# CPL: CRITICAL PLANNING STEP LEARNING BOOSTS LLM GENERALIZATION IN REASONING TASKS

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#### Abstract

Post-training large language models (LLMs) to develop reasoning capabilities has proven effective across diverse domains, such as mathematical reasoning and code generation. However, existing methods primarily focus on improving task-specific reasoning, but have not adequately addressed the model's generalization capabilities across a broader range of reasoning tasks. To tackle this challenge, we introduce Critical Planning Step Learning (CPL), which leverages Monte Carlo Tree Search (MCTS) to explore diverse planning steps in multi-step reasoning tasks. Based on long-term outcomes, CPL learns step-level planning preferences to improve the model's planning capabilities and, consequently, its general reasoning capabilities. Furthermore, while effective in many scenarios for aligning LLMs, existing preference learning approaches like Direct Preference Optimization (DPO) struggle with complex multi-step reasoning tasks due to their inability to capture fine-grained supervision at each step. We propose Step-level Advantage Preference Optimization (Step-APO), which integrates an advantage estimate for step-level preference pairs obtained via MCTS into the DPO. This enables the model to more effectively learn critical intermediate planning steps, thereby further improving its generalization in reasoning tasks. Experimental results demonstrate that our method, trained exclusively on GSM8K and MATH, not only significantly improves performance on GSM8K (+10.5%) and MATH (+6.5%), but also enhances out-of-domain reasoning benchmarks, such as ARC-C (+4.0%), BBH (+1.8%), MMLU-STEM (+2.2%), and MMLU (+0.9%).

## 1 Introduction

Recent studies focus on enhancing the reasoning capabilities of large language models (LLMs) through various approaches, including collecting high-quality and domain-specific data (Gunasekar et al., 2023; Shao et al., 2024; Dubey et al., 2024), designing elaborate prompting techniques (Wei et al., 2023; Yao et al., 2023a;b), and developing advanced optimization algorithms (Ouyang et al., 2022; Rafailov et al., 2023; Ethayarajh et al., 2024; Yuan et al., 2023). Among these approaches, training on model-generated synthetic data is a promising method. Specifically, recent work (Feng et al., 2023; Chen et al., 2024; Xie et al., 2024) leverages Monte Carlo Tree Search (MCTS) (Kocsis & Szepesvári, 2006) to iteratively collect reasoning paths to boost LLM's reasoning capabilities.

MCTS strikes a balance between exploration and exploitation, utilizing its look-ahead ability to obtain high-quality step-level supervision. However, a primary challenge with MCTS for LLMs is the high inference latency and the vast search space, which limits the diversity of explored reasoning paths. Additionally, existing methods primarily focus on enhancing task-specific or domain-specific reasoning capabilities, such as for math or code. This has led to significant improvements in specific tasks but has not adequately addressed the model's

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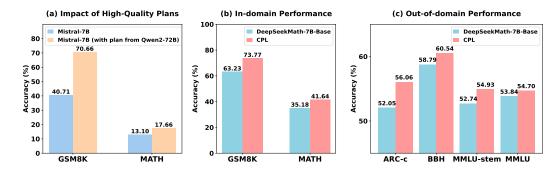


Figure 1: Impact of High-Quality Plans. (a): Mistral 7B benefits significantly from a well-crafted plan provided by Qwen2-72B. Comparison between the DeepSeekMath-7B-Base model and our CPL-trained model. (b) Our CPL method significantly outperforms the baselines in in-domain tasks. (c) CPL also demonstrates substantial improvements in out-of-domain reasoning tasks, proving its ability to generalize across a wider range of reasoning tasks.

generalization abilities across various reasoning tasks. For instance, AlphaMath (Chen et al., 2024) greatly boosts mathematical tasks, its performance on other reasoning tasks, such as BBH (Suzgun et al., 2022) and ARC-C (Clark et al., 2018), did not show significant improvement.

To improve transfer performance on a broader range of reasoning tasks. We propose that effectively learning planning strategies to solve complex problems is crucial for improving LLM's reasoning capabilities and generalization. Approaches (Hao et al., 2023; Yao et al., 2023b) explore using LLMs to generate both reasoning traces and task-specific actions in an interleaved manner to boost reasoning capabilities. We suggest that task-specific actions are the execution steps that follow a plan and are often more closely tied to task-specific skills, such as mathematical computation. In contrast, generating planning-based reasoning traces helps models develop more task-agnostic skills, leading to improved generalization. Our preliminary experiments show that a weaker model benefits significantly from a well-crafted plan provided by a more capable model (see Figure 1 (a)). This underscores that learning effective planning is crucial for handling complex reasoning tasks.

Thus, we introduce Critical Planning Step Learning (CPL) to efficiently explore diverse planning strategies via MCTS within the vast search space. This involves devising a step-by-step plan to solve the problem, with the final step providing the full solution based on the plan and the final answer. This approach generates a plan tree, where high-quality planning step preferences is obtained from the final result.

Preference learning approaches like Direct Preference Optimization (DPO) (Rafailov et al., 2023) has proven effective for aligning LLMs. However, it struggles on complex multi-step reasoning tasks, where the model often fails to identify erroneous steps and learn spurious correlations from the flawed steps, ultimately hindering model generalization (Hwang et al., 2024). Recent works propose Step-DPO (Setlur et al., 2024; Lai et al., 2024) to learn step-level preferences in complex reasoning tasks. A key challenge with Step-DPO lies in the vast search space of reasoning steps, where the selection of appropriate preference data for model optimization is crucial. Current approaches often rely on heuristic methods, with the most common strategy being to identify the first error step as dispreferred. However, we argue that this approach fails to fully explore the step-level search space, limiting the model's optimization potential. To overcome this, we propose Step-level Advantage Preference Optimization (Step-APO) to better leverage step preference data. By incorporating advantage estimates between chosen and rejected plans from MCTS, Step-APO enables the model to learn fine-grained preferences between plan steps, allowing it to identify critical plan steps and de-emphasize erroneous ones. This further improves the generalization of LLM in reasoning tasks.

We conduct extensive experiments on both in-domain and out-of-domain reasoning datasets. Our results demonstrate that CPL significantly enhances the model's overall reasoning performance. Specifically, when trained exclusively on GSM8K and MATH, the model

not only shows significant improvement in mathematical tasks including GSM8K(+10.5%) and MATH(+6.5%), but also achieves better performance on out-of-domain benchmarks, including ARC-C (+4.0%), BBH (+1.8%), MMLU-STEM (+2.2%), and MMLU (+0.9%).

To conclude, our work makes the following contributions: 1) We introduce CPL, which leverages MCTS to explore planning steps and learn step-level planning preferences, enhancing the model's general reasoning capabilities. 2) We introduce Step-APO to further enhance the learning of critical planning steps. 3) We achieve significant improvements in both in-domain and out-of-domain tasks.

# 2 Related Work

Search-Guided Reasoning in LLMs Recent advancements (Feng et al., 2023; Chen et al., 2024; Xie et al., 2024) in enhancing LLM reasoning capabilities have focused on integrating Monte Carlo Tree Search (MCTS) to collect trajectories and train models, resulting in notable advancements for reasoning tasks. For example, AlphaMath Chen et al. (2024) employs MCTS to automatically generate process supervision, leading to significant improvements in mathematical reasoning. However, these MCTS-based training methods encounter challenges such as vast search spaces, limited solution diversity for LLMs. Furthermore, there is limited research on how these methods generalize to other reasoning tasks and enhance overall reasoning capabilities. To address these issues, we propose a method for searching over plan steps and learning critical plan steps for problem-solving, which aims to enhance generalization across a range of reasoning tasks.

Direct Preference Optimization (DPO) Algorithms DPO (Rafailov et al., 2023) uses solution-level preference data for model optimization but has notable limitations. It struggles with multi-step reasoning tasks because it cannot effectively correct specific errors within the reasoning process (Hwang et al., 2024). Moreover, training on model-generated positive data can amplify spurious correlations from incorrect intermediate steps, leading to poor generalization (Setlur et al., 2024). Recent work proposes step-level DPO (Setlur et al., 2024; Lai et al., 2024) to address these issues by providing the fine-grained error identification needed for improving reasoning capabilities. For example, SELF-EXPLORE Hwang et al. (2024) identifies the first incorrect step in a solution and constructs step-level preference data to guide model improvement. Unlike these heuristic methods, we propose Step-APO to fully explore the step-level search space and achieve the maximum optimization potential.

# 3 Methods

Our Critical Planning Step Learning (CPL) framework is illustrated in Figure 2. In this section, we first introduce our planning based MCTS, which enables the LLM to learn critical planning steps. Next, we present our Step-APO in detail to further explore the potential of step-level preference learning in multi-step reasoning task. Finally, we describe how we iteratively optimize the policy model and value model.

#### 3.1 Critical Planning Step Learning with MCTS

MCTS builds a reasoning tree iteratively and autonomously explores step-level reasoning traces, which can be used to optimize LLMs. Existing methods (Chen et al., 2024; Xie et al., 2024) that leverage MCTS to collect data for training usually focus on exploring solution steps within the entire search space or on simultaneously exploring both plans and solutions. To improve transfer performance across a broader range of reasoning tasks, we propose learning effective and diverse planning, which enables the model to acquire more task-agnostic capabilities and thereby achieve better generalization. We first create a step-by-step plan to solve the problem, with the final step presenting the full solution and final answer based on the plan. The prompt is provided in the Appendix A.1. Ultimately, we obtain a plan tree and high-quality planning step supervision through iterative search simulations with MCTS (Figure 2).

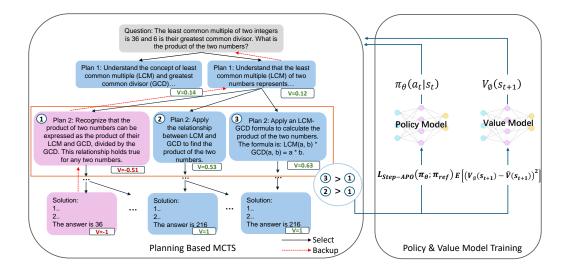


Figure 2: CPL boosts model performance via iterative process over planning based MCTS and step-level preference learning. Left: Example of an MCTS-generated plan tree, exploring diverse planning strategies in the vast search space. CPL generates step-by-step plans, which lead to the final solution and answer. State value V is updated via a bottom-up reward propagation from the terminal node to the root, and used to assign preferences. Right: Step-level preferences from MCTS are used to update the policy and value models. Our Step-APO integrates value estimates for preference pairs into DPO, assigning different optimization weights to emphasize critical steps. The value model is optimized using MSE loss.

Specifically, given the plan tree  $\mathcal{T}$ , each node represents a state  $\mathbf{s}_t$ , and each edge represents an action  $\mathbf{a}_t$ , which corresponds to a reasoning step that leads to the next state  $\mathbf{s}_{t+1}$ . Under the same parent node, different sibling nodes form a set of step-level preference pairs, with each node having its own value  $V(\mathbf{s}_t)$  representing the expected future reward under state  $\mathbf{s}_t$ . These values can be obtained through the MCTS process, which involves four key operations: selection, expansion, evaluation, and backup. To enhance efficiency, we use a value model to estimate rewards for intermediate steps, with the final integration of both policy and value models guiding the search process. Next, we describe the four steps of MCTS.

Selection: We use the PUCT algorithm to guide the selection process with the following formula, where N represents the visit count:

$$\arg \max_{\mathbf{a}_t} \left[ Q(\mathbf{s}_t, \mathbf{a}_t) + c_{\text{puct}} \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t) \frac{\sqrt{N(\mathbf{s}_t)}}{1 + N(\mathbf{s}_t, \mathbf{a}_t)} \right]. \tag{1}$$

**Expansion and Evaluation**: During expansion, we sample multiple possible candidate actions for the next step. During evaluation, the final answer in the terminal action is evaluated with the ground truth, otherwise, the value is predicted by the value model.

**Backup:** Once a terminal node is reached, we perform a bottom-up update from the terminal node back to the root. We update the visit count N, the state value V, and the transition value Q as follows:

$$Q(\mathbf{s}_t, \mathbf{a}_t) \leftarrow r(\mathbf{s}_t, \mathbf{a}_t) + V(\mathbf{s}_{t+1})$$
 (2)

$$V(\mathbf{s}_t) \leftarrow \sum_{a} N(\mathbf{s}_{t+1}) Q(\mathbf{s}_t, \mathbf{a}_t) / \sum_{a} N(\mathbf{s}_{t+1})$$

$$N(\mathbf{s}_t) \leftarrow N(\mathbf{s}_t) + 1.$$
(3)

$$N(\mathbf{s}_t) \leftarrow N(\mathbf{s}_t) + 1.$$
 (4)

# 3.2 Step-APO

Unlike mainstream approaches (Hwang et al., 2024; Lai et al., 2024) that learn step-level preferences by identifying the first error step and sampling a corresponding preferred step, while potentially yielding more accurate preferences, this method lacks sufficient exploration of the vast reasoning trace space. Given the large variations in advantage differences across different data pairs, we propose Step-APO, which introduces advantage estimates for preference pairs into DPO. This enables the model to more effectively learn critical intermediate planning steps, thereby further improving its reasoning capabilities. Next, We will provide its derivation and analysis from the perspective of its gradient.

#### 3.2.1 Preliminaries

The Classical RL Objective RLHF approaches (Ziegler et al., 2020; Bai et al., 2022; Ouyang et al., 2022) usually first learn a reward function from human feedback, then optimize it with a policy gradient-based method like PPO (Schulman et al., 2017) with an entropy-bonus using the following multi-step RL objective:

$$\max_{\pi_{\theta}} \mathbb{E}_{\mathbf{a}_{t} \sim \pi_{\theta}(\cdot|\mathbf{s}_{t})} \left[ \sum_{t=0}^{T} (r(\mathbf{s}_{t}, \mathbf{a}_{t}) + \underbrace{\beta \log \pi_{\text{ref}}(\mathbf{a}_{t}|\mathbf{s}_{t})}_{\text{KL penalty}}) + \beta \mathcal{H}(\pi_{\theta}) | \mathbf{s}_{0} \sim \rho(\mathbf{s}_{0}) \right], \tag{5}$$

where  $r(\mathbf{s}_t, \mathbf{a}_t)$  denotes the step-level reward function, followed by a KL penalty that aims to ensure the learned policy  $\pi_{\theta}$  does not deviate significantly from the reference policy  $\pi_{\text{ref}}$ .  $\pi_{\text{ref}}$  is typically produced via supervised fine-tuning.

**Direct Preference Optimization** DPO (Rafailov et al., 2023) uses the well-known closed-form optimal solution, which establishes a mapping between the reward model and the optimal policy under the KL divergence, obtaining the reward as:

$$r(\mathbf{x}, \mathbf{y}) = \beta \log \pi^*(\mathbf{y}|\mathbf{x}) - \beta \log \pi_{\text{ref}}(\mathbf{y}|\mathbf{x}) - Z(\mathbf{x}), \tag{6}$$

where  $\mathbf{x}$  denotes the prompt and y denotes the response,  $\pi^*$  is the optimal policy and  $Z(\mathbf{x})$  is the partition function that normalizes it. Substituting eq. (6) into the Bradley Terry preference model, and leverage the maximum likelihood objective, DPO derives the loss:

$$\mathcal{L}_{\text{DPO}}(\pi_{\theta}; \pi_{\text{ref}}) = -\mathbb{E}_{(\mathbf{x}, \mathbf{y}^w, \mathbf{y}^l) \sim \mathcal{D}} \left[ \log \sigma \left( \beta \log \frac{\pi_{\theta}(\mathbf{y}^w \mid \mathbf{x})}{\pi_{\text{ref}}(\mathbf{y}^w \mid \mathbf{x})} - \beta \log \frac{\pi_{\theta}(\mathbf{y}^l \mid \mathbf{x})}{\pi_{\text{ref}}(\mathbf{y}^l \mid \mathbf{x})} \right) \right], \quad (7)$$

where  $\sigma$  denotes the logistic function,  $\mathbf{y}^w$  and  $\mathbf{y}^l$  denote the preferred and dis-preferred responses to the prompt  $\mathbf{x}$ .

#### 3.2.2 Deriving the Step-APO Objective

In the general maximum entropy RL setting (Ziebart, 2010), the optimal policy  $\pi^*(\mathbf{a}|\mathbf{s})$  of multi-step RL objective in eq. (5) is:

$$\pi^*(\mathbf{a}_t|\mathbf{s}_t) = e^{(Q^*(\mathbf{s}_t,\mathbf{a}_t) - V^*(\mathbf{s}_t))/\beta},\tag{8}$$

where  $Q^*(\mathbf{s}, \mathbf{a})$  is the optimal Q-function which models the total future reward from  $(\mathbf{s}_t, \mathbf{a}_t)$  under  $\pi^*$ . The optimal value function  $V^*$  estimates the total future reward under state  $\mathbf{s}_t$ , and it's a function of  $Q^*$  (Rafailov et al., 2024).

Under the reward r with a KL divergence penalty, the relationship between Q-function and step-level reward function can be established with the Bellman equation as follows:

$$Q^*(\mathbf{s}_t, \mathbf{a}_t) = r(\mathbf{s}_t, \mathbf{a}_t) + \beta \log \pi_{\text{ref}}(\mathbf{a}_t | \mathbf{s}_t) + V^*(\mathbf{s}_{t+1}). \tag{9}$$

By log-linearizing the optimal policy in eq. (8) and substituting in the Bellman equation from eq. (9) (Nachum et al., 2017; Rafailov et al., 2024), we have below equation which is precisely the optimal advantage function  $A^*(\mathbf{s}, \mathbf{a}) = Q^*(\mathbf{s}, \mathbf{a}) - V^*(\mathbf{s})$ :

$$\beta \log \frac{\pi^*(\mathbf{a}_t|\mathbf{s}_t)}{\pi_{\text{ref}}(\mathbf{a}_t|\mathbf{s}_t)} = r(\mathbf{s}_t, \mathbf{a}_t) + V^*(\mathbf{s}_{t+1}) - V^*(\mathbf{s}_t). \tag{10}$$

Unlike DPO utilize response-level Bradley Terry model, we introduce step-level Bradley Terry preference model to learn fine-grained step-level preference:

$$p^*(\mathbf{a}^w \succeq \mathbf{a}^l | \mathbf{s}) = \frac{\exp(r(\mathbf{s}, \mathbf{a}^w))}{\exp(r(\mathbf{s}, \mathbf{a}^w)) + \exp(r(\mathbf{s}, \mathbf{a}^l))}.$$
 (11)

By substituting eq. (10) into eq. (11) and leveraging the negative log-likelihood loss, we derive the objective for step-APO:

$$\mathcal{L}_{\text{Step-APO}}(\pi_{\theta}; \pi_{\text{ref}}) = -\mathbb{E}_{(\mathbf{s}_{t}, \mathbf{a}_{t}^{w}, \mathbf{a}_{t}^{l}) \sim \mathcal{D}} \left[ \log \sigma \left( \beta \log \frac{\pi_{\theta}(\mathbf{a}_{t}^{w} \mid \mathbf{s}_{t})}{\pi_{\text{ref}}(\mathbf{a}_{t}^{w} \mid \mathbf{s}_{t})} + V(\mathbf{s}_{t}) - V(\mathbf{s}_{t+1}^{w}) \right. \\ \left. - \left( \beta \log \frac{\pi_{\theta}(\mathbf{a}_{t}^{l} \mid \mathbf{s}_{t})}{\pi_{\text{ref}}(\mathbf{a}_{t}^{l} \mid \mathbf{s}_{t})} + V(\mathbf{s}_{t}) - V(\mathbf{s}_{t+1}^{l}) \right) \right] \right] \\ = -\mathbb{E}_{(\mathbf{s}_{t}, \mathbf{a}_{t}^{w}, \mathbf{a}_{t}^{l}) \sim \mathcal{D}} \left[ \log \sigma \left( \beta \log \frac{\pi_{\theta}(\mathbf{a}_{t}^{w} \mid \mathbf{s}_{t})}{\pi_{\text{ref}}(\mathbf{a}_{t}^{w} \mid \mathbf{s}_{t})} - V(\mathbf{s}_{t+1}^{w}) \right. \\ \left. - \beta \log \frac{\pi_{\theta}(\mathbf{a}_{t}^{l} \mid \mathbf{s}_{t})}{\pi_{\text{ref}}(\mathbf{a}_{t}^{l} \mid \mathbf{s}_{t})} + V(\mathbf{s}_{t+1}^{l}) \right) \right]. \tag{12}$$

where  $V(\mathbf{s}_{t+1}^w) - V(\mathbf{s}_{t+1}^l)$  denotes the advantage of  $\mathbf{s}_{t+1}^w$  to  $\mathbf{s}_{t+1}^l$  from the same start state.

To understand the difference between our step-APO and other step-DPO, we will analyze the gradient of the  $\mathcal{L}_{\text{Step-APO}}$ :

$$\nabla_{\theta} \mathcal{L}_{\text{Step-APO}}(\pi_{\theta}; \pi_{\text{ref}}) = -\beta \mathbb{E}_{(\mathbf{s}_{t}, \mathbf{a}_{t}^{w}, \mathbf{a}_{t}^{l}) \sim \mathcal{D}} \left[ \sigma \left( \hat{r}_{\theta}(\mathbf{s}_{t}, \mathbf{a}_{t}^{l}) - \hat{r}_{\theta}(\mathbf{s}_{t}, \mathbf{a}_{t}^{w}) + V(\mathbf{s}_{t+1}^{w}) - V(\mathbf{s}_{t+1}^{l}) \right) \right] \left[ \nabla_{\theta} \log \pi(\mathbf{a}_{t}^{w} \mid \mathbf{s}_{t}) - \nabla_{\theta} \log \pi(\mathbf{a}_{t}^{l} \mid \mathbf{s}_{t}) \right].$$

$$(13)$$

where  $\hat{r}_{\theta}(\mathbf{s}_{t}, \mathbf{a}_{t}) = \beta \log \frac{\pi_{\theta}(\mathbf{a}_{t}|\mathbf{s}_{t})}{\pi_{\text{ref}}(\mathbf{a}_{t}|\mathbf{s}_{t})}$ . Intuitively, the gradient of the loss function  $\mathcal{L}_{\text{Step-APO}}$  increases the likelihood of the preferred completions  $\mathbf{a}_{t}^{w}$  and decreases the likelihood of dispreferred completions  $\mathbf{a}_{t}^{l}$ . Importantly, besides the examples are weighed by how much higher the  $\hat{r}_{\theta}$  incorrectly orders the completions, the examples are also weighted by how much higher the advantage of  $\mathbf{a}_{t}^{w}$  is compared to  $\mathbf{a}_{t}^{l}$ . Our experiments prove the importance of this weighting.

# 3.3 Iterative Training of Policy and Value Model

As shown in Figure 2, our approach employs iterative training for policy and value models. Our policy model  $\pi_{\theta}$  and value model  $v_{\phi}$  are two separate models, both adapted from the same base model. We add a value head for the value model, which is randomly initialized in the first round. However, as the MCTS simulations proceed in the first round, rewards from terminal nodes are back-propagated to the intermediate nodes, reducing the negative impact of the random value initialization.

For policy model training, we first supervised fine-tune (SFT) it using collected correct paths, then apply our Step-APO (Eq. 8) using collected step-level preference data both from MCTS. Notably,  $V(\mathbf{s}^w_{t+1})$  and  $V(\mathbf{s}^l_{t+1})$  in eq.8 , obtained from MCTS, represent the values of the corresponding states. The difference between these values reflects the advantage difference of the two actions under the same previous state  $\mathbf{s}_t$ :

$$A(\mathbf{s}_{t}, \mathbf{a}_{t}^{w}) - A(\mathbf{s}_{t}, \mathbf{a}_{t}^{l}) = Q(\mathbf{s}_{t}, \mathbf{a}_{t}^{w}) - V(\mathbf{s}_{t}) - (Q(\mathbf{s}_{t}, \mathbf{a}_{t}^{l}) - V(\mathbf{s}_{t})) = V(\mathbf{s}_{t+1}^{w}) - V(\mathbf{s}_{t+1}^{l}).$$
(14)

For value model optimization, we sue a mean squared error (MSE) loss between the value model's predict and values from MCTS. With the updated policy and value models, we can advance to the next-round MCTS, iterating this training process to enhance the models.

#### 4 Experiments

# 4.1 Implementation Details

We iteratively generate data via MCTS and train our policy and value models in two rounds. In each round, planning steps and final solution steps are generated by the policy model using MCTS to solve the given problem. The value model was employed to assist in evaluating the step plans during MCTS. At the end of each round, the generated data was used to train both the policy model and the value model.

Model Architecture We utilize the DeepSeekMathBase-7B (Shao et al., 2024) as our initial policy model and add a randomly initialized value head to this model, serving as the initial value model. We then optimize these two separate models and use the updated models for the next round of data generation.

Datasets We construct our training data using the GSM8K (Cobbe et al., 2021) and MATH (Hendrycks et al., 2021b) datasets. The GSM8K dataset consists of 7,473 training and 1,319 test problems, while the MATH dataset contains 7,500 training and 5,000 test problems. From these datasets, we exclusively extracted question-answer pairs from the training sets of GSM8K and MATH, omitting the human-annotated solution. This resulted in a total of 15k question-answer pairs to construct our training data.

Training Data Generation via MCTS For each problem, we utilize MCTS to generate multiple step-level plans and final solutions. In the first round, we generate data from a subset of 5k question-answer pairs, consisting of 4k from the MATH and 1k from GSM8K, for efficiency. We carefully design prompts and 2-shot demonstrations to guide the model's output, see Appendix A.1 for details. MCTS is run for 200 simulations in this phase to mitigate the impact of the random initialization of the value model. Starting from the second round, with the fine-tuned model from the first round, we use the full set of 15k question-answer pairs for data generation. A 2-shot prompt formatted in XML is used, and MCTS is executed for 100 simulations. During the MCTS expansion phase, we expanded 5 child nodes for the root node and 3 child nodes for other nodes. We apply a temperature of 0.7 to encourage diverse generation.

We list the statistic for the generated data in two rounds in Table 1. For plan step preference data, we categorize sibling nodes as "preferred" if their value is greater than 0 and "dispreferred" if their value is less than 0, forming preference pairs from any combination. For the final solution step data, we only create pairs between the max value (>0) and the min value (<0). This is based on our experimental findings that an excess of solution data can negatively impact the performance on out-of-domain reasoning tasks, whereas increasing the emphasis on planning data improves performance in both mathematical and other reasoning tasks. Table 1 shows that Round 2 generates more correct responses, indicating a stronger policy and value model.

Table 1: Statistic for the generated data in two rounds

Round Num	Avg Depths	Pos:Neg	Plan Pairs Count	Solution Pairs Count
Round 1	4.18	1:3.16	18742	16506
Round 2	3.80	1:1.23	24707	24633

Training Details For the policy model, we first randomly select up to four correct responses per problem for supervised fine-tuning (SFT), resulting in approximately 50k SFT data per round. Next, we use step-level preference data from MCTS to train the model with our Step-APO algorithm. The statistics for preference data are listed in Table 1. For the value model, we use values from MCTS for partial solutions as labels to update the model. This allows the value model to score both partial plans and complete responses. The SFT data for the value model consists of approximately 200k examples in Round 1. The training hyperparameters are provided in the Appendix A.2. Notably, because the value difference for final solution step preference pairs is 2, while the value difference for other plan steps ranges between 0.6 and 0.8, we apply a scaling factor of 0.3 to the values of solution steps. In the second round of training, we use the data from the second round to train the base model, rather than the Round 1 model.

# 4.2 EVALUATION REASONING TASKS

We evaluate our method on both mathematical tasks and other out-of-domain reasoning tasks.

Mathematical tasks. We evaluate our in-domain capabilities on MATH and GSM8K test set in a zero-shot setting. We use vLLM (Kwon et al., 2023) for inference during evaluation and the math evaluation toolkit by Zhang et al. (2024).

Out-of-domain reasoning tasks. We select three benchmarks for evaluating out-of-domain reasoning: BIG-Bench Hard (BBH) (Suzgun et al., 2022), ARC-C (Clark et al., 2018), and MMLU-STEM (MMLU) (Hendrycks et al., 2021a). BBH consists of 23 challenging tasks requiring multi-step reasoning, designed to test capabilities beyond the performance of language models, particularly in cases where traditional few-shot methods underperform. ARC-C focuses on commonsense reasoning and complex science-related questions, posing a significant challenge for models to handle nuanced scientific concepts. MMLU-STEM is a subset of the MMLU benchmark, covering subjects like mathematics, physics, and engineering, aiming to assess the model's performance in STEM disciplines. We employ few-shot prompting using lm-evaluation-harness (Gao et al., 2024) for evaluation on these benchmarks.

#### 4.3 Results on Mathematical Tasks

As shown in Table 2, our CPL significantly boosts performance on in-domain tasks. In both rounds, Step-APO consistently improves results over the SFT significantly. Additionally, Round 2 outperforms Round 1 in both SFT and Step-APO, demonstrating that the updated policy and value models generate better data through MCTS, further improving performance.

Table 2: Model performance on MATH and GSM8K, DeepSeekMath-Base results are reproduced, with the originally reported numbers in parentheses. Best results are **bolded**.

Model	GSM8K	MATH
DeepSeekMath-Base (4-shot)	63.23(64.20)	35.18(36.20)
CPL(Round 1 SFT)	63.79	36.3
CPL(Round 1 Step-APO)	71.06	40.56
CPL(Round 2 SFT)	69.75	39.16
CPL(Round 2 Step-APO)	73.77	41.64

#### 4.4 Results on Out-of-domain Reasoning Tasks

From Table 3, we can see that our approach also achieves significant improvements on OOD tasks, demonstrating that CPL enhances the model's generalization ability across diverse reasoning tasks. Compared to AlphaMath, which was trained on the same 15k dataset using the REACT format for 3 round, our performance on these OOD reasoning tasks is noticeably better. Notably, AlphaMath even shows a decrease in performance on certain tasks, such as a 2.2 drop in BBH.

#### 4.5 Advantage of Planning-based Learning

In our preliminary experiments, we aim to verify whether planning-based learning outperforms solution-based learning on OOD tasks. We conducted these experiments on the GSM8K and MATH training set and evaluated on BBH. Specifically, we compared CoT-formatted SFT with our planning-based prompt SFT, both of which were fine-tuned using model self-generated data, filtered based on the correctness of the answer. In this experiment, we sampled only one response per problem for training. The results in Table 4 demonstrate that planning-based learning enhances performance on BBH, whereas CoT SFT does not show significant improvements.

Table 3: Model performance on out-of-domain tasks. Best results are **bolded**. We use 25-shot for ARC-C, 3-shot CoT for BBH, 5-shot for MMLU-STEM (MMLU).

Model	ARC-C	ввн	MMLU-STEM (MMLU)
DeepSeekMath-Base	52.05	58.79	52.74(53.84)
AlphaMath	53.41	56.63	<b>55.31</b> (54.55)
CPL(Round 1 SFT)	54.44	59.68	54.58(54.22)
CPL(Round 1 Step-APO)	55.55	60.18	55.15(54.66)
CPL(Round 2 SFT)	54.95	59.93	55.44(54.44)
CPL(Round 2 Step-APO)	56.06	60.54	54.93( <b>54.70</b> )

Table 4: Advantage of Planning-base Learning

Model	BBH(3-shot CoT)
DeepSeekMath-Base CoT SFT	58.79 58.92
Planning-based Learning SFT	59.5

#### 4.6 Advantage of Step-APO

We aim to analyze the advantages of Step-APO over non-advantage integrated step-DPO. Our experiments reveal that Step-APO achieves superior performance on both in-domain and out-of-domain tasks. This demonstrates that our method, by reinforcing important steps through preference learning, leads to more effective model optimization.

Table 5: Advantage of Step-APO

Model	GSM8K	MATH	ARC-C	BBH	MMLU-STEM(MMLU)
DeepSeekMath-Base	63.23	35.18	52.05	58.79	52.74(53.84)
Round 2 SFT	69.75	39.16	54.95	59.93	<b>55.44</b> (54.44)
Round 2 Step-DPO	72.80	41.47	55.63	60.40	55.20(54.68)
Round 2 Step-APO	73.77	41.64	56.06	60.54	54.93( <b>54.70</b> )

#### 5 Conclusion

In this work, we propose that learning planning can improve a model's reasoning and generalization capabilities. By focusing on finer-grained learning of plan step preferences through our Step-APO, the model can identify critical planning steps within the reasoning trace, further enhancing its reasoning ability. Although we trained on GSM8K and MATH data, our approach has demonstrated general improvements on other reasoning tasks such as BBH, ARC-C, and MMLU-STEM.

Finding an effective way to improve transfer performance to more reasoning tasks and enhance overall model generalization in reasoning remains an open and important research question that has yet to be fully addressed. We believe that learning the critical planning steps for solving a problem is crucial for enhancing the model's reasoning capabilities. At the same time, the relative advantages between these planning steps are important for optimization. Additionally, the diversity of preference data is essential for learning various planning strategies. In future work, we plan to explore the application of our method to other types of data, such as code. Additionally, we will continue to refine our approach, exploring various improvements such as enhancing the diversity of planning steps to better capture a broader range of planning step preferences.

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#### A Appendix

#### A.1 PROMPT USED IN MCTS

Prompts for Round 1 and Round 2 are listed below.

# Round 1 2-shot prompt

You are a powerful agent with advanced reasoning and planning capabilities. Answer the questions as best you can.

#### !!!Remember:

- 1. Your answer should have two sections: "Plans" and "Detailed Implementation".
- 2. In the "Plans" section, you should outline step-by-step plans for solving the problem. These plans might include extracting key information, forming sub-questions, analyzing aspects, etc. Each step should introduce new insights, avoid overly abstract or generic actions. End each step with "<endstep>".
- 3. In the "Detailed Implementation" section, provide detailed steps that correspond to each plan, and conclude with "The final answer is \boxed{answer}.<endsolution>"

The following is a template for your answer:

Question: The input question

#### Plans:

Plan 1: Describe the first plan step.<endstep>Plan 2: Describe the second plan step<endstep>...

# Plan N: Describe the final plan step<endstep>

# Detailed Implementation:

- 1. Execute the first plan step
- 2. Execute the second plan step

. . .

N. Execute the final plan step

The final answer is \boxed{answer}.<endsolution>

The following are 2 demonstration examples.

Question: Natalia sold clips to 48 of her friends in April, and then she sold half as many clips in May. How many clips did Natalia sell altogether in April and May?

#### Plans:

Plan 1: Analyze the total number of clips sold in April.<endstep>
Plan 2: Calculate the number of clips sold in May by applying the
"half as many" condition to the number sold in April.<endstep>
Plan 3: Sum the results from April and May to determine the overall
total of clips sold over the two months.<endstep>

# Detailed Implementation:

- 1. Natalia sold 48 clips in April.
- 2. The number of clips sold in May is  $\frac{48}{2}=24$ .
- 3. The total number of clips sold in April and May combined is 48+24=72.

The final answer is  $\boxed{72}$ .<endsolution>

Question: If  $x^2+y^2=1$ , what is the largest possible value of |x|+|y|?

#### Plans:

Plan 1: Understand that the equation  $x^2+y^2=1$  defines a circle centered at the origin with a radius of 1. To maximize |x|+|y|, we need to consider points on this circle that maximize the sum of the absolute values of x and y.<

Plan 2: Recognize that |x|+|y| is maximized when both |x| and |y| are large. The maximum sum occurs along lines where x and y contribute equally, specifically along the lines y=x and y=-x.<

Plan 3: Identify the points of intersection between the lines y=x and y=-x with the circle  $x^2+y^2=1$ . These points are expected to yield the maximum value of |x|+|y|.<br/>endstep>

Plan 4: Evaluate |x|+|y| for the intersection points to determine the maximum possible value. <endstep>

#### Detailed Implementation:

- 1. The circle  $x^2+y^2=1$  is centered at the origin with a radius of 1. We need to find the points on this circle that maximize the sum |x|+|y|.
- 2. To maximize |x|+|y|, the sum is largest when both |x| and |y| are large. This occurs along the lines y=x and y=-x, where x and y contribute equally to the sum.

```
3. The intersection points are
$\left(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}}\right)$,
$\left(\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}}\right)$,
$\left(-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}}\right)$, and
$\left(-\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}}\right)$.
4. For these points, calculate $|x|+|y|$. For
$\left(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}}\right)$,
$|x|+|y|=\sqrt{2}$. The same value applies to the other points.
Therefore, the maximum value is $\sqrt{2}$$.
The final answer is $\boxed{\sqrt{2}}$$.
Now! It's your turn.
```

## Round 2 XML 2-shot prompt

```
<question>
Question: Natalia sold clips to 48 of her friends in April, and then
she sold half as many clips in May. How many clips did Natalia sell
altogether in April and May?
</question>
<plan>
<step>
Plan 1: Analyze the total number of clips sold in April.
</step>
<step>
Plan 2: Calculate the number of clips sold in May by applying the
"half as many" condition to the number sold in April.
</step>
<step>
Plan 3: Sum the results from April and May to determine the overall
total of clips sold over the two months.
</step>
</plan>
<solution>
1. Natalia sold 48 clips in April.
2. The number of clips sold in May is \frac{48}{2}=24.
3. The total number of clips sold in April and May combined is
$48+24=72$.
The final answer is \begin{tabular}{l} \begin{tab
</solution>
<question>
If x^2+y^2=1, what is the largest possible value of |x|+|y|?
</question>
<plan>
<step>
Plan 1: Understand that the equation x^2+y^2=1 defines a circle
centered at the origin with a radius of 1. To maximize |x|+|y|, we
need to consider points on this circle that maximize the sum of the
absolute values of $x$ and $y.
</step>
Plan 2: Recognize that |x|+|y| is maximized when both |x| and
$|y|$ are large. The maximum sum occurs along lines where $x$ and
y$ contribute equally, specifically along the lines y=x$ and y=-x.
</step>
```

```
<step>
Plan 3: Identify the points of intersection between the lines $y=x$
and y=-x with the circle x^2+y^2=1. These points are expected to
yield the maximum value of |x|+|y|.
</step>
<step>
Plan 4: Evaluate |x|+|y| for the intersection points to determine
the maximum possible value.
</plan>
<solution>
1. The circle x^2+y^2=1 is centered at the origin with a radius of
1. We need to find the points on this circle that maximize the sum
|x| + |y| .
2. To maximize |x|+|y|, the sum is largest when both |x| and
$|y|$ are large. This occurs along the lines $y=x$ and $y=-x$, where
$x$ and $y$ contribute equally to the sum.
3. The intersection points are
\left(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}}\right)
\left(\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}}\right)
\left(-\frac{1}{\sqrt{2}}\right), \frac{1}{\sqrt{2}}\right), 
\left(-\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}}\right).
4. For these points, calculate |x|+|y|. For
\left(\frac{1}{\sqrt{2}}\right), \frac{1}{\sqrt{2}}\right)
|x|+|y|=\sqrt{2}. The same value applies to the other points.
Therefore, the maximum value is $\sqrt{2}$.
The final answer is $\boxed{\sqrt{2}}.
</solution>
```

# A.2 Implementation Details

Table 6: Key Hyperparameters of CPL

Hyperparameter	Value
$c_{puct}$	1.5
Simulations $N$	200 (for round 1) or 100
Expand child nodes	5 (for root) or 3
Temperature	0.7
Max depth	6
SFT batch size	512
SFT learning rate	1e-5
SFT epochs	5  (for round 1) or  3
Step-APO batch size	64
Step-APO $\beta$	0.3
Step-APO learning rate	1e-6
Step-APO epochs	2
Solution step scaling factor	0.3
Lr scheduler type	cosine
Warmup ratio	0.1

**Experiment Environments** We implement our Step-APO in Llama Factory (Zheng et al., 2024) and use Llama Factory as the training framwork. We use vLLM (Kwon et al., 2023) as the inference framework. We train all models with DeepSpeed ZeRO Stage2 (Rajbhandari et al., 2021), Flash Attention 2 (Dao, 2023).

The key hyperparameter of CPL is listed in Table 6.