Entropy-Regularized Process Reward Model

Abstract

Large language models (LLMs) have shown promise in performing complex multi-step reasoning, yet they continue to struggle with mathematical reasoning, often making systematic errors. A promising solution is reinforcement learning (RL) guided by reward models, particularly those focusing on process rewards, which score each intermediate step rather than solely evaluating the final outcome. This approach is more effective at guiding policy models towards correct reasoning trajectories. However, traditional process reward models diverge from typical RL practices and can limit model generalization. In this work, we propose an entropy-regularized process reward model (ER-PRM) that addresses these limitations by integrating KL-regularized Markov Decision Processes (MDP) to balance policy optimization with the need to prevent the policy from shifting too far from its initial distribution. We derive a novel reward construction method and introduce an automatic labeling mechanism based on the theoretical results. Our experiments on the MATH and GSM8K benchmarks demonstrate that ER-PRM consistently outperforms existing process reward models, achieving 1% improvement on GSM8K and 2-3% improvement on MATH under best-of-N evaluation. These results highlight the efficacy of entropy-regularization in enhancing LLMs' reasoning capabilities.

1 Introduction

Large language models (LLMs) have demonstrated remarkable performance across numerous tasks, particularly in the challenging area of mathematical reasoning (OpenAI et al., 2024; Yang et al., 2024; Dubey et al., 2024). A key factor behind these successes is the use of synthetic data, as explored in works such as Meta-MathQA (Yu et al., 2023), MAmmoTH (Yue et al., 2023), and Open-MathInstruct (Toshniwal et al., 2024b). Open-source models fine-tuned on these synthetic datasets have shown significant improvements in test accuracy on standard mathematical reasoning benchmarks such as MATH (Hendrycks et al., 2021) and GSM8K (Cobbe et al., 2021). Following supervised fine-tuning, reinforcement learning (RL) has received considerable attention as a technique for further improving models' reasoning abilities by aligning the model's behavior with human values and goals, especially after the release of OpenAI-o1 model[1].

The RL methods used in the current literature on LLM reasoning can be broadly categorized into two approaches. The first category focuses on training-time alignment, where RL is used to fine-tune the model to maximize an RL metric evaluated by a reward model. Examples include PPO (Schulman et al., 2017), GRPO (Shao et al., 2024). More recently, scaling inference-time computation has also been shown to enhance model performance by using reward models to guide LLM decoding. Techniques such as best-of-n sampling (Dong et al., 2023) and Monte Carlo tree search (MCTS) (Xie et al., 2024) are representative examples of this approach. All these methods require an external reward model to provide a reward signal to update the model parameters or rank the candidate responses. Regardless of the specific RL method, the quality of the reward function remains the most crucial factor, as it sets the upper bound for the algorithm's performance.

One distinct feature of complex mathematical reasoning is that models typically require multiple steps of reasoning before producing the final answer (Wei et al., 2023). Accordingly, there are generally two types of reward models in the mathematical domain: the outcome reward model (ORM) and the process reward model (PRM). ORM provides an overall score for the quality of the final

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[1] https://openai.com/index/introducing-openai-o1-preview/

Figure 1: Illustration of ER-PRM, along with other baseline methods to construct the process reward data and outcome reward data. The key idea of ER-PRM is to calculate the process reward from the sampling trajectories under entropy-regularization.

answer, while PRM assigns a score to each step in the reasoning process, providing more fine-grained feedback. Existing works (Wang et al., 2024; Lightman et al., 2023) show that PRM outperforms ORM by a considerable margin. For instance, in Lightman et al. (2023), if we use the PRM to select the final output from the candidate responses, we can achieve a test accuracy of 78.2%, as compared to the ORM with 72.4% and majority voting of 69.6%. Furthermore, PRM is more interpretable because it mirrors human behavior when evaluating reasoning paths. The PRM model is able to guide the policy model's decoding at each individual step or rerank candidate answers to enhance accuracy and consistency during generation.

Inspired by the superior performance of PRM, researchers have spent great efforts recently in the training of PRM. To get the process annotation for the PRM, one can ask humans to label the data at each step (Lightman et al., 2023), which is extremely expensive and inefficient. Since then, researchers have explored alternative labeling techniques. One representative example is the automatic labeling technique introduced by Math-Shepherd (Wang et al., 2024). The main idea of Math-Shepherd is to interpret the score of each step as its potential to deduce the correct final answer. Then, we can sample multiple trajectories starting from the intermediate step, and use the ratio of correct trajectories as a proxy for this score. The Math-Shepherd has proved as an effective way to generate high-quality process reward scores and even outperform human-labeled data.

Despite its effectiveness, Math-Shepherd considers a traditional Markov Decision Process (MDP)

framework, which differs from the typical RL practice used with LLMs. Since the introduction of reinforcement learning from human feedback (RLHF), the standard approach has been using a entropy-regularized reward relative to a reference model (often the initial model) (Ouyang et al., 2022; Bai et al., 2022). This also applies to RL in reasoning tasks where we formulate the problem as a entropy-regularized MDP (Shao et al., 2024; Xiong et al., 2024b; Zhong et al., 2024). The main goal here is to balance optimizing the reward and staying close to the original policy, which is crucial because we start with a well-trained LLM, and we do not want the model to deviate too far from this initial strong foundation policy. In recognition of this gap, in this paper, we formulate the multi-step mathematical reasoning task under the entropy-regularized MDP framework, derive the mathematical principles of the process reward construction, and propose practical algorithms. Our contributions are summarized as follows.

- We propose the entropy-regularized process reward, a novel method for labeling the process reward score with entropy regularization.
- Based on the labeled data, we train a new process reward model to improve the performance.
- On the MATH and GSM8K datasets, we achieve significant improvements using the best-of-N evaluation method. Furthermore, by employing the reward model with rejection sampling, we observe a substantial enhancement in the performance of the policy model.
- To further boost the process reward model research, we will release all the data, code, and checkpoints to the community.

2   Related Work

Mathematical Reasoning and Synthetic Data Generation.   Mathematical problem solving has become an important research area for assessing the LLMs' reasoning ability. A line of works proposes to prompt LLMs to solve the complex reasoning task in a step-by-step manner, known as the Chain-of-Thought (CoT) prompting (Wei et al., 2023; Zhou et al., 2022; Zhu et al., 2022; Tong et al., 2024), which has been a standard practice in reasoning task. Despite this, general chatbots still struggle with solving mathematical problems using natural language reasoning, as evidenced by standard benchmarks (Cobbe et al., 2021; Hendrycks et al., 2021). To address this, numerous works have proposed generating synthetic data and fine-tuning LLMs on these datasets to improve their reasoning abilities. Representative examples include Meta-MathQA (Yu et al., 2023), MAmmoTH (Yue et al., 2023), MMIQC (Liu and Yao, 2024), ToRA (Gou et al., 2023), Open-MathInstruct (Toshniwal et al., 2024b), and Dart-Math (Tong et al., 2024). These works use teacher models (e.g., ChatGPT) to generate multiple responses per problem and filter incorrect or low-quality responses using ground-truth answers, preserving only the correct ones. This process is also referred to as rejection sampling or best-of-n sampling in the literature (Dong et al., 2023; Yuan et al., 2023). Notably, all these datasets are generated through step-by-step reasoning, emphasizing the importance of stepwise thinking for reasoning tasks.

Applying RL to Mathematical Reasoning.   Inspired by the tremendous successes of RL in making general chatbot such as Chat-GPT and Claude, researchers have started applying RL to mathematical reasoning tasks. One line of work applies deep RL methods such as PPO (Schulman et al., 2017) and GRPO (Shao et al., 2024) to optimize external reward signals (described later). Another approach adapts direct preference learning algorithms for mathematical problem solving. For example, Jiao et al. (2024); Yuan et al. (2024) apply DPO and KTO algorithms to reasoning tasks. Furthermore, Xie et al. (2024); Xiong et al. (2024b); Pang et al. (2024) adapt online iterative DPO, originally developed for chat tasks (Xiong et al., 2024a; Xu et al., 2023), to achieve improved performance for CoT reasoning. Recently, inference-time RL methods have also attracted significant attention, particularly following the release of OpenAI-o1 model.

These methods utilize external reward models to guide model decoding or to select the best answer among multiple candidate responses. Notable examples include best-of-n sampling (Dong et al., 2023; Lightman et al., 2023) and Monte Carlo Tree Search (MCTS) (Xie et al., 2024; Chen et al., 2024a; Lai et al., 2024). As these methods typically require generating multiple responses during inference, they have also inspired the passion of scaling the inference compute.

In particular, we notice that all the deep RL method, online iterative direct preference learning algorithms, and inference-time RL methods like BoN sampling and MCTS require a reward model in their algorithm framework, thus can benefit from our study.

Reward Modeling in Mathematical Reasoning. Due to the presence of the ground-truth answer, the reward model in mathematical reasoning is not trained in a pairwise comparison way in the application of RLHF (Bai et al., 2022; Ouyang et al., 2022; Dong et al., 2024). Generally, reward models for mathematical reasoning can be broadly categorized into Outcome Reward Models (ORM) and Process Supervision Reward Models (PRM). ORM provides a response-level score to evaluate the overall quality of a response, whereas PRM assigns scores to individual steps in the reasoning process, offering more fine-grained feedback. The promising results (as mentioned in the introduction) in Lightman et al. (2023) has sparked the passions across a wide range of community to study the construction of PRMs. However, training PRMs requires stepwise human annotation, which is often infeasible for open-source communities. To address this, Math-Shepherd (Wang et al., 2024) introduced a novel method that efficiently acquires process reward labels. This approach generates multiple potential completions in parallel until the final answer is reached. Then, we can use the ratio of trajectories with correct final answer to evaluate the correctness of current step. Following this work, several studies have leveraged process supervision and MCTS to enhance RLHF pipelines, including stepwise DPO with MCTS (Chen et al., 2024b), an automated MCTS-based PRM framework (Luo et al., 2024), MCTS Self-Refine (Zhang et al., 2024), and process generation based solely on the final answer (Chen et al., 2024a). These studies have greatly improved the efficiency of process supervision, inspiring us to use automatic labeling

to ensure obtaining high-quality process supervision data.

3 Approach

In this section, we present a novel reward formulation from an entropy perspective that utilizes KL-Regularization to smooth out the reward calculation of PRM, which we refer to as Entropy-Regularized PRM (ER-PRM). This formulation is followed by the derivation of obtaining the optimal policy model through RLHF using our entropy-regulated process reward calculation approach. Subsequently, we compare our approach with Wang et al. (2024); Luo et al. (2024) and then demonstrate that our methodology is more robust than those proposed aggregation-based reward calculation due to their dependency on initial policy model.

3.1 Task Formulation and Optimal Policy

We consider training an LLM for reasoning. Given prompt x, the LLM produces L-step reasoning chain $a = [a^1, \ldots, a^L]$. The reward $r(a, x)$ indicates whether the result of the reasoning chain is correct or not. We want to find LLM, denoted by a policy $\pi_*(a|x)$, that optimizes $\pi \in \Pi$ with the KL-regularized loss function

$$\mathcal{L}(\pi) = -\mathbb{E}_x \mathbb{E}_{a \sim \pi(\cdot|x)} \left[r(a, x) - \frac{1}{\eta} \ln \frac{\pi(a|x)}{\pi_0(a|x)} \right]$$

where π_0 is the initial policy model, a pretrained LLM, and π is the model being fine-tuned. According to Lemma 1, the minimizer for $\mathcal{L}$ is

$$\pi_*(a|x) = \frac{\pi_0(a|x)e^{\eta r(a,x)}}{\mathbb{E}_{a \sim \pi_0}e^{\eta r(a,x)}} \propto \pi_0(a|x)e^{\eta r(a,x)}.$$

3.2 Multi-step Reasoning

Let $a^{[l]} = [a^1, \ldots, a^l]$, be partial reasoning up to step l, and $a^{-[l]} = [a^{l+1}, \ldots, a^L]$ be the completion of the partial reasoning from step $l + 1$. We define the intermediate reward by $e^{\eta r(a^{[l]}, x)} = \mathbb{E}_{a^{-[l]} \sim \pi_0} e^{\eta r(a,x)}$. Thus, we have

$$\pi_*(a^{-[l]}|x, a^{[l]}) = \frac{\pi_0(a^{-[l]}|x, a^{[l]})e^{\eta r(a,x)}}{\mathbb{E}_{a^{-[l]} \sim \pi_0(\cdot|x, a^{[l]})}e^{\eta r(a,x)}},$$

and we obtain

$$\pi_*(a^{[l]}|x) = \frac{\pi_0(a^{[l]}|x)e^{\eta r(a^{[l]}, x)}}{\mathbb{E}_{a^{[l]} \sim \pi_0}e^{\eta r(a^{[l]}, x)}}.$$

$$r(a^{[l]}, x) = \frac{1}{\eta} \ln \mathbb{E}_{a^{-[l]} \sim \pi_0} e^{\eta r(a,x)}. \quad (1)$$

The partial reward according to this formula is our definition of entropy regularized process reward. We can optimize partial reasoning step $\pi(a^{[l]}|x)$ using this process reward.

An important property of this formulation is that our process reward model can be computed by using the reference policy π_0 to generate the completion. In comparison, in traditional RL, the reward depends on the optimal policy that generates the completion. Therefore in the traditional RL, one has to learn reward and policy simultaneously. This is not necessary in our entropy-based approach. As one can see, equation 1 employs soft optimism over paths generated by the reference policy. More generally, the reward can be computed using any policy including the optimal policy. In this case, the equivalent formula becomes

$$r(a^{[l]}, x) = -\frac{1}{\eta} \ln \mathbb{E}_{a^{-[l]} \sim \pi_*} e^{-\eta r(a,x)}, \quad (2)$$

where we have used the following fact to express equation 1 using π_*:

$$\pi_0(a^{-[l]}|x, a^{[l]}) = \frac{\pi_*(a^{-[l]}|x, a^{[l]})e^{-\eta r(a,x)}}{\mathbb{E}_{a^{-[l]} \sim \pi_*}e^{-\eta r(a,x)}}.$$

Intuitively, equation 2 implements soft pessimism over paths generated by the optimal policy. It can be shown that the reward of this model is equivalent to the reward computed using the reference policy in equation 1. As we have already pointed out, the fact that entropy-regularized process reward model can be computed using the reference policy is a key advantage of entropy regularization approach. In this paper, we will use equation 1 to compute our process reward models, and demonstrate its advantage over previous approaches empirically.

We note that the process reward has two formulations: when completions are generated from the initial policy π_0, it is soft-max, and when completions are generated from the optimal policy, it is soft-min. If one trains LLM and reward model simultaneously using examples generated by the updated LLM, then one needs to gradually turn from soft max to soft min during the training process.

4 Experimental Settings

Process Reward Model We use two widely adopted mathematical datasets, GSM8K (Cobbe et al., 2021) and MATH (Hendrycks et al., 2021) in our experiments. We generate and label our process

(a) Best-of-N evaluation on GSM8K

(b) Best-of-N evaluation on MATH500

Figure 2: Best-of-N evaluation results on GSM8K and MATH500 datasets with **Mistral-MetaMath-7b** as the generator. The Hard-label PRM is the same setting as Math-Shepherd.

(a) Best-of-N evaluation on GSM8K

(b) Best-of-N evaluation on MATH500

Figure 3: Best-of-N evaluation results on GSM8K and MATH500 datasets with **deepseek-math-7b-rl** as the generator. The Hard-label PRM is the same setting as Math-Shepherd.

reward data using automatic labeling with entropy regularization, similar to Math-Shepherd (Wang et al., 2024). For each problem in the training dataset, we sample 15 solutions with step-by-step rationale. For each step, we use the completer to sample 16 paths to reach the final answer. The process reward score for each step is calculated by Equation 1, using initial policy π_0. In our experiments, we use Mistral-7b (Jiang et al., 2023) fine-tuned on MetaMath Dataset (Yu et al., 2024) as the generator and the completer. In total, we have 280K data and 1.5 million step annotations. We train our reward models using Llama-3.1-8B (Dubey et al., 2024). We use the whole test set of GSM8K, and the MATH500 introduced in Lightman et al. (2023) for evaluation. We use the best-of-N strategy to evaluate our reward models. For

each problem in the test set, we randomly sample N solutions from the **Mistral-MetaMath-7b** and the **deepseek-math-7b-rl** generators. Each step in each response is given a score by the reward model. We select the response with the highest score as the final answer. The score for each response is represented using the lowest score among all the steps.

To demonstrate the effectiveness of our method, we compare our models with the hard-label process reward model (Hard-label PRM), vanilla soft-label process reward model (Soft-label PRM), and outcome reward model (ORM). For Hard-label PRM, one reasoning step will be labeled good as long as it can reach the final correct answer. For Soft-label PRM, the step score is approximated by the probability of reaching the final correct answer. For the

ORM, it will assign an overall score for the entire mathematical reasoning. We train the Hard-label PRM, Soft-label PRM, and ORM using the above settings. We consider two training settings. The first one is auto-regressive training where special tokens are inserted after each step, and the reward model is trained on these tokens with cross-entropy loss between the prediction and the ground-truth process reward. The dataset format is similar to Math-Shepherd (Wang et al., 2024). The second one is regression training where the reward model is trained to predict a real number as the score given the question and current steps with mean-square error (MSE) loss. The results for regression training are in Section 6.2.

Improving Policy Model with PRM We also design experiments to improve our policy model **Mistral-MetaMath-7b** using RLHF where we adopt the rejection sampling fine-tuning strategy (Dong et al., 2023) on the MATH training set and OpenMathInstruct-2 dataset (Toshniwal et al., 2024b). For each question, we sample 16 responses and rank them with the reward model. We select the responses with the highest reward score and fine-tune our policy models on these data. The fine-tuned policy models are evaluated on GSM8K and MATH using Top-1 accuracy under a zero-shot CoT setting. We compare different policy models guided by our reward model and guided by other baseline reward models.

5   Experimental Results

5.1   Auto-Regressive Training Results

The results of our model compared with several baseline methods are shown in Figure 2 and Table 2, which are all trained in an auto-regressive way. When the policy model is Mistral-MetaMath-7b, as N increases, the best-of-N accuracy for most of the models keeps increasing except the Outcome Reward Model (ORM). In particular, ER-PRM outperforms other baselines in all evaluation settings.

Our model demonstrates consistent improvements, with more substantial gains observed on the more challenging datasets. Concretely, on MATH, which presents harder questions compared with GSM8K, the gap widens significantly, highlighting our method's more pronounced effectiveness in tackling complex datasets. Additionally, the considerable difference between our model and the majority voting results further validates the strength of our labeling strategy, establishing our model

as a reliable approach for mathematical multi-step reasoning.

For the deepseek-math-7b-rl policy model, the accuracy increases slowly when N increases from 4 to 64 on GSM8K. And the increment on the MATH dataset is also slower than the case where we use Mistral as the policy model. We observe the performance drop for ORM reward models, indicating its instability for out-of-distribution generated data. The reason for the smaller performance gain is that, our process reward data is generated from a weaker model Mistral-MetaMath-7b. The reward model might only understand the behavior of the weak model. For certain steps where the weak model fails to produce the correct answer, the reward model is likely to assign these steps a low score. However, a stronger model may be capable of deriving the correct answer in such cases.

We notice that the Hard-label PRM also demonstrates similar strong performance for best-of-N evaluation, and is effective as Soft-label PRM in some cases, especially when N is large. We attribute this to the semi-supervised learning process during the hard-label training. The labels during the Markov Decision Process are only an estimation of the process reward instead of a precise value. The Hard-label setting is a way to reduce the noise during the training.

We note that here the Hard-label setting adopts the same labeling strategy with Math-Shepherd (Wang et al., 2024), trained with the same base model as ER-PRM to ensure a fair comparison. Our model outperforms Math-Shepherd in all settings on GSM8K and MATH, demonstrating the ability to better rank and select candidate responses. It shows that ours are intrinsically competent reward models compared to the open-source models with high consistency and robustness.

5.2   RLHF Results

Due to the fine-grained reward nature of Soft-Label PRM compared to Hard-Label PRM, which is a closer approach to our entropy formulation; we choose to verify the effectiveness of our auto-regressive Entropy-Regularized Process Reward Model (ER-PRM) by comparing it against the auto-regressive Soft-Label PRM in RLHF via RAFT algorithm (Dong et al., 2023). Table 1 summarizes the performance improvements achieved using the **Mistral-MetaMath-7b** as the initial baseline policy model.

During initial tests, we observed that the base-

(a) Best-of-N evaluation on GSM8K

(b) Best-of-N evaluation on MATH500

Figure 4: Best-of-N evaluation results on GSM8K and MATH500 datasets with **Mistral-MetaMath-7b** as the generator with different η settings.

(a) Best-of-N evaluation on GSM8K

(b) Best-of-N evaluation on MATH500

Figure 5: Best-of-N evaluation results on GSM8K and MATH500 datasets with **Mistral-MetaMath-7b** as the generator. The reward models are trained using regression. They are also compared with the auto-regressive training strategy.

Mistral-MetaMath-7b	GSM8K	MATH
Baseline	77.9	28.6
+ Soft-Label PRM	78.7	30.1
+ ER-PRM (ours)	79.5	32.8

Table 1: Zero-shot CoT evaluation for policy model **Mistral-MetaMath-7b** improved via Rejection Sampling Fine-tuning.

line policy model exhibited signs of overfitting to the training data from GSM8K and MATH, resulting in only marginal performance gains after RLHF on the original training set, particularly for GSM8K. To address this, we incorporated out-of-domain data from OpenMathInstruct-2 (Toshniwal et al., 2024a), augmenting GSM8K and MATH with 12,500 additional new questions each. For each question, the initial policy model generated 16 candidate rationales, which were then evaluated by both ER-PRM and Soft-Label PRM to select the highest-scoring rationale as training data for RLHF.

For GSM8K, we utilized the correct rationales of the augmented data identified by both PRMs, followed by a single round of RAFT. For MATH, we combined the MATH training set with the correct augmented data and applied the same RLHF strategy above. Our ER-PRM outperformed the other approach by surpassing 0.8% and 2.7% on GSM8K and MATH, respectively, indicating its superior capability in guiding the optimal policy model and its robustness in handling more complex

task settings.

In general, our RLHF approach achieved superior performance in evaluating the policy model in GSM8K and MATH, with our ER-PRM consistently having 1-2% higher best-of-N accuracy in both the in-domain and out-of-domain datasets than the soft-label baseline, showcasing the stability and effectiveness of our entropy-regularized reward formulation in selecting accurate rationales from varying quality data sources.

6   Analysis

6.1   Entropy-Regularized Reward Analysis

To better interpret our entropy-regularized method, we change the hyper-parameter η to regularize the penalty of the entropy during automatic process reward labeling and train the reward model on GSM8K and MATH separately. We then evaluate our models using the best-of-N strategy on each dataset. Note that when $\eta \to 0$, the labeling strategy is vanilla soft labeling. When $\eta \to \infty$, the labeling strategy is hard labeling. We show the performance change as η changes, and intend to find the optimal η for these two datasets.

The result is shown in Figure 4 for best-of-N performance on each η. We observe that there is a peak performance for each dataset and then the performance drops when η is too large or small. The experiments show that $\eta = 1$ or $\eta = 2$ is the best for hard dataset MATH. $\eta = 15$ is the best for easy dataset GSM8K. Larger η represents a larger penalty on the entropy for the process rewards where they are pushed higher and closer to the hard label estimation, while smaller η represents a small penalty on the entropy for the process rewards. We conclude that to achieve the best performance on automatic process reward labeling, a more fine-grained estimation of the reward scores should be applied. Simply applying hard label estimation may introduce too much noise for reward model training. We also notice that vanilla soft label estimation may not be an optimal strategy, as the performance is relatively bad when η is small ($\eta = 0.1$) for both datasets.

Considering the difficulty of the GSM8K and MATH datasets, We may need a larger entropy penalty for the process reward for the hard dataset, and a relatively smaller entropy penalty estimation for the easy dataset.

6.2   Regression Training Strategy

In addition to training the reward model in an auto-regressive way, we also explore the reward models with the regression training strategy, where we train the model to output a score directly given a problem and current steps. The best-of-N evaluation results are shown in Figure 5. The performance of best-of-N increases as N becomes larger. Our reward model still outperforms the Soft-label and Hard-label settings. We also identify it as a method to train reward models. However, we notice that auto-regressive training could yield better results for reward models than regression training. On both GSM8K and MATH datasets, the best-of-N accuracies are consistently lower than the models trained using the auto-regressive strategy. Especially on MATH, there is a significant gap of the accuracy between the two training methods. One hypothesis is that auto-regressive training integrates the steps, reducing the total number of training steps, which in turn leads to less forgetting. For the MATH dataset, since there are more reasoning steps per question, splitting them into multiple training samples increases the difficulty for the reward models to learn. It is also possible that the reasoning steps in auto-regressive training are continuous and coherent, allowing the reward model to better learn the process of assigning rewards.

7   Conclusion

In this paper, we demonstrate the potential of process reward models (PRMs) in enhancing the performance of large language models (LLMs) on complex mathematical reasoning tasks. By leveraging the fine-grained feedback provided by PRMs, we achieve a notable improvement over traditional outcome reward models (ORMs), as PRMs better capture the multi-step reasoning required for such tasks. To enhance the process reward model, we formulate the multi-step reasoning in the entropy perspective and then derive the process reward score by a new aggregation method. The effectiveness of our automatic labeling process rewards, coupled with entropy-regularized reinforcement learning techniques, highlights the importance of balancing reward optimization with policy stability. Our model outperforms baseline ORMs and PRMs by a large margin on the MATH and GSM8K benchmarks. Furthermore, we apply our process reward model to improve the policy model and observe a significant improvement after rejection sampling.

8 Limitations

Although our method demonstrates the potential to improve the reward models and the policy models with rejection fine-tuning, we have not conducted large-scale online RLHF experiments such as PPO (Schulman et al., 2017), due to the limitation of the computational resources. Future work could explore more policy models training for mathematical reasoning using more RLHF methods, combined with ER-PRM.

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A Technical Lemma

Lemma 1 (Solution of KL-regularized Optimization)
Given a loss functional with respect to $p(\cdot|x)$,

written as

$$\mathbb{E}_{w \sim p(\cdot)}\Big[- U(w) + \eta D_{\mathrm{KL}}\big(p(\cdot), p_0(\cdot)\big)\Big]$$

$$= \eta D_{\mathrm{KL}}\Big(p(\cdot), p_0(\cdot)\exp\Big(\frac{1}{\eta}U(\cdot)\Big)\Big)$$

$$- \eta \cdot \log \underbrace{\mathbb{E}_{w \sim p_0(\cdot)}\exp\Big(\frac{1}{\eta}U(w)\Big)}_{C_r},$$

where the minimizer of the loss functional is $p^*(w) = \frac{1}{C_r}p_0(w)\exp\Big(\frac{1}{\eta}U(w)\Big)$, *also known as Gibbs distribution.*

See Proposition 7.16 and Theorem 15.3 of Zhang (2023) for a detailed proof.

B   Best-of-N Evaluation Results

In this section, we list the performance of the best-of-N evaluation of ER-PRM and other baselines in Tables. The results for the reward models with policy model **Mistral-MetaMath-7b** are shown in Table 2, which corresponds to Figure 2. The results for the reward models with policy model **deepseek-math-7b-rl** are shown in Table 3, which corresponds to Figure 3.

The results for Section 6.1 in Analysis are shown in Table 4 and Table 5, corresponding to the GSM8K and MATH datasets. The results for Section 6.2 are shown in Table 6.

Best-of-N	GSM8K						MATH500					
	Ours	Soft-label PRM	Hard-label PRM	ORM	Math-Shepherd	Majority-Voting	Ours	Soft-label PRM	Hard-label PRM	ORM	Math-Shepherd	Majority-Voting
N=4	86.05	85.97	85.44	84.54	85.22	81.20	35.0	33.6	34.0	34.4	32.6	28.8
N=8	87.79	86.88	87.19	86.20	85.37	82.18	37.2	37.0	34.0	36.2	33.0	32.4
N=16	88.78	87.11	88.48	86.88	86.35	83.47	39.2	38.6	38.4	37.4	35.4	34.0
N=32	89.23	88.25	89.01	86.66	86.66	84.00	40.8	38.6	38.4	39.0	37.6	35.4
N=64	89.54	88.10	89.16	85.90	87.26	83.55	41.8	38.4	39.8	39.2	37.6	36.4
Top1@acc	78.09						29.4					

Table 2: Best-of-N evaluation for policy model **Mistral-MetaMath-7b**. The reward models are trained using **auto-regressive** strategy

Best-of-N	GSM8K					MATH500				
	Ours	Soft-label PRM	Hard-label PRM	ORM	Math-Shepherd	Ours	Soft-label PRM	Hard-label PRM	ORM	Math-Shepherd
N=4	89.46	89.39	88.70	88.77	87.26	52.6	51.4	51.8	52.6	52.4
N=8	89.91	89.61	88.93	89.09	88.78	55.8	54.8	55.4	55.0	55.6
N=16	90.22	90.22	89.76	89.01	89.08	55.6	54.8	55.4	55.2	55.2
N=32	90.45	90.45	89.84	89.01	88.70	56.0	55.0	55.0	55.0	54.4
N=64	90.67	90.45	89.84	88.10	88.63	57.0	55.4	55.6	53.4	53.4
Top1@acc	88.17					51.0				

Table 3: Best-of-N evaluation for policy model **deepseek-math-7b-rl**. The reward models are trained using **auto-regressive** strategy

Best-of-N	GSM8K							
	$\eta = 0.1$	$\eta = 1$	$\eta = 2$	$\eta = 5$	$\eta = 8$	$\eta = 10$	$\eta = 15$	$\eta = 20$
N=4	83.93	84.69	84.99	84.38	85.22	84.69	84.91	84.53
N=8	85.14	85.82	86.43	86.35	86.73	86.28	86.66	86.43
N=16	85.29	85.75	86.05	87.11	87.57	87.04	87.72	87.04
N=32	86.13	85.52	86.43	87.72	87.87	88.02	88.78	87.11
N=64	86.13	85.90	86.35	88.17	88.25	88.48	88.78	87.19

Table 4: Best-of-N evaluation for different η values on GSM8K dataset

Best-of-N	MATH							
	$\eta = 0.1$	$\eta = 1$	$\eta = 2$	$\eta = 5$	$\eta = 8$	$\eta = 10$	$\eta = 15$	$\eta = 20$
N=4	35.0	34.0	35.0	33.2	32.4	33.2	33.2	31.8
N=8	35.8	37.2	39.0	35.0	36.0	35.8	35.6	33.8
N=16	39.0	38.6	40.0	37.0	39.4	38.6	39.0	37.4
N=32	39.8	39.8	40.2	38.6	39.2	39.4	38.6	38.8
N=64	38.6	41.0	40.2	37.4	38.2	40.0	40.2	39.4

Table 5: Best-of-N evaluation for different η values on MATH dataset

Best-of-N	GSM8K			MATH500		
	Ours	Soft-label PRM	Hard-label PRM	Ours	Soft-label PRM	Hard-label PRM
N=4	84.84	84.60	84.60	33.6	31.4	31.8
N=8	86.80	86.05	86.73	33.6	33.0	33.0
N=16	87.95	87.41	87.41	36.2	35.0	35.6
N=32	88.40	87.87	87.71	37.0	35.0	36.6
N=64	88.40	88.24	88.17	36.8	34.2	36.4

Table 6: Best-of-N evaluation, trained using **regression**