{\pi_{\text{ref}}(y_l \mid x)} \right) \right]$$
(10)

where  $\sigma$  is the logistic function,  $\beta$  is a parameter controlling the deviation from the base reference policy  $\pi_{ref}$ , namely the initial model  $\pi^{LLM}$ . In practice, the language model policy  $\pi_{\theta}$  is also initialized to  $\pi^{LLM}$ . For one answer, denoted as  $y_w \succ y_l | x$  where  $y_w$  and  $y_l$  denotes the preferred and dispreferred completion amongst (y1, y2) respectively.

#### D DETAILS OF BERRY-TREE INFERENCE FRAMEWORK

# D.1 OVERVIEW

Berry-Tree is an inference framework specifically designed for complex multi-model reasoning tasks, addressing the need to improve inference efficiency and accuracy in intricate tree search processes. This framework is particularly suited for large-scale reasoning tasks that involve the integration of multiple models and algorithms. By incorporating advanced tree search methods, robust concurrency handling, and lightweight inference engines, Berry-Tree significantly enhances inference speed and resource utilization. This report provides a detailed explanation of the system architecture and key technologies of Berry-Tree, along with preliminary performance evaluation results.

# D.2 SYSTEM ARCHITECTURE OVERVIEW

Figure 9 demonstrates the architecture of Berry-Tree which is divided into several layers, each handling different functional requirements. The **Data Management Layer** is responsible for the serialization and deserialization of data, ensuring efficient data read/write operations across models and systems. The **Tree Search Methods Layer** incorporates MCTS (Monte Carlo Tree Search), ToT (Tree of Thoughts), and A\* algorithms to optimize the inference process and explore multiple reasoning paths. Additionally, Berry-Tree includes a **Reliability Layer**, which ensures load balancing and failover support in highly concurrent scenarios, guaranteeing the stability of inference tasks. Finally, the **Inference Engines Layer** integrates efficient inference engines such as vLLM, FastAPI, and HuggingFace TGI to enable parallelized and efficient task processing.

#### D.3 KEY TECHNICAL COMPONENTS

**Data Management:** Berry-Tree employs serialization and describilization techniques, specifically using formats like JSON and CSV, to efficiently store and transfer checkpoint data from tree

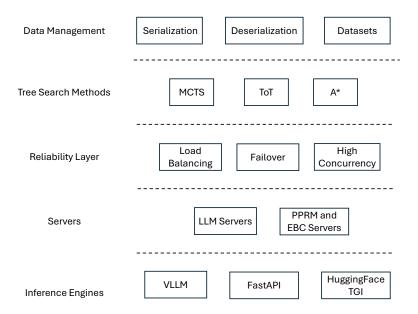


Figure 9: Architecture Design of Berry-Tree

search reasoning processes. The framework stores this data along with hash values to ensure integrity and allows for quick restoration of tree search states in memory when needed. Furthermore, Berry-Tree leverages the HuggingFace Datasets library to handle core data inputs for both training and inference. It supports seamless loading of datasets such as GSM8K and MATH from the HuggingFace Hub, enhancing its flexibility and ensuring compatibility with diverse reasoning tasks.

**Tree Search Methods:** Berry-Tree support multiple tree search algorithms, with MCTS being central to handling large-scale complex reasoning tasks by leveraging random simulation and statistical analysis to optimize the search space. The Tree of Thoughts (ToT) further extends the exploration depth and breadth of reasoning paths, helping the system manage uncertainty. A\* is applied in pathfinding tasks, offering efficient heuristic search capabilities.

**Reliability Design:** To ensure the stability and continuity of inference tasks, Berry-Tree incorporates load balancing and failover mechanisms. During high-concurrency operations, the load balancer distributes workloads across different servers, preventing server overload. The failover mechanism ensures that tasks can seamlessly transition to backup servers in case of partial server failures.

**Server Architecture:** The framework's server architecture is divided into two segments: one dedicated to executing Large Language Model (LLM) inference and the other designated explicitly for handling PPRM (Pairwise Preference Reward Model) and EBC (Enhanced Borda Count) processes. This modular design allows the framework to allocate computational resources flexibly, improving overall efficiency.

**Inference Engines:** Inference engines of Berry-Tree include VLLM (a lightweight language model inference engine), FastAPI (a high-performance web framework), and HuggingFace TGI (Text Generation Inference engine). These engines collectively enable the system to maintain high efficiency and stability while handling multi-model inference tasks, with robust support for high-concurrency demands.

#### D.4 Preliminary Performance Evaluation

In a preliminary performance evaluation, we utilize **16 A100 GPUs** to run the LLaMA3.1-8B-instruct model for large-scale inference tasks, while **4 A100 GPUs** are used to run the Gemma2-2B-it model as PPRM servers. The test dataset consists of **1319 GSM8K test samples**.

We conduct **16 MCTS rollouts** to parallelize the inference tasks via Berry-Tree. The results indicate that the total inference time is **1 hour and 25 minutes**, with an average inference time of approximately **3.87 seconds per sample**. These results demonstrate strong parallel inference capabilities of Berry-Tree under the given hardware configuration.

This preliminary performance evaluation highlights the efficiency of Berry-Tree, particularly in handling complex reasoning tasks. Although these results are based on initial experiments, future evaluations with varying hardware configurations and more complex task scenarios could provide deeper insights into the system's performance.

#### D.5 SYSTEM SCALABILITY AND OPTIMIZATION

The modular design of Berry-Tree allows for future scalability and optimization. For instance, the system can be flexibly integrated with additional inference engines, support alternative tree search methods, or accommodate more diverse language models. This flexibility makes it adaptable to various applications, such as natural language reasoning, mathematical problem-solving, and pathfinding tasks. Future optimization directions will include enhancing inference speed, improving concurrency handling, and strengthening fault-tolerance and load management mechanisms to ensure stability and reliability in large-scale deployment scenarios.

# E CONVERGENCE ANALYSIS OF THE ENHANCED BORDA COUNT (EBC) METHOD

In this appendix section, we provide a rigorous mathematical proof that the quantile scores evaluated by the Enhanced Borda Count (EBC) method converge to the true quantile scores of solutions in the actual quality distribution as the number of samples increases.

#### E.1 DEFINITIONS AND ASSUMPTIONS

**Solution Set**: Let  $A = \{a_1, a_2, \dots, a_n\}$  be a finite set of n solutions (answers).

**True Quality Scores**: Each solution  $a_i$  has a true quality score  $Q^*(a_i) \in \mathbb{R}$ , drawn from a continuous distribution  $P_Q$ .

**True Ranking**: The true ranking  $R^*$  is induced by ordering the solutions in decreasing order of their true quality scores  $Q^*(a_i)$ .

**True Pairwise Preference Probabilities**: The true probability that solution  $a_i$  is preferred over  $a_j$  is defined as:

$$P^*(a_i \succ a_j) = \mathbb{P}(Q^*(a_i) > Q^*(a_j)) + \frac{1}{2}\mathbb{P}(Q^*(a_i) = Q^*(a_j)). \tag{11}$$

Given the continuity of  $P_Q$ , we have  $\mathbb{P}(Q^*(a_i) = Q^*(a_j)) = 0$ , so:

$$P^*(a_i \succ a_j) = \begin{cases} 1, & \text{if } Q^*(a_i) > Q^*(a_j), \\ 0, & \text{if } Q^*(a_i) < Q^*(a_j). \end{cases}$$
 (12)

**Estimated Preference Probabilities**: For T independent samples, the estimated preference probability is:

$$P_T(a_i \succ a_j) = \frac{1}{T} \sum_{t=1}^T X_t^{(i,j)}, \tag{13}$$

where  $X_t^{(i,j)}$  are independent Bernoulli random variables with success probability  $P^*(a_i \succ a_j)$ .

**Convergence Assumption:** As  $T \to \infty$ ,  $P_T(a_i \succ a_j)$  converges almost surely to  $P^*(a_i \succ a_j)$ .

**Preference Matrix**: Construct the estimated preference matrix  $M_T$  and the true preference matrix  $M^*$  as:

$$M_T[i,j] = \begin{cases} 1, & \text{if } P_T(a_i \succ a_j) \ge 0.5, \\ 0, & \text{otherwise.} \end{cases} \qquad M^*[i,j] = \begin{cases} 1, & \text{if } P^*(a_i \succ a_j) = 1, \\ 0, & \text{if } P^*(a_i \succ a_j) = 0. \end{cases}$$
(14)

**Transitive Closure**: Let  $C_T$  and  $C^*$  be the transitive closures of  $M_T$  and  $M^*$ , respectively.

**Borda Counts**: Compute the Borda count for each solution:

$$B_T(a_i) = \sum_{j \neq i} C_T[i, j], \quad B^*(a_i) = \sum_{j \neq i} C^*[i, j].$$
 (15)

#### **Estimated Ranking and Quantile Scores:**

- Estimated ranking  $R_T$ : Order solutions by decreasing  $B_T(a_i)$ .
- Estimated quantile score:

$$Q_g(a_i) = 1 - \frac{\text{rank}_T(a_i) - 1}{n - 1}.$$
(16)

• True quantile score:

$$Q_g^*(a_i) = 1 - \frac{\operatorname{rank}^*(a_i) - 1}{n - 1}.$$
(17)

### E.2 OBJECTIVE

To prove that as  $T \to \infty$ , the estimated quantile scores  $Q_g(a_i)$  converge almost surely to the true quantile scores  $Q_q^*(a_i)$ :

$$\lim_{T \to \infty} Q_g(a_i) = Q_g^*(a_i), \quad \forall a_i \in A.$$
 (18)

#### E.3 PROOF

#### **Step 1: Convergence of Estimated Preference Probabilities**

By the Strong Law of Large Numbers (SLLN), since  $X_t^{(i,j)}$  are i.i.d. Bernoulli random variables with success probability  $P^*(a_i \succ a_j)$ , we have:

$$\lim_{T \to \infty} P_T(a_i \succ a_j) = P^*(a_i \succ a_j) \quad \text{almost surely.}$$
 (19)

# **Step 2: Convergence of Preference Matrix** $M_T$ **to** $M^*$

Since  $P_T(a_i \succ a_j)$  converges to  $P^*(a_i \succ a_j)$  and  $P^*(a_i \succ a_j) \in \{0, 1\}$ , for sufficiently large T, we have:

$$M_T[i,j] = M^*[i,j], \quad \forall i \neq j, \tag{20}$$

almost surely.

Justification: Because  $P_T(a_i \succ a_j)$  converges to either 0 or 1, and  $P_T(a_i \succ a_j) \neq 0.5$  almost surely for large T.

# Step 3: Convergence of Transitive Closure $C_T$ to $C^*$

The transitive closure is a deterministic function of the preference matrix. Therefore, since  $M_T \to M^*$ , it follows that:

$$C_T \to C^*$$
 as  $T \to \infty$ , (21)

almost surely.

# **Step 4: Convergence of Borda Counts** $B_T(a_i)$ **to** $B^*(a_i)$

Given that  $C_T \to C^*$ , the Borda counts converge:

$$B_T(a_i) = \sum_{j \neq i} C_T[i, j] \to B^*(a_i) = \sum_{j \neq i} C^*[i, j], \tag{22}$$

almost surely.

#### Step 5: Convergence of Estimated Ranking $R_T$ to True Ranking $R^*$

Since the Borda counts  $B_T(a_i)$  converge to  $B^*(a_i)$ , and assuming that all  $Q^*(a_i)$  are distinct (due to the continuity of  $P_O$ ), the rankings induced by  $B_T(a_i)$  converge to the true rankings:

$$R_T \to R^* \quad \text{as } T \to \infty,$$
 (23)

almost surely.

# **Step 6: Convergence of Quantile Scores** $Q_g(a_i)$ **to** $Q_g^*(a_i)$

Since  $\operatorname{rank}_T(a_i) \to \operatorname{rank}^*(a_i)$ , we have:

$$Q_g(a_i) = 1 - \frac{\operatorname{rank}_T(a_i) - 1}{n - 1} \to Q_g^*(a_i) = 1 - \frac{\operatorname{rank}^*(a_i) - 1}{n - 1},\tag{24}$$

almost surely.

#### Conclusion

Therefore, we have shown that:

$$\lim_{T \to \infty} Q_g(a_i) = Q_g^*(a_i), \quad \forall a_i \in A, \tag{25}$$

which means that the EBC method's estimated quantile scores converge almost surely to the true quantile scores of the solutions.

#### E.4 FINITE SAMPLE ANALYSIS AND CONVERGENCE RATE

## Lemma 1: Hoeffding's Inequality for Preference Probability Estimates

For each pair  $(a_i, a_j)$ ,  $P_T(a_i \succ a_j)$  is the sample mean of T i.i.d. Bernoulli trials with success probability  $P^*(a_i \succ a_j)$ . By Hoeffding's inequality:

$$\mathbb{P}\left(|P_T(a_i \succ a_j) - P^*(a_i \succ a_j)| \ge \epsilon\right) \le 2\exp(-2T\epsilon^2). \tag{26}$$

# Lemma 2: Uniform Convergence over All Pairs

Apply the union bound over all N = n(n-1)/2 pairs:

$$\mathbb{P}\left(\exists (i,j) : |P_T(a_i \succ a_j) - P^*(a_i \succ a_j)| \ge \epsilon\right) \le N \cdot 2\exp(-2T\epsilon^2). \tag{27}$$

Set the right-hand side equal to  $\delta$  to solve for T:

$$T \ge \frac{1}{2\epsilon^2} \ln \left( \frac{2N}{\delta} \right). \tag{28}$$

# Lemma 3: Correctness of Preference Matrix with High Probability

Given that  $P^*(a_i \succ a_i) \in \{0, 1\}$ , for any  $0 < \epsilon < 0.5$ , if:

$$|P_T(a_i \succ a_j) - P^*(a_i \succ a_j)| < \epsilon, \tag{29}$$

then  $M_T[i,j] = M^*[i,j]$  because  $P_T(a_i \succ a_j)$  will be greater than 0.5 when  $P^*(a_i \succ a_j) = 1$ , and less than 0.5 when  $P^*(a_i \succ a_j) = 0$ .

# Lemma 4: Probability of Correct Ranking

From Lemma 2 and 3, with probability at least  $1 - \delta$ ,  $M_T = M^*$ , and thus  $C_T = C^*$ , leading to  $R_T = R^*$  and  $Q_g(a_i) = Q_g^*(a_i)$ .

#### **Convergence Rate Analysis**

To achieve this with confidence level  $1 - \delta$ , the required number of samples per pair is:

$$T \ge \frac{1}{2\epsilon^2} \ln \left( \frac{n(n-1)}{\delta} \right). \tag{30}$$

For small  $\delta$  and  $\epsilon$  < 0.5, T scales logarithmically with the number of solutions n.

#### E.5 ADDRESSING PRACTICAL CONSIDERATIONS

In practice, the true preference probabilities may not be exactly 0 or 1 due to noise or overlapping quality scores. To accommodate this:

• Extended Preference Model: Assume  $P^*(a_i \succ a_j)$  is a strictly increasing function of  $\Delta Q_{ij}^* = Q^*(a_i) - Q^*(a_j)$ , such as:

$$P^*(a_i \succ a_j) = F(\Delta Q_{ij}^*), \tag{31}$$

where F is a cumulative distribution function (CDF).

• Margin Condition: Define a margin m > 0 such that for all  $i \neq j$ :

$$|P^*(a_i \succ a_i) - 0.5| \ge m. \tag{32}$$

This ensures a minimum separation between preference probabilities.

Modified Sample Complexity: With the margin condition, Hoeffding's inequality becomes:

$$\mathbb{P}(M_T[i,j] \neq M^*[i,j]) \le 2\exp(-2Tm^2). \tag{33}$$

To achieve  $\mathbb{P}\left(M_T=M^*\right)\geq 1-\delta$ , we need:

$$T \ge \frac{1}{2m^2} \ln \left( \frac{n(n-1)}{\delta} \right). \tag{34}$$

• Convergence under Noise: Even with noisy preference probabilities, as long as there is a margin m > 0, the convergence of  $Q_g(a_i)$  to  $Q_g^*(a_i)$  still holds with high probability for sufficiently large T.

#### E.6 FINAL CONCLUSION

We have provided a rigorous proof that the EBC method's estimated quantile scores  $Q_g(a_i)$  converge almost surely to the true quantile scores  $Q_g^*(a_i)$  as the number of samples T approaches infinity. The finite sample analysis demonstrates that the convergence rate depends logarithmically on the number of solutions and inversely on the square of the margin m between preference probabilities.

# F PSEUDO-CODE OF MAIN ALGORITHMS

#### G CASE STUDY

Algorithm 1: Ehanced Borda Count (EBC) Method: Process for computing transitive closure using Floyd-Warshall algorithm and reranking entities based on quantile rewards

```
Data: M (Binary Reward Matrix), P (Pairwised Preference Reward model)
   Result: Q (quantile rewards), R (ranked node list), L (ranked layers of nodes)
 1 Function FillTransitiveClosure (M):
       C \leftarrow \text{all-zero matrix from size of } M
       C[i,j] \leftarrow -1 \text{ for all } i,j
       C[i,j] \leftarrow \operatorname{sign}(M[i,j]-0.5) if M[i,j] \neq -1 else -1
       for k = 0 to |C| - 1 do
5
           for i = 0 to |C| - 1 do
                for j = 0 to |C| - 1 do
                    if C[i,k] = C[k,j] then
 8
                     C[i,j] \leftarrow C[i,k]
                     end
10
                end
11
           end
12
       end
13
       return Updated C
14
15 Function BordaCount (C):
       D \leftarrow outdegree of each node from C
16
       R \leftarrow \operatorname{argsort}(-D)
17
       L \leftarrow Define layers using unique values in D
18
       return R , L
20 Function Rerank (R, L, C, P):
       G \leftarrow \operatorname{Group} R \text{ by } L
21
       R \leftarrow Sort each group in G using local comparisons computed by P
22
       L, C \leftarrow \text{Update } L, C \text{ by } R
       return R, L, Updated C
25 Function CalculateQuantileScores (R, L):
       Q \leftarrow \emptyset
26
       S_L \leftarrow \{1 - \frac{l}{\max(L)} : l \in L\}
27
       Q[x] \leftarrow S_L[\text{layer of } x] \text{ for each } x \in R
28
       return Q
30 Function EnhancedBordaCount (M, q):
       C \leftarrow \texttt{FillTransitiveClosure}(M)
       R, L \leftarrow BordaCount(C)
32
       R, L, C \leftarrow \operatorname{Rerank}(R, L, C, P)
33
       Q \leftarrow \texttt{CalculateQuantileScores}(R, L)
34
       return Q, R, L
35
```

# Algorithm 2: Self-Refine applied to Monte Carlo Tree Search (SR-MCTS) Method **Input:** Initial state $s_0$ , search tree $\mathcal{T}$ , max nodes $N_{max}$ , exploration constant c**Output:** Ranked solution list S1 Initialize search tree $\mathcal{T}$ with root node $s_0$ ; 2 while number of nodes $N(\mathcal{T}) < N_{max}$ do /∗ Selection Phase \*/ Select a node $s_i$ which met the dynamic pruning rule from T using UCT: 3 $a = \arg\max_{a \in A(s)} \left( Q(s,a) + c \cdot \sqrt{\frac{\ln N(s)}{N(s,a)}} \right)$ /\* Expansion Phase Expand $s_i$ by generating a successor node s' using the rewriting process $R(s_i, c_i)$ , where $c_i = C(s_i)$ is a critique of the current state; Add the new node s' to $\mathcal{T}$ ; /\* Evaluation Phase Compute the value Q(s') of the new node with Enhanced Borda Count (EBC) method: $Q(s') = \alpha Q_q(s') + (1 - \alpha)Q_l(s')$ where $Q_g(s')$ is the global value from the win-loss matrix M and $Q_l(s')$ is the local value from adjacent nodes in $\mathcal{T}$ ; /\* Backpropagation Phase \*/ 7 Propagate Q(s') back to its parent node $s_i$ , updating $s_i$ 's Q value: $Q(s_i) = (1 - \gamma)Q(s_i) + \gamma Q(s')$ /\* Check for tree growth limit \*/ if $N(\mathcal{T}) \geq N_{max}$ then break; end 10 11 end

12 return Ranked solution list S

Table 6: Prompts Overview

Component	Details		
Generate the first solution	Please wrie a answer for this question. The Answer should format as '#### Reasoning Process #### Verification #### Final Answer'. The Final Answer should format as \boxed{Final Answer}		
Generate Critique	Let's think step by step.  Analyze this weak Answer, write a strict Critic/Reflection for error re-correct and Hints/Guidelines for maximum improvement.  Let's think step by step.		
Rewriting	Please write a better answer for this question refer to the comments. The Answer should format as '#### Reasoning Process #### Verification #### Final Answer'. The Final Answer should format as \boxed{Final Answer} Let's think step by step.		
Instruction of PPRM	Problem: First Answer: Second Answer: Is First Answer better than Second Answer?		

Table	7.	Problem	Solving	Overview
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Component	Details
Problem Statement	Lee used to be able to run the 400-meter hurdles two seconds faster than Gerald would run the 400-meter hurdles. But Gerald changed his diet, which improved his speed by 10%. If Lee runs the 400-meter hurdles in 38 seconds, how fast can Gerald, with his improved diet, run the 400-meter hurdles, in seconds?
First Attempt	Reasoning Process:  1. Gerald's original time: 40 seconds (Lee's time + 2 seconds).  2. Calculate improvement: 10% of 40 seconds = 4 seconds.  3. New time: 40 + 4 = 44 seconds.
	Verification: Calculated time based on Lee's current time and original difference. Final Answer: 44 seconds.
Critique of First Attempt	Reflection:  1. Lack of clear explanation.  2. Inaccurate percentage increase representation.  3. Incorrect verification.  4. Insufficient mathematical notation.
	Error Re-correction:  1. Gerald's original time: $40$ seconds.  2. New time: $40 - 4 = 36$ seconds.
Improved Answer	Reasoning Process:  1. Lee runs in 38 seconds. 2. Gerald's original time: 40 seconds. 3. Improvement: 4 seconds. 4. New time: 36 seconds.
	Final Answer: 36 seconds.