# AgentPro: Enhancing LLM Agents with Automated Process Supervision

**Anonymous ACL submission** 

## Abstract

Large language model (LLM) agents have demonstrated significant potential for addressing complex tasks through mechanisms such as chain-of-thought reasoning and tool invocation. However, current frameworks lack explicit supervision during the reasoning process, which may lead to error propagation across reasoning chains and hinder the optimization of intermediate decision-making stages. This paper introduces a novel framework, AgentPro, which enhances LLM agent performance by automated process supervision. AgentPro employs Monte Carlo Tree Search to automatically generate step-level annotations, and develops a process reward model based on these annotations to facilitate fine-grained quality assessment of reasoning. By employing a rejection sampling strategy, the LLM agent dynamically adjusts generation probability distributions to prevent the continuation of erroneous paths, thereby improving reasoning capabilities. Extensive experiments on four datasets indicate that our method significantly outperforms existing agent-based LLM methods (e.g., achieving a 6.32% increase in accuracy on the HotpotQA dataset), underscoring its proficiency in managing intricate reasoning chains.

# 1 Introduction

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Recent advancements in large language models (LLMs), such as GPT-4 (OpenAI, 2023), PaLM (Anil et al., 2023), and LLaMA (Dubey et al., 2024), have showcased impressive capabilities in semantic understanding, knowledge reasoning, and cross-task generalization. Meanwhile, research indicates that LLM-based agents can effectively decompose complex, multi-step tasks through chainof-thought prompting and tool invocation mechanisms (Schick et al., 2024). This has led to significant advancements in mathematical problemsolving (Lightman et al., 2023) and in scenarios involving embodied interaction (Shridhar et al., 2020; Wei et al., 2022; Yao et al., 2023).

Despite the demonstrated potential of LLM agents in managing complex tasks, existing frameworks face significant challenges in utilizing process supervision to train and improve these agents. Conventional approaches, such as ReAct (Yao et al., 2022b), which decomposes tasks through alternating reasoning trajectory generation and actions; and Reflexion (Shinn et al., 2024), which uses self-reflection mechanisms for policy iteration, primarily concentrate on the accuracy of final task outcomes while neglecting explicit supervision of intermediate reasoning steps. This design leads to two major issues. First, the lack of real-time error detection and correction mechanisms allows local errors to propagate along reasoning chains during extended inferences (Lightman et al., 2023). Second, the absence of mechanisms in output feedback optimization to discern subtle differences in reasoning quality hinders the identification of optimal decision paths (Wang et al., 2024). For example, QueryAgent (Huang et al., 2024) utilizes environmental feedback for self-correction. However, this feedback primarily relates to task outcomes and fails to pinpoint specific errors in the process.

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In mathematical reasoning tasks, process supervision techniques, such as the use of Process Reward Models (PRMs), have proven to be highly effective (Lightman et al., 2023). However, integrating PRMs into LLM agents remains underexplored, primarily due to the substantial costs associated with manual, step-wise supervision. Specifically, creating training datasets for PRMs necessitates human labeling to assess the correctness of each step. Therefore, developing cost-effective, automated process supervision methods is essential for improving the reasoning capabilities and robustness of LLM agents in handling complex tasks.

In this paper, we present AgentPro, a novel framework for LLM **Agent**s that incorporates an Automated **Process** Supervision mechanism to address complex tasks such as reasoning and decision

making. Our approach employs Monte Carlo Tree Search (MCTS) (Wang et al., 2024; Świechowski 086 et al., 2023) to generate step-level labels, which 087 facilitate the training of a process reward model (PRM). The PRM improves its comprehension by learning from automatically annotated data, thereby 090 providing detailed evaluations of each reasoning step. Our goal is to improve the reasoning abilities of an LLM agent by applying the Rejection Sampling (RS) (Liu et al., 2023; Yuan et al., 2023) 094 strategy within the framework of reinforcement learning from human feedback (Bai et al., 2022). This approach adjusts the generation probability distributions based on feedback from the PRM, thereby minimizing error propagation along reasoning paths. We evaluated AgentPro's performance across four distinct datasets in various task do-101 mains, demonstrating its substantial enhancements 102 in both the accuracy and robustness of LLM agents 103 when addressing complex tasks. Specifically, our 104 method achieved a 6.32% increase in accuracy on 105 the HotpotQA dataset within multi-hop question answering scenarios, highlighting its proficiency in handling intricate reasoning chains. 108

Our main contributions are as follows:

 We present the first LLM agent framework that integrates automated process supervision to optimize reasoning and decision-making tasks. Our framework conducts real-time quality evaluation at each step, effectively mitigating the issue of error propagation found in traditional approaches.

- We propose an automated label generation algorithm based on Monte Carlo Tree Search (MCTS) that minimizes the cost of step-wise annotation for training PRMs, thereby facilitating the feasibility of large-scale process supervision.
- We conduct extensive experiments on four datasets, considering both reasoning and decision-making scenarios. The results indicate that our method achieves superior performance compared to existing agent-based methods.

# 2 Related Work

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# 2.1 Large Language Model Agent

LLM agents (Yao et al., 2023; Sumers et al., 2023; Gong et al., 2023) exhibit exceptional reasoning capabilities across a variety of problem domains, including embodied environments and reasoning tasks. CAMEL (Li et al., 2023) introduces a multiagent role-playing framework that guides agents in task completion by utilizing initial prompts and detailed constraints while ensuring alignment with human intentions. AutoAgents (Chen et al., 2023) emphasize the autonomous generation of language agents to adapt to diverse task requirements. ExpeL (Zhao et al., 2024) achieves continuous performance enhancement and transfer learning in decision-making tasks by autonomously collecting experiences and extracting knowledge through natural language. Existing approaches primarily focus on the final outcomes. In contrast, our approach addresses error propagation in extensive reasoning chains by providing explicit process supervision of the intermediate reasoning steps. 135

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# 2.2 Reasoning-Action Framework

Integrating actions with reasoning enhances the efficiency and accuracy of LLMs in multi-step, conditional problems (Ding et al., 2023; Gong et al., 2023; Chen et al., 2023; Huang et al., 2024; Arora et al., 2024). ReAct (Yao et al., 2022b) integrates reasoning with action generation, decreasing hallucination in chain-of-thought processes. AUTOACT (Qiao et al., 2024) introduces a self-planning framework for question-answering that facilitates agent learning from scratch, addressing limitations of single-model systems. LLM+AL (Ishay and Lee, 2025) merges LLMs with action languages, utilizing their strengths in semantic parsing, commonsense generation, and automated reasoning tasks. However, these methods do not thoroughly evaluate the quality of intermediate steps, and we address this by employing rejection sampling for dynamic error correction during reasoning.

# 2.3 Process Reward Model

PRM enhances the accuracy of reasoning by supervising and emphasizing intermediate steps, rewarding correct inferences and penalizing errors, in contrast to traditional methods that solely concentrate on final outcomes (Uesato et al., 2022; Lightman et al., 2023; Wang et al., 2024; Zhang et al., 2025). It allows for more precise pattern learning and handles the misalignment between correct conclusions and flawed derivations. For example, Math-Shepherd (Wang et al., 2024) employs automated annotation to provide step-level rewards, and DeepMind's Process Advantage Verifiers assign rewards based on the correctness probability changes at each step (Setlur et al., 2024). However, existing PRM implementations are limited to math problems. Our work expands PRM to a wider range of reasoning and decision-making tasks.

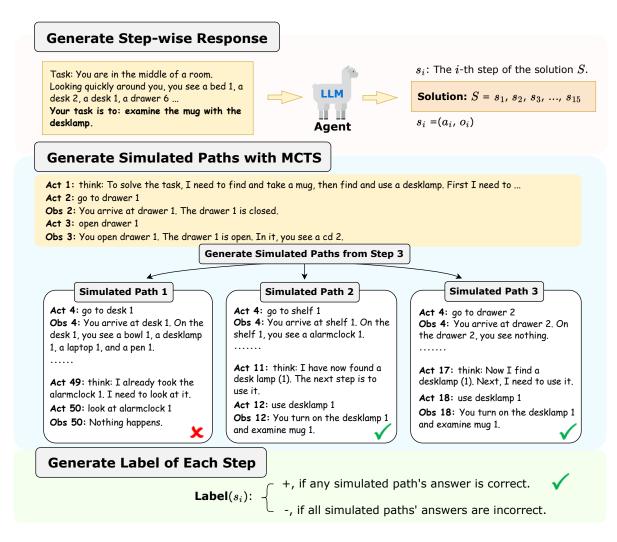


Figure 1: Overview of the Monte Carlo Tree Search-driven automatic labeling framework. First, the LLM Agent generates a solution S for a given task q. Then, MCTS is employed to simulate multiple decision-making paths for a given step  $s_i$  (in this case i = 3). Finally, the results of these simulations determine if the step  $s_i$  is labeled as correct or incorrect, depending on whether any of the simulated trajectories reach the correct final answer.

# 3 Method

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Existing LLM frameworks often lack robust verification mechanisms to ensure the accuracy of intermediate steps in complex problem-solving tasks. Furthermore, manual annotation methods are prohibitively expensive. To address these challenges, we propose a novel framework, AgentPro, designed to enhance the reasoning capabilities of LLM agents while minimizing costs.

AgentPro comprises two core components:

LLM Agent: The LLM Agent M<sub>agent</sub> is the core component responsible for generating step-by-step solutions (responses) and is the agent to be fine-tuned in the end. Given a query q, the agent generates a solution S ← M<sub>agent</sub>({q}), where S = {s<sub>1</sub>, s<sub>2</sub>, s<sub>3</sub>, ..., s<sub>K</sub>} represents the sequence of steps and K de-

notes the total number of steps in the solution. For decision-making tasks such as in AlfWorld, each step  $s_i$  can defined as  $s_i = (a_i, o_i)$ , where  $a_i$  is an executable action (e.g., "Go to desk 1") and  $o_i$  is an optional observation from the environment (e.g., "You arrive at desk 1 and see a bowl 1 on the desk").

 Process Reward Model: The process reward model (PRM), denoted as M<sub>prm</sub>, is utilized to assess the step-wise accuracy of a solution S. It assigns a score to each step s<sub>i</sub> to quantify the correctness of that specific step.

Building on these two components, we devised a three-phase optimization framework that utilizes Monte Carlo Tree Search to automatically generate a training dataset for the PRM  $M_{\rm prm}$ , which is then employed to improve the reasoning abilities of the

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LLM Agent M<sub>agent</sub> through reinforcement learning.
The framework functions as follows:

- 1. Automated Process Annotation: We employ the LLM Agent to produce multi-step trajectories, with each intermediate step  $s_i$  being automatically annotated using labels obtained from MCTS simulations. This phase facilitates the creation of a self-supervised dataset, which is subsequently used to train the PRM.
  - 2. Training of the Process Reward Model: Utilizing the annotated steps from Phase 1, we fine-tune the PRM  $M_{prm}$  to accurately predict correctness scores for each individual step  $s_i$ , thereby equipping the PRM with the capability to assess step-wise validity within complex problem-solving scenarios.
  - 3. Reinforcement Learning: We adopted the rejection sampling strategy, a technique within the framework of reinforcement learning from human feedback (RLHF), to enhance the capabilities of our LLM Agent  $M_{\text{agent}}$ , where the PRM  $M_{\text{prm}}$  functions as the reward model.

# 3.1 Gathering Step-Wise Trajectories

To enable effective process supervision, it is essential to ensure that the answers from the LLM Agent are generated in a step-by-step manner. A robust base model is critical for generating structured, step-wise responses, leveraging its contextual understanding and reasoning capabilities developed through extensive training on large-scale corpora. Consequently, a good base model ensures the high quality of the generated responses. In our setting, we utilize pre-trained LLMs, such as LLaMA-3.1-8B-Instruct (Dubey et al., 2024), as the base model for our agent.

Meanwhile, every step of a response must be meticulously documented to facilitate the subsequent automatic labeling process, which is crucial for training the PRM. For each query q, the LLM agent performs a comprehensive semantic analysis to extract crucial information and delineate the inherent reasoning framework. This analysis involves consulting its internal knowledge base to construct logically coherent reasoning or decisionmaking trajectories. Specifically, the solution  $S \leftarrow M_{\text{agent}}(\{q\})$  must be delineated in a step-wise manner and presented as  $S = \{s_1, s_2, s_3, \dots, s_K\}$ . Then the trajectory  $T_q$  can be represented as: For example, for a given decision-making task (query) q illustrated in Fig. 1 within the AlfWorld scenario, the agent generates a solution S comprising K = 15 steps. Thus, the trajectory for task q can be represented as  $T_q = \{q, s_1, s_2, \dots, s_{15}\}$ .

# 3.2 Monte Carlo Tree Search-Driven Automatic Labeling

To systematically evaluate the quality of each step  $s_i$  generated by the LLM agent  $M_{\text{agent}}$ , we define the following criterion: a step  $s_i$  is deemed high-quality if it contributes to deriving the ground-truth answer  $A_{\text{correct}}$ . This criterion aligns with the fundamental objective of multi-step reasoning and decision-making tasks, where intermediate steps should progressively lead to a correct final result. Our goal is to design a method to automatically assess the contribution of each step.

Monte Carlo Tree Search (MCTS) (Świechowski et al., 2023) is a heuristic search algorithm renowned for its effectiveness in navigating complex decision spaces under uncertainty. Building upon its strong simulation performance, we introduce an MCTS-based automatic labeling framework for training the PRM. For each step  $s_i$ , we generate m simulated paths  $p_1^i$  to  $p_m^i$  for  $s_i$  using the path from query q to  $s_i$  in the trajectory  $T_q$ described by Eq. 1. Each path  $p_i^j$  is constructed as:

$$p_j^i \leftarrow M_{\text{agent}}(\{q, s_1, \dots, s_i\}) \tag{2}$$

Let  $A_{\text{final}}^{(j)}$  denote the final answer of the *j*-th path  $p_j^i$ . The label for  $s_i$  is determined based on whether any of the *m* paths from  $p_1^i$  to  $p_m^i$  result in  $A_{\text{correct}}$ :

$$\text{Label}(s_i) = \begin{cases} + & \text{if } \exists j \in [1,m], \ A_{\text{final}}^{(j)} = A_{\text{correct}}, \\ - & \text{if } \forall j \in [1,m], \ A_{\text{final}}^{(j)} \neq A_{\text{correct}}. \end{cases}$$
(3)

As illustrated in Fig. 1, we generated m = 3 simulated paths from  $p_1^3$  to  $p_3^3$  for step  $s_3$ . Given that the task q in AlfWorld pertains to decision-making, each step  $s_i$  can be represented as  $s_i = (a_i, o_i)$ , where  $o_i$  is optional. Consequently, each path  $p_j^3$  is derived from  $p_j^3 \leftarrow M_{\text{agent}}(\{q, a_1, a_2, o_2, a_3, o_3\})$ . Since the outcomes of both path  $p_2^3$  and path  $p_3^3$ lead to the correct answer, "You turn on desk lamp 1 and examine mug 1", we label step  $s_3$  as "+".

Utilizing the MCTS-based automatic labeling framework, we label each step  $s_i$  within trajectory  $T_q$ . Upon completion of the labeling process for all steps across all queries  $Q = \{q_j\}_{j=1}^N$ , we generate a labeled dataset  $D_{prm} = \{d_j\}_{j=1}^N$ . This dataset consists of N samples, each corresponding to one

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$$T_q = \{q, s_1, s_2, s_3, \dots, s_K\}$$
(1)

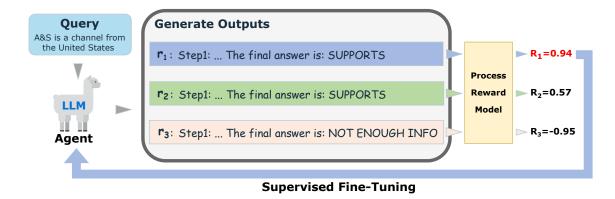


Figure 2: Overview of the training process for LLM Agent  $M_{\text{agent}}$ . For a given query q, the agent generates multiple step-wise responses, and each response  $r_i$  is subsequently evaluated by the PRM  $M_{\text{prm}}$ . The agent is then fine-tuned based on the response  $r_*$  with the highest reward score  $R_*$ . The whole process will repeat until the agent converges.

of the N queries in set Q. For each data sample  $d_j$ , the input  $X = \{q_j, s_1^j, s_2^j, \ldots, s_K^j\}$ , which represents the trajectory  $T_q^j$  generated from the *j*-th query  $q_j$  that includes K steps. The output (label) y is an array of K elements, where each element corresponds to the label associated with step  $s_i$ :

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$$d_j = (\underbrace{\{q_j, s_1^j, \dots, s_K^j\}}_X, \underbrace{\{y_{s_1}^j, y_{s_2}^j, \dots, y_{s_K}^j\}}_y)$$
(4)

where  $y_{s_i}^j$  represents the label of step  $s_i^j$ , Label $(s_i^j)$ .

# 3.3 Process Reward Model Training

We utilize the dataset  $D_{prm}$  in Sec. 3.2 to train our process reward model  $M_{prm}$ , enabling it to evaluate step-wise responses in complex problem-solving scenarios. The PRM is also constructed based on a pre-trained LLM. We adopt the full parameter finetuning strategy for training, where all parameters of  $M_{prm}$  are optimized by gradient descent to minimize prediction errors in step-wise assessments:

$$\mathcal{L}_{prm} = -\frac{1}{N} \frac{1}{K} \sum_{j=1}^{N} \sum_{i=1}^{K} CrossEntropy(y_{s_i}^j, \hat{y}_{s_i}^j) \quad (5)$$

where  $\hat{y}_{s_i}^j$  denotes the predicted correctness score for step  $s_i^j$  of the *j*-th training sample, while CrossEntropy signifies the cross entropy loss.

This full-parameter fine-tuning strategy effectively utilizes fine-grained supervisory labels from the training data, enabling the trained PRM to accurately determine if each generated step  $s_i$  logically progresses toward resolving the problem. Consequently, it provides high-quality reward scores for training LLM agents.

# 3.4 LLM Agent Training

Drawing on the principles of reinforcement learning (Kaelbling et al., 1996), we introduce an optimization mechanism that employs rejection sampling (Liu et al., 2023) to enhance the performance of our LLM agent. This mechanism involves iteratively generating multiple step-wise responses by the LLM agent  $M_{\text{agent}}$ , evaluating these responses using our well-trained PRM  $M_{\text{prm}}$ , and selecting the response with the highest reward score to train the LLM agent through supervised fine-tuning. 344

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Specifically, for each query q, the LLM agent  $M_{\text{agent}}$  first generates n candidate responses, ranging from  $r_1$  to  $r_n$ , defined as  $r_j \leftarrow M_{\text{agent}}(\{q\})$ . Similar to the solution S described in Sec. 3.1, each response  $r_j$  should be generated in a stepwise format:  $r_j = \{s_1, s_2, s_3, \ldots, s_K\}$ . The PRM  $M_{\text{prm}}$  will evaluate each step  $s_i$  in  $r_j$  and assign a label  $l_i$  (+ or -) to  $s_i$ , along with the probability  $P_i$  for generating that label. The reward score  $R_j$  for response  $r_j$  is then calculated as the average probability of the label values across all steps. During calculation, we negate those probabilities associated with negatively labeled steps to reflect our disinclination towards incorrect steps:

$$R_{j} = \frac{1}{K} \sum_{i=1}^{K} \left( \mathbb{I}(l_{i} = +) \cdot P_{i} - \mathbb{I}(l_{i} = -) \cdot P_{i} \right)$$
(6)

where  $\mathbb{I}$  is the indicator function. The response  $r_*$  with the highest reward score  $R_*$  is selected as the optimal response for further training:

$$r_* = \operatorname*{arg\,max}_{r_j} R_j \tag{7}$$

After selecting the optimal responses for all queries, we utilize these responses to fine-tune the

LLM agent  $M_{\text{agent}}$ . Consistent with Sec. 3.3, we employ the full-parameter fine-tuning strategy on  $M_{\text{agent}}$  to maximize the likelihood of replicating the optimal reasoning steps:

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$$\mathcal{L}_{agent} = -\frac{1}{N_r} \sum_{i=1}^{N_r} \sum_{t=1}^{T_i} \log P(y_{i,t}|x_i) \quad (8)$$

where  $x_i$  is the *i*-th query (prompt) among  $N_r$  training samples,  $y_i$  is the step-wise response for  $x_i$ ,  $y_{i,t}$  is the *t*-th word of  $y_i$ , and  $T_i$  is the length of  $y_i$ .

Fig. 2 illustrates an example of the agent training process, wherein the agent generates three stepwise responses. The first response, which exhibits the highest reward score ( $R_1 = 0.94$ ), is chosen for training the agent. The training process is repeated until the agent develops sufficient capabilities to manage complex multi-step reasoning tasks.

In summary, our framework enhances the performance of the LLM agent through MCTS-based automated process supervision and rejection sampling training strategy. For additional details on the algorithm, please refer to Appendix A.

# 4 Experiments

# 4.1 Experimental Setup

**Datasets.** We selected four representative benchmark datasets to evaluate the performance of our method: FEVER (Thorne et al., 2018), HotpotQA (Yang et al., 2018), ALFWorld (Shridhar et al., 2020), and WebShop (Yao et al., 2022a). The FEVER dataset is utilized for assessing fact extraction and verification. HotpotQA serves as a benchmark for knowledge-intensive, multi-hop question answering. ALFWorld provides an embodied simulation environment for executing multi-step tasks in domestic contexts. Finally, WebShop functions as a benchmark for complex decision-making, simulating multi-modal interactions and product filtering in online shopping settings.

Baselines. We compare our method with four base-411 line methods: Act (Yao et al., 2022b), ReAct (Yao 412 et al., 2022b), Reflexion (Shinn et al., 2024), and 413 ExpeL (Zhao et al., 2024). The Act method gen-414 erates responses through single-step predictions 415 without explicit reasoning abilities. ReAct adopts a 416 more structured approach by integrating reasoning 417 418 and action in a feedback loop to enhance task performance. Reflexion uses verbal reinforcement to 419 enable agents to learn from past mistakes, thereby 420 improving the quality of reasoning. ExpeL, the 421 state-of-the-art agent-based method, focuses on 422

autonomously gathering experience from a set of training tasks to enhance the capabilities of LLM. Implementation. Following ReAct, we use success rate (SR) as the evaluation metric: exact matching for HotpotQA and FEVER, timely task completion for ALFWorld, and purchasing an item matching all attributes for WebShop. We utilize the LLaMA-3.1-8B-Instruct model (Dubey et al., 2024) as the LLM agent for our method and all baselines. For FEVER and HotpotQA, Wikipedia information is appended to questions for additional context, a common practice among all baselines. For MCTS, we conduct m = 3 simulations to determine the label for each step. Regarding rejection sampling, n = 4 different responses are generated over T = 5 iterations during the training of our LLM agent. All results are averaged across three different random seeds. For further implementation details, please refer to Appendix B.

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## 4.2 Main Results

Fig. 3 illustrates the average success rates of various methods across all four datasets. Results show that our method consistently outperforms existing baselines, which underscores the effectiveness of process supervision in enhancing the reasoning and sequential decision-making abilities of LLM agents. Specifically, in tasks requiring fine-grained factual inference (e.g., FEVER) and multi-hop reasoning (e.g., HotpotQA), our method systematically refines the reasoning process step by step using PRM. This leads to accuracy gains of 3.59% and 6.32%, respectively, over the best-performing baseline, ExpeL. These improvements suggest that PRM effectively identifies flawed reasoning paths and minimizes error accumulation, which is prevalent in traditional single-step predictions.

Furthermore, results from the ALFWorld environment demonstrate the impact of process rewards on physical reasoning. Across 134 household interaction scenarios, our approach achieves a 40.88% success rate, outperforming the best baseline, Reflexion (34.08%). This suggests that the automatically generated step-level annotations successfully capture environmental state transitions. The most significant improvement is observed in the Web-Shop tasks, where our method achieves a 52.67% success rate, which is substantially higher than ExpeL (38.00%) and Reflexion (40.67%). This finding indicates that PRM's ability to evaluate the quality of actions (such as price comparison and option matching), which helps the agent to build bet-

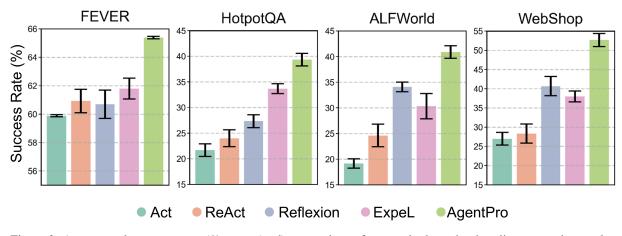


Figure 3: Average task success rates (%, mean±std) comparison of our method to other baselines on various tasks.

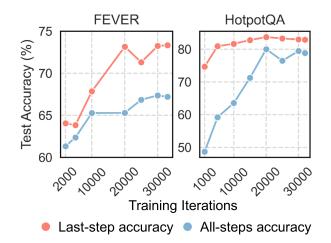


Figure 4: Performance of the trained process reward model (PRM) on the FEVER and HotpotQA datasets.

ter decision-making chains in shopping scenarios. All these experiments confirm that PRM, trained automatically using step-wise labels from MCTS, significantly improves the LLM agents.

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## 4.3 Effectiveness of Process Reward Model

To evaluate the effectiveness of the trained process reward model (PRM), we employ two performance metrics: *last-step accuracy* and *all-steps accuracy*. Last-step accuracy measures the PRM's ability to correctly evaluate the label of the final reasoning step. In contrast, all-steps accuracy calculates the average accuracy of the PRM across all reasoning steps, thereby reflecting its overall capacity to assess the entire reasoning process.

As shown in Fig. 4, the PRM exhibits significant progressive convergence on both the FEVER and HotpotQA datasets. During the training iterations from 2,000 to 20,000, both last-step accuracy and all-steps accuracy display a consistent upward trend, with convergence speed showing

Table 1: Performance comparison (%) of different methods with the deepseek-llm-7b-chat model structure.

Dataset	Act	ReAct	Reflexion	ExpeL	AgentPro
Fever	40.01	44.89	49.97	51.87	57.07
WebShop	20.00	14.00	27.00	24.00	39.00

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marked nonlinearity. Specifically, on the FEVER dataset, last-step accuracy increases by 9% during this phase. Conversely, between 20,000 and 33,000 iterations, performance stabilizes, yielding only a marginal increase of 0.17%. On the HotpotQA dataset, all-steps accuracy reaches 80.00% by 20,000 iterations, after which improvements become negligible, maintaining stable performance for the remainder of training. Although all-steps accuracy is slightly lower than last-step accuracy, it remains adequate (78.82%) for the PRM to correctly evaluate and score the reasoning steps. Overall, these results indicate that the PRM demonstrates excellent stability during training and effectively scores the reasoning steps.

# 4.4 Impact of Model Structure

To validate the robustness of our method across different base models, we conducted comparative experiments using the *deepseek-llm-7b-chat* (Bi et al., 2024) model architecture. This model has a similar parameter size to LLaMA-3.1-8B-Instruct but features a significantly different architecture. Table 1 illustrates that although the deepseek model exhibits weaker reasoning abilities compared to llama, our method consistently surpasses all other baselines. Notably, for the knowledge reasoning tasks in FEVER, our method surpasses the best baseline, ExpeL, by 5.2%. For the interactive decisionmaking tasks in WebShop, the success rate of our

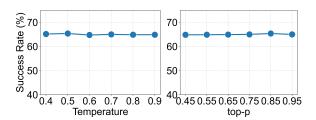


Figure 5: Impact of hyperparameters on agent performance for the FEVER dataset.

method reaches 39%, significantly outperforming the best baseline (27%). These results indicate that guiding the reasoning path of the LLM agent with PRM significantly boosts reasoning capabilities, irrespective of the base model architecture.

# 4.5 Ablation Studies

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Hyperparameter sensitivity. We investigate the impact of the hyperparameters top\_p and temperature of our method on LLM agent performance in generating step-wise responses. As shown in Fig. 5, when the temperature is fixed at 0.5, adjusting top\_p within the range of 0.45 to 0.95 leads to less than a 0.54% variation in accuracy on the FEVER dataset (65.38% compared to 64.84%). This finding indicates that the model exhibits strong robustness to these hyperparameters. Similarly, fixing top p at 0.85 and varying the temperature between 0.4 and 0.9 results in model accuracy remaining consistently within a 0.62% range, peaking at 65.38% at a temperature of 0.5. Notably, even under extreme temperature settings such as 0.4, the model maintained performance levels above 64.76%. This highlights the positive effect of process supervision mechanisms on the stability of the step-wise generation process.

Effect of MCTS simulation iterations. Table 2 548 shows how different numbers of MCTS simula-549 tion iterations impact the agent performance of 550 our method on the HotpotQA dataset. The results 551 demonstrate a significant increase in accuracy from 552 32% to 39% as the number of simulations rises from 1 to 3. Increasing the simulations to 5 yields 554 a marginal improvement of 2% (from 39% to 41%). Beyond 5 simulations, the performance stabilizes at 42%. These findings suggest that the MCTS al-558 gorithm effectively identifies crucial path information within the first three simulations, and provides empirical evidence that a balance can be achieved between computational efficiency and model performance, as three simulations are adequate for 562

Table 2: Success rates (%) of our method with different number of MCTS iterations on the HotpotQA dataset.

No. of MCTS iterations	1	3	5	7	9
Accuracy	32	39	41	42	42

Table 3: Accuracy (%) of our method with various number of generated responses during rejection sampling.

No. of Responses	3	4	5	6	7	8
AlfWorld	38	40	41	42	42	43
WebShop	47	50	52	54	55	55

achieving near-optimal outcomes.

Effect of number of generated responses during rejection sampling. We evaluated the effect of the number of generated responses (n) during rejection sampling on the performance of our method observed on the AlfWorld and Webshop datasets. As illustrated in Table 3, there is a clear pattern of "diminishing marginal returns" associated with increasing n. For instance, in the AlfWorld tasks, performance levels off when n reaches 6, with a marginal improvement from 42% to 43%. Similarly, in WebShop tasks, the accuracy improved from 47% to 55% when n increased from 3 to 7, with no notable improvements beyond this point. This pattern indicates that while initial increases in the number of generated responses significantly enhance the diversity and quality of candidate responses, further increases eventually result in minimal gains as the selection mechanism driven by the reward model reaches stabilization.

# 5 Conclusion

This paper presents AgentPro, a novel framework designed to improve the reasoning and decisionmaking abilities of LLM agents through automated process supervision and rejection sampling. Our framework leverages Monte Carlo Tree Search to automatically generate step-level labels and train a process reward model, which greatly reduces error propagation in the responses generated by large language model agents and facilitates real-time quality assessment of these responses. Extensive experiments on four datasets demonstrate that our method significantly enhances the accuracy and robustness of LLM agents. This work provides a scalable solution to the challenges associated with manual process supervision in complex and practical realworld tasks, thereby broadening the applicability of LLM agents across various domains.

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# 6 Limitation

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In contrast to prompt-based methods, our method necessitates further training of large language models to develop the process reward model and en-604 hance the LLM agent. Specifically, we utilize 605 MCTS to generate labels for intermediate steps and 607 need to fine-tune all model parameters, which results in increased computational resource usage and extended training time. It is important to note that while our approach incurs higher training costs due to additional fine-tuning and inference of large lan-611 guage models, it remains significantly more cost-612 effective compared to manual process supervision 613 requiring human labeling. In the future, we aim to 614 explore more efficient training strategies, such as 615 parameter-efficient fine-tuning and distillation tech-616 niques, to minimize resource consumption during 617 the training process. 618

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# A Algorithm Details

The details of our method are formally delineated in Algorithms 1 and 2. Our framework functions across three distinct phases:

Phase 1: Automated Step Annotation via MCTS (Alg. 1, lines 1-24). For each query qk from the Query Set Q, an initial step-wise solution S is generated using the LLM agent Magent (line 4). Then, for each step si in S, we generate m MCTS simulations (lines 8-14) through path expansion. A step si is labeled positively (+) if any simulation path results in the correct final answer Acorrect (line 17). Otherwise a negative label (-) is assigned if no path concludes correctly (line 19). Then, the dataset Dprm is constructed (lines 22-23) for training the PRM.

• Phase 2: Process Reward Model Training (Alg. 1, lines 25-29). We conducted supervised, full-parameter fine-tuning of the model  $M_{\rm prm}$  across  $E_{\rm prm}$  epochs utilizing the annotated dataset  $D_{\rm prm}$ . This procedure enabled  $M_{\rm prm}$  to acquire precise, step-wise evaluative capabilities essential for the subsequent training in rejection sampling.

• Phase 3: LLM Agent Training via PRM-Guided Rejection Sampling (Alg. 2). In each round t, we generate n candidate paths from  $r_1$  to  $r_n$  for each query q using  $M_{\text{agent}}$  (line 8). Subsequently, we compute the reward score  $R_i$  for each *j*-th response  $r_i$  (lines 10-12) and select the response  $r_*$  with the highest reward score among all evaluated responses (line 15). The dataset  $\mathcal{D}_{rs}$  is then updated to include these responses (line 16), which facilitates the full-parameter fine-tuning of  $M_{\text{agent}}$  (lines 18-20). Over T iterations,  $M_{\text{agent}}$  incrementally optimizes its alignment with trajectories that yield high rewards, while  $M_{\rm prm}$  remains unchanged during the whole rejection sampling training process.

# **B** Implementation Details

# **B.1** Details of datasets

As illustrated in Table 4, our study utilized four datasets: FEVER, HotpotQA, ALFWorld, and WebShop. The FEVER dataset initially comprised of 145,000 training and 19,000 test samples, and we selected 30,000 training samples to train the process reward model and 9,999 test samples to evaluate the performance of LLM agents. For HotpotQA, we analyzed its performance using 100 validation tasks from the distractor dev split of the dataset, which is also used by Expel, ReAct and Reflexion in their studies. In the case of ALF-World, we utilized the same set of 134 solvable tasks previously used by Expel, ReAct and Reflexion. Likewise, the evaluation of the WebShop tasks involved the same 100 tasks as those used in prior studies by Expel, ReAct, and Reflexion. 859

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	Algorithm 1: MCTS-Based Automatic La-					
b	beling and PRM Training					
	Input: LLM agent $M_{agent}$ , PRM model					
	$M_{\rm prm}$ , Query set $Q$ , number of					
	MCTS simulations $m$ , PRM training					
	epochs $E_{prm}$					
	<b>Output:</b> Trained PRM model $M_{\rm prm}$					
	Phase 1: Auto-labeling with MCTS					
2	$D_{prm} \leftarrow \emptyset$					
	for each query $q_k \in Q$ do					
4	$S \leftarrow M_{\text{agent}}(\{q_k\})$					
5	$//S = \{s_1, s_2, s_3, \dots, s_K\}$					
6	for each step $s_i \in S$ do					
7	$correct_flag \leftarrow False$					
8	for $j = 1$ to $m$ do					
9	$\begin{bmatrix} p_j^i \leftarrow M_{\text{agent}}(\{q_k, s_1, \dots, s_i\}) \end{bmatrix}$					
10	<b>if</b> $A_{final}^{(j)} = A_{correct}$ then					
11	$ $ $ $ $correct_flag \leftarrow True$					
12	break					
13	end					
14	end					
15	if correct_flag then					
16	// Label $s_i$ as +					
17	$y_{s_i}^k \leftarrow +$					
18	else					
19	$      y_{s_i}^k \leftarrow -$					
20	end					
21	end					
22	$d_k =$					
	$(\{q_k, s_1^k, \dots, s_K^k\}, \{y_{s_1}^k, y_{s_2}^k, \dots, y_{s_K}^k\})$					
23	$\begin{bmatrix} (\{q_k, \sigma_1, \dots, \sigma_K\}, \{g_{s_1}, g_{s_2}, \dots, g_{s_K}\}) \\ D_{prm} \leftarrow D_{prm} \cup \{d_k\} \end{bmatrix}$					
	end					
20 27	Update $M_{\rm prm}$ via supervised					
	full-parameter fine-tuning on D <sub>mm</sub>					

full-parameter fine-tuning on  $D_{prm}$ 

# 28 end

29 return  $M_{prm}$ 

Dataset	<b>Training Set Size</b>	Training Samples Used	Test Set Size	Test Samples Used
FEVER	145,449	30,000	19,998	9,999
HotpotQA	90,443	30,000	7,405	100
ALFWorld	3,553	355	134	134
WebShop	10,587	1,000	500	100

Table 4: Training and Test Set sizes for each dataset, along with sampled data for training and evaluation.

As detailed in Sec. 4.3, to assess the efficacy of the trained process reward model (PRM), we divided the 30,000 FEVER and HotpotQA training samples into a reward training set (24,000 samples, 80%) and a reward test set (6,000 samples, 20%).

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## B.2 Computational and Storage Resources

All our experiments were conducted on a single machine with 1TB RAM and 256-core AMD EPYC 7742 64-Core Processor @ 3.4GHz CPU. We use the NVIDIA H100 GPU with 80GB memory. The software environment settings are: Python 3.9.21, PyTorch 2.5.1 with CUDA 12.4 on Ubuntu 22.04.4 LTS. Specifically, the computational experiments were conducted using two NVIDIA H100 GPUs with 80 GB of memory each. We utilized the Llama-3.1-8B-Instruct as the base model, which possesses a total of 8 billion parameters; each model checkpoint demanded 106 GB of disk space. To improve inference efficiency, we incorporated the vLLM framework (Kwon et al., 2023), which features optimized attention computation and enhanced memory management.

The time required for processing varies across different datasets. For example, each stage of the FEVER dataset's processing pipeline requires varying amounts of time. The generation of step-wise responses phase takes about 25 minutes and 33 seconds, focusing on generating responses in a stepby-step manner for each claim. Following that, Monte Carlo Tree Search (m=3) is a more computationally intensive process, lasting approximately 5 hours and 12 minutes to evaluate all generated steps. Next, training the process reward model for  $E_{prm} = 5$  epochs requires 11 hours and 25 minutes, during which the model learns to assign reward scores to step-by-step responses. For a single round of the rejection sampling process, where multiple responses are generated for each claim (n=4), the process takes 45 minutes and 15 seconds. Afterward, the reward scores for all generated responses are calculated, which takes 8 hours and 53 minutes because vllm cannot be used here to calculate the

probability of every generated token, therefore the original transformer library is applied here which is much more slower than vllm. Lastly, the model undergoes supervised fine-tuning, taking 2 hours and 26 minutes to further improve its performance based on labeled data. This entire pipeline sums up to around 33 hours and 34 minutes for completion.

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## **B.3** Hyperparameters

In our experiments, we use the vllm and the transformer library to generate step by step responses. The sampling process is controlled by a temperature of 0.9, which adjusts the randomness of the output, and a top-p value of 0.85 for nucleus sampling, determining the smallest set of tokens to consider based on cumulative probability. The model generates a maximum of 2048 tokens per output, with a repetition penalty of 1.0 to discourage repetitive phrases. Additionally, the tokenizer processes the text before it is passed to the model for generation and decodes the output back into human-readable text. All these parameters were conducted through grid search and the hyper-parameters with the best performance are selected as the final parameters. We generated three different responses for Monte Carlo Tree Search with seeds 0, 1 and 3407. For Rejection Sampling, we run five iterations, and for every iteration we generate four different responses with seeds 0, 3407, 314159, 271828, respectively.

The LLaMA-Factory library is used to fine-tune the large language models, including the process reward model and the LLM agent. In our experiments, the adopted fine-tuning approach involves full fine-tuning with the SFT (Supervised Fine-Tuning) stage. Training is conducted using Deep-Speed, which is well-suited for large-scale training environments and incorporates ZeRO-3 optimization. The maximum input sequence length is constrained to 2048 tokens. During training, the batch size per device is set to 1, and gradient accumulation is used over 2 steps to simulate a larger batch. The learning rate is set to 1.0e-5 with a cosine learning rate scheduler, a warmup ratio of 0.1, and Algorithm 2: LLM Agent Training Process

**Input:** LLM agent  $M_{\text{agent}}$ , PRM model  $M_{\rm prm}$ , Query set Q, number of candidate responses n, training iterations T, LLM Agent training epochs  $E_{rs}$ 

**Output:** Optimized LLM agent  $M_{agent}$ 

1 Phase 3: Rejection Sampling

I	r hase 5. Rejection Sampling
2	for round $t = 1$ to $T$ do
3	$D_{rs} \leftarrow \emptyset;$
4	for each query $q \in Q$ do
5	// Generate n candidate responses
6	for $j = 1$ to $n$ do
7	// $r_j = \{s_1, s_2, s_3, \dots, s_K\}$
8	$r_i \leftarrow M_{\text{agent}}(\{q\})$
9	// Generate labels and associated
	probabilities for every step of
	current response $r_j$
10	$\{(l_i, P_i)\}_{i=1}^K \leftarrow M_{\text{prm}}(r_j)$
11	// Calculate the reward score $R_j$
	for current response $r_j$
12	$R_{i} = \frac{1}{K} \sum_{i=1}^{K} (\mathbb{I}(l_{i} = +) \cdot P_{i})$
	$-\mathbb{I}(l_i = -) \cdot P_i)$
13	end
14	// Select the best response
15	$r_* = \arg\max_{r_i} R_j$
16	$D_{rs} \leftarrow D_{rs} \cup \{(q, r_*)\}$
17	end
18	for epoch $e = 1$ to $E_{rs}$ do
19	Update $M_{\text{agent}}$ via supervised
	full-parameter fine-tuning on $D_{rs}$
20	end
21	end
22	return M <sub>agent</sub>
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training will run for  $E_{rs} = 5$  epochs and T = 5iterations. Every epoch will train the model for 2250 steps. Mixed precision training with bf16 is enabled for efficiency. The training pipeline uses 16 workers for data preprocessing. For evaluation, 10% of the dataset is used for validation, with the batch size set to 1 for evaluation as well.

#### С License

Our implementation employs the LLaMA-3.1-8B-Instruct model (Dubey et al., 2024), a cutting-edge large language model tailored for a range of natural language processing (NLP) tasks, including question answering and text generation. This model is subject to the LLaMA 3.1 Community License

Agreement. Additionally, the LLaMA-Factory, which facilitates efficient training and deployment of large language models and is likely employed for fine-tuning LLaMA models, is governed by the Apache-2.0 license (Zheng et al., 2024). The vLLM framework, designed to optimize large language models for both training and inference with a focus on efficient memory usage and computational performance, adheres to the Apache-2.0 License (Kwon et al., 2023).

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Our implementation also utilizes the transformers library, a widely recognized open-source tool for NLP that offers easily accessible pre-trained models for various tasks such as text classification, question answering, and translation. This library, supporting multiple architectures including BERT, GPT, and T5, is governed by the Apache-2.0 License (Wolf et al., 2020).

Regarding datasets, the FEVER dataset (Thorne et al., 2018), utilized for fact verification where models determine the veracity of claims against provided texts, is licensed under the Apache-2.0 License. The HotpotOA dataset (Yang et al., 2018), used for multi-hop question answering that requires synthesizing information from multiple documents, operates under the Apache-2.0 License. The ALF-World dataset (Shridhar et al., 2020), designed for training agents in virtual environments through natural language for interactive task-oriented dialogue and situated learning, is available under the MIT License. Lastly, the WebShop dataset (Yao et al., 2022a), aimed at developing conversational agents for e-commerce applications where users interact with a shopping assistant, is also available under the MIT License.

#### **Experiment Details and Discussion** D

Table 5 presents the detailed numerical values of all the datasets depicted in Fig. 3, serving as a reference for further analysis and comparison.

The ablation studies discussed in Section 4.5 1007 conclusively show that our method ensures robust 1008 hyperparameter selection and exhibits distinct convergence behaviors during critical processes like 1010 MCTS simulations and rejection sampling. These 1011 findings affirm the effectiveness of our method in 1012 reducing the need for manual adjustments of hy-1013 perparameters, while the automated process supervision framework improves the model's resilience 1015 to parameter fluctuations by optimizing explicit 1016 reasoning paths. Importantly, these experimen-1017

Method	FEVER	HotpotQA	ALFWorld	WebShop
Act	$59.89{\pm}0.08$	$21.67 \pm 1.25$	$19.15 {\pm} 0.93$	$27.00 \pm 1.63$
ReAct	$60.92 {\pm} 0.83$	$24.00{\pm}1.63$	$24.62{\pm}2.20$	$28.33 {\pm} 2.49$
Reflexion	$60.69 {\pm} 1.00$	$27.33{\pm}1.25$	$34.08{\pm}0.93$	$40.67 {\pm} 2.49$
ExpeL	$61.80{\pm}0.73$	$33.67 {\pm} 0.94$	$30.34{\pm}2.46$	$38.00{\pm}1.41$
AgentPro	65.39±0.09	39.33±1.25	40.88±1.22	52.67±1.70

Table 5: The specific numerical results from the experiments shown in Fig. 3.

1018tal results offer practical implications for deploy-1019ment: users can efficiently manage computational1020resources by moderately decreasing the number of1021MCTS simulations and rejection sampling itera-1022tions without compromising performance.

# E Prompt Templates

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# E.1 Prompt for generating step by step responses

For the FEVER dataset, we employed the prompt illustrated in Fig. 6 to guide the LLM agent in generating detailed, step-by-step responses to the corresponding claims. Similarly, for the HotpotQA dataset, we used the prompt shown in Fig. 7 to direct the agent toward producing step-wise responses to the questions. For both the AlfWorld and WebShop datasets, we applied the prompts from the ReAct dataset to generate step-by-step, action-based outputs from the LLM agent.

# E.2 Prompt for MCTS

Fig. 8 presents the prompt used for labeling each step in the Monte Carlo Tree Search. This prompt contains the original trajectories before the current step that awaits labeling.

# E.3 Prompt for process reward model

Fig. 9 shows the prompt employed to train the process reward model. This prompt annotates each step in the responses generated by the LLM agent, assigning a single binary label (+ or -) to each step.

# F Case Study

In this section, we present a detailed case study on the FEVER dataset to illustrate the entire process of our AgentPro framework. This includes generating step-by-step answers, utilizing Monte Carlo Tree Search to train the process reward model, and employing the rejection sampling strategy to train our LLM agent. This comprehensive demonstration aims to provide a clear and efficient understanding of our framework. First of all, we need to generate step-by-step responses for a given claim by our pre-trained LLM agent. Take the claim "The 84th Academy Awards' winners included Beginners" as an example, Fig. 10 illustrates how our LLM agent  $M_{agent}$  generates a step-by-step solution for the claim: the agent analyzes the claim, verifies the ceremony year (2012), checks the film's eligibility (2011 release), and finally confirms its award (Best Supporting Actor).

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Next, we need to use Monte Carlo Tree Search to label each step generated in Fig. 10, in order to create the training set required for training the process reward model. Fig. 11 showcases three MCTS simulations, with each simulation exploring alternative reasoning paths:

- **Response 1** correctly identifies *Beginners*' Best Supporting Actor and gives the **SUP-PORTS** conclusion.
- **Response 2** erroneously attributes a Best Original Screenplay win but still reaches a **SUP-PORTS** conclusion.
- **Response 3** mistakenly assumes that "Beginners" was solely a Best Picture nominee, which results in the conclusion of **NOT ENOUGH INFO**.

We employ the same pre-trained LLM agent as in Fig. 10 to generate all three responses. Given that the correct response to the claim is **SUP-PORTS**, and 2 out of the 3 responses arrived at this conclusion, our method consequently autoannotates this step (Step 2) as correct (+).

After labeling all four steps in Fig. 10 via MCTS, we generated a sample based on the claim for training the process reward model, as illustrated in Fig. 12. Notably, all steps in the original response (as shown in Fig. 10) received a positive label, demonstrating the effectiveness of our LLM agent in step by step reasoning on this claim. We will use the method described from Fig. 10 to Fig. 12 to generate training samples for the process reward model.

After training the process reward model, we can 1096 then employ the Rejection Sampling strategy to 1097 train our LLM agent. For instance, consider the 1098 claim "A&E is a channel from the United States" 1099 in the FEVER dataset. Initially, our LLM agent 1100 is tasked with generating multiple, step by step re-1101 sponses based on this claim, using the prompt as 1102 depicted in Fig. 13 with Wikipedia background 1103 information. Figures 14 and 15 present four candi-1104 date responses, among which three conclude with 1105 SUPPORTS and one with NOT ENOUGH INFO. 1106

Subsequently, the trained PRM evaluates the 1107 four candidate responses and selects the one with 1108 the highest average probability as the sample to 1109 fine-tune our LLM agent. As depicted in Fig. 16, 1110 the PRM assigns labels to each step of the re-1111 sponses and calculates the associated probabilities. 1112 A higher probability signifies higher confidence 1113 in the correctness of that label. We then negate 1114 those probabilities associated with negatively la-1115 beled steps to reflect our disinclination towards 1116 incorrect steps and calculate the average of all the 1117 probabilities across the steps. This average prob-1118 ability quantifies the likelihood of each candidate 1119 response being correct, which is essentially the re-1120 ward value of PRM. Finally, the response with the 1121 highest average probability, in this case, the second 1122 response, is selected as the training sample for fur-1123 ther supervised fine-tuning of our LLM agent. This 1124 method is consistently applied to each sample in 1125 the training set during rejection sampling. 1126

> The procedure shown from Figures 13 to 16 is repeated through multiple rounds until the agent can reliably generate high-quality responses appropriate to the current dataset.

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Prompt for generating step by step responses (FEVER)
You are an assistant tasked with analyzing claims and determining their validity. Your goal is to evaluate whether a given Claim is SUPPORTS, REFUTES, or if there is NOT ENOUGH INFO.
Follow these guidelines strictly:
1. Carefully analyze the information provided in the Claim.
2. Think step by step and provide reasoning for your conclusion.
3. At the end of your analysis, choose one of the following outcomes:
- SUPPORTS
- REFUTES
- NOT ENOUGH INFO
The final result must follow this format:
Step 1: [Solution process for Step 1].
Step 2: [Solution process for Step 2].
"The final answer is: [SUPPORTS/REFUTES/NOT ENOUGH INF0]
Claim: The 84th Academy Awards' winners included Beginners.
Evaluate the claim step by step and determine its validity.
Your response must end with:
"The final answer is: [SUPPORTS/REFUTES/NOT ENOUGH INFO]"

Figure 6: Example prompt for generating step-by-step responses on the FEVER dataset.

# Prompt for generating step by step responses (HotpotQA)

Solve a question answering task with steps. Please think step by step to determine the answer to the question. Question: [Insert your question here]. Step 1:[Provide the solution process for Step 1]. Step 2:[Provide the solution process for Step 2]. Step 3:[Provide the solution process for Step 3]. The final answer is: [Provide the final answer]. Based on the example above, solve the following question step by step. The number of steps to solve the problem is not limited. Your response to me must end with: The final answer is: [Provide the final answer] Question: What nationality were the Tag team wrestlers the Haas Brothers?

Figure 7: Example prompt for generating step-by-step responses on the HotpotQA dataset.

# **Prompt for MCTS**

You are an assistant tasked with analyzing question and determining their validity. Your goal is to evaluate whether a given claim is SUPPORTS, REFUTES, or if there is NOT ENOUGH TNFO. Follow these guidelines strictly: 1. Carefully analyze the information provided in the Claim. 2. Think step by step and provide reasoning for your conclusion. 3. At the end of your analysis, choose one of the following outcomes: - SUPPORTS - REFUTES - NOT ENOUGH INFO The final result must follow this format: Step 1: [Solution process for Step 1]. Step 2: [Solution process for Step 2]. . . . The final answer is: [SUPPORTS/REFUTES/NOT ENOUGH INFO] Continue generating the steps for the claim in a step-by-step manner. Each response must contain only the solution steps and, when available, the final answer in the specified format. The final answer should be given as: 'The final answer is: [SUPPORTS/REFUTES/NOT ENOUGH INFO]'. No other explanations or symbols are allowed. If the final answer has already been reached, output the final answer directly in the specified format. Claim: The 84th Academy Awards' winners included Beginners.

Figure 8: Example prompt for MCTS.

## Prompt for process reward model

Label each step: if a step contributes to deriving the correct result, mark it as '+'. If a step hinders the derivation of the correct result, mark it as '-'. Claim: The 84th Academy Awards' winners included Beginners. Step 1: Analyze the Claim: The Claim states that the 84th Academy Awards' winners included "Beginners." This implies that "Beginners" is a film that won at least one category at the 84th Academy Awards. Step 2: Recall the year the 84th Academy Awards took place. The 84th Academy Awards ceremony was held in 2012. Step 3: Check if "Beginners" is a film released in 2011, which would make it eligible for the 84th Academy Awards. After verifying, it is confirmed that "Beginners" is a 2011 film directed by Mike Mills. Step 4: Verify if "Beginners" won any awards at the 84th Academy Awards. Upon reviewing the list of winners, it is confirmed that "Beginners" indeed won the award for Best Supporting Actor for Christopher Plummer's performance. The final answer is: SUPPORTS

Figure 9: Example prompt for training the process reward model.

# Trajectory for generating a step by step response

Claim: The 84th Academy Awards' winners included Beginners.

## Response:

**Step 1:** Analyze the Claim: The Claim states that the 84th Academy Awards' winners included "Beginners." This implies that "Beginners" is a film that won at least one category at the 84th Academy Awards.

**Step 2:** Recall the year the 84th Academy Awards took place. The 84th Academy Awards ceremony was held in 2012.

**Step 3:** Check if "Beginners" is a film released in 2011, which would make it eligible for the 84th Academy Awards. After verifying, it is confirmed that "Beginners" is a 2011 film directed by Mike Mills.

Step 4: Verify if "Beginners" won any awards at the 84th Academy Awards. Upon reviewing the list of winners, it is confirmed that "Beginners" indeed won the award for Best Supporting Actor for Christopher Plummer's performance.

The final answer is: SUPPORTS

Figure 10: Trajectory for generating a step-by-step response on a claim in the FEVER dataset.

# **Trajectory for MCTS**

## Claim and Step 1&2:

The 84th Academy Awards' winners included Beginners.

**Step 1:** Analyze the Claim: The Claim states that the 84th Academy Awards' winners included "Beginners." This implies that "Beginners" is a film that won at least one category at the 84th Academy Awards.

**Step 2:** Recall the year the 84th Academy Awards took place. The 84th Academy Awards ceremony was held in 2012.

## First Response:

Step 3: Determine the nominees and winners of the 84th Academy Awards to verify if
"Beginners" won in any category. The 84th Academy Awards took place in 2012, and "The
Artist" won the award for Best Picture, Best Director, and several other categories.
Step 4: Verify if "Beginners" won any awards at the 84th Academy Awards. "The Artist"
received the award for Best Picture, but "Beginners" received a win for Best Supporting
Actor for Christopher Plummer.

**Step 5:** Since "Beginners" won a category at the 84th Academy Awards, we can conclude that the claim is accurate.

The final answer is: SUPPORTS

## Second Response:

Screenplay.

Step 3: Identify major films from 2011, the year before the 84th Academy Awards.
"Beginners" is a film released in 2011 and received critical acclaim.
Step 4: Check the 84th Academy Awards winners. The 84th Academy Awards took place in 2012
and recognized the best in film for 2011. "Beginners" won the award for Best Original

Step 5: Determine if the claim is supported by the information. The claim that
"Beginners" is a film that won at least one category at the 84th Academy Awards is
supported by the fact that it won the award for Best Original Screenplay.
The final answer is: SUPPORTS

## Third Response:

Step 3: Research the winners of the 84th Academy Awards. According to my knowledge, the
84th Academy Awards, held in 2012, had a number of winners but most notable were "The
Artist" as the Best Picture and Michel Hazanavicius for Best Director.
Step 4: Look up the nominees for Best Picture to confirm if "Beginners" was among them.
"Beginners" was indeed a nominee for Best Picture at the 84th Academy Awards but not the
actual winner.

The final answer is: NOT ENOUGH INFO

Figure 11: Trajectory for MCTS simulation on the same claim in Fig. 10 with m = 3 simulations.

Generated sample for training the process reward model
Label each step: if a step contributes to deriving the correct result, mark it as '+'. If
a step hinders the derivation of the correct result, mark it as '-'.
Claim: The 84th Academy Awards' winners included Beginners.
Step 1: Analyze the Claim: The Claim states that the 84th Academy Awards' winners
included "Beginners." This implies that "Beginners" is a film that won at least one
category at the 84th Academy Awards.
Step 2: Recall the year the 84th Academy Awards took place. The 84th Academy Awards
ceremony was held in 2012.
Step 3: Check if "Beginners" is a film released in 2011, which would make it eligible for
the 84th Academy Awards. After verifying, it is confirmed that "Beginners" is a 2011 film
directed by Mike Mills.
Step 4: Verify if "Beginners" won any awards at the 84th Academy Awards. Upon reviewing
the list of winners, it is confirmed that "Beginners" indeed won the award for Best
Supporting Actor for Christopher Plummer's performance.
The final answer is: SUPPORTS
Output:
Step 1: +
Step 2: +
Step 3: +
Step 4: +

Figure 12: Generated sample for training the process reward model for the claim in Fig. 10.

## Prompt for rejection sampling

You are an assistant tasked with analyzing claims and determining their validity. Your goal is to evaluate whether a given Claim is SUPPORTS, REFUTES, or if there is NOT ENOUGH INFO. Follow these guidelines strictly: 1. Carefully analyze the information provided in the Claim. 2. Think step by step and provide reasoning for your conclusion. 3. At the end of your analysis, choose one of the following outcomes: - SUPPORTS - REFUTES - NOT ENOUGH INFO The final result must follow this format: Step 1: [Solution process for Step 1]. Step 2: [Solution process for Step 2]. The final answer is: [SUPPORTS/REFUTES/NOT ENOUGH INFO] Claim: A&E is a channel from the United States. Background Information about the Claim: The information about A&E is as follows: A or a is the first letter and the first vowel letter of the Latin alphabet, used in the modern English alphabet, and others worldwide. Its name in English is a (pronounced /\u02c8e\u026a/ AY), plural aes. It is similar in shape to the Ancient Greek letter alpha, from which it derives. The uppercase version consists of the two slanting sides of a triangle, crossed in the middle by a horizontal bar. The lowercase version is often written in one of two forms: the double-storey |a| and single-storey |\u0251|. The latter is commonly used in handwriting and fonts based on it, especially fonts intended to be read by children, and is also found in italic type..\n\nThe information about United States is as follows:\nThe United States of America (USA), commonly known as the United States (U.S.) or America, is a country primarily located in North America. It is a federal union of 50 states and a federal capital district, Washington, D.C. The 48 contiguous states border Canada to the north and Mexico to the south, with the State of Alaska in the northwest and the archipelagic State of Hawaii in the Pacific Ocean. The United States also asserts sovereignty over five major island territories and various uninhabited islands. The country has the world's third-largest land area, second-largest exclusive economic zone, and third-largest population, exceeding 340 million. Its three largest metropolitan areas are New York, Los Angeles, and Chicago, and its three most populous states are California, Texas, and Florida. Paleo-Indians migrated across the Bering land bridge more than 12,000 years ago, and formed various civilizations and societies. Evaluate the claim step by step and determine its validity. Your response must end with: The final answer is: [SUPPORTS/REFUTES/NOT ENOUGH INFO]

Figure 13: Example prompt for the claim "A&E is a channel from the United States" during rejection sampling, where Wikipedia information is appended as background information.

## Trajectory for rejection sampling (1th&2th response)

## First response:

Step 1: Determine the relevance of the provided information to the claim. The provided information about A&E and the United States seems unrelated at first glance, as one pertains to the Latin alphabet and the other is about a country. However, looking closely, "A&E" can refer to "Arts & Entertainment," a global cable and satellite television network. This network is often associated with the United States.

**Step 2:** Check if "A&E" refers to a television network that originated or is headquartered in the United States. From general knowledge, A&E (Arts & Entertainment) is a well-known cable television network in the United States. While it has global presence, its origins and a significant portion of its content are tailored to the American audience, making it a US-centric channel.

**Step 3:** Analyze the definition of A&E in relation to its original context of the claim. Since the provided background information about A&E does not directly mention its association with television, it is unclear whether the claim refers to the original Latin letter or the television network. However, the lack of any information suggesting an alternative meaning of A&E in the context of the United States makes it more plausible that the claim refers to the television network, which is indeed based in the United States.

**Step 4:** Determine the validity of the claim. Considering the information about A&E as a television network, the claim that A&E is a channel from the United States is true. A&E (Arts & Entertainment) is indeed a television channel that originated in the United States.

The final answer is: SUPPORTS

## Second response:

Step 1: Analyze the Claim: The claim is that A&E is a channel from the United States. The
key components of the claim are "A&E" and "United States."

**Step 2:** Identify relevant information from the background: We have information about A&E, which describes it as an English alphabet letter, but it also mentions the word "A&E," which could refer to several things. We also have extensive information about the United States, describing its geography, population, and other characteristics.

Step 3: Consider the context of the acronym A&E: The provided background information
about the letter "A" and "E" in the Latin alphabet does not directly relate to the
context of a TV channel. However, A&E is indeed an acronym that can be expanded to mean
"Arts and Entertainment." A search of the internet would show that A&E is an American pay
television network that airs content related to documentary, drama, and reality TV.
Step 4: Connect the information to the claim: Since A&E refers to the Arts and

Entertainment network, which is indeed based in the United States, this would support the claim that A&E is a channel from the United States.

Step 5: Evaluate the information for consistency and reliability: Based on external
knowledge, the information is consistent and reliable.

The final answer is: SUPPORTS

Figure 14: Generated responses for the claim "A&E is a channel from the United States" during rejection sampling (1th&2th response).

# Trajectory for rejection sampling (3th&4th response)

### Third response:

**Step 1:** Identify the components of the claim. The claim is about A&E being a channel from the United States. The two main components are A&E (a channel) and the United States (a country).

**Step 2:** Analyze the information provided about A&E in the background. The given text about A&E discusses its origin, pronunciation, shape, and usage in different fonts, but does not mention its location or origin country.

**Step 3:** Analyze the information provided about the United States in the background. The given text about the United States describes its geographical location, size, population, and history, but does not mention any TV channels or media networks by name.

Step 4: Determine the relevance of the information. The text about A&E does not mention
its location or affiliation, while the text about the United States does not mention any
media networks. There is no direct information linking A&E to the United States.
Step 5: Draw a conclusion. Since there is no direct information in the provided
background that links A&E to the United States, the claim is unsubstantiated by the given
information.

The final answer is: NOT ENOUGH INFO

## Fourth response:

Step 1: Analyze the claim "A&E is a channel from the United States." The claim is about a
media channel named A&E, not the letter 'a'. Therefore, this claim is unrelated to the
background information about the letter 'a' provided in the background information.
Step 2: Look for information about A&E in the background information. There is no mention
of A&E in the background information.

**Step 3:** Search for external information about A&E. From external knowledge, A&E is known to be a channel that is a joint venture between Hearst Communications and Disney-ABC Television Group. A&E stands for Arts and Entertainment. A&E networks is a US-based American cable television network.

**Step 4:** Determine the origin of A&E based on the external information. Given the external information that A&E is a joint venture between US-based companies, it is plausible that A&E has its origins in the United States.

The final answer is: SUPPORTS

Figure 15: Generated responses for the claim "A&E is a channel from the United States" during rejection sampling (3th&4th response).

rajectory for rejection sampling (scoring)				
First respo	nse:	Second response:		
	Probability:		Probability:	
Step 1: -	0.8839759230613708	<b>Step 1:</b> +	0.9885740280151367	
Step 2: +	0.9774795174598694	Step 2: -	0.958041250705719	
Step 3: +	0.9435433745384216	Step 3: +	0.9999788999557495	
Step 4: +	0.9968554973602295	Step 4: +	0.9999936819076538	
		Step 5: +	0.9998918771743774	
Average Probability: 0.5085		Average Probability: 0.6061 🗸		
Third respo	nse:	Fourth response:		
	Probability:		Probability:	
Step 1: -	0.9888468384742737	Step 1: -	0.9190813302993774	
Step 2: -	0.9226863980293274	Step 2: -	0.9998040795326233	
Step 3: -	0.8883765935897827	Step 3: +	0.9996646642684937	
Step 4: -	0.9999895095825195	Step 4: +	0.9998919963836674	
Step 5: -	0.9771665334701538			
Average Prol	bability: -0.9552	Average Pro	bability: 0.0202	

Figure 16: The scoring process of the process reward model for the four responses shown in Fig. 14 and Fig. 15. The response with the highest average probability (the second response) is selected as the training sample for subsequent supervised fine-tuning.