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Self-Play Preference Optimization for Language Model Alignment

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Abstract

010 Traditional reinforcement learning from human feedback (RLHF) approaches relying on paramet-012 ric models like the Bradley-Terry model fall short in capturing the intransitivity and irrationality in human preferences. Recent advancements sug-015 gest that directly working with preference probabilities can yield a more accurate reflection of human preferences, enabling more flexible and 018 accurate language model alignment. In this pa-019 per, we propose a self-play-based method for lan-020 guage model alignment, which treats the problem as a constant-sum two-player game aimed at identifying the Nash equilibrium policy. Our approach, dubbed Self-Play Preference Optimization (SPPO), approximates the Nash equilibrium 025 through iterative policy updates and enjoys a theoretical convergence guarantee. Our method can 027 effectively increase the log-likelihood of the cho-028 sen response and decrease that of the rejected 029 response, which cannot be trivially achieved by 030 symmetric pairwise loss such as Direct Preference Optimization (DPO) and Identity Preference Optimization (IPO). In our experiments, using only 60k prompts (without responses) from the 034 UltraFeedback dataset and without any prompt 035 augmentation, by leveraging a pre-trained preference model PairRM with only 0.4B parameters, SPPO can obtain a model from fine-tuning Mistral-7B-Instruct-v0.2 that achieves the state-039 of-the-art length-controlled win-rate of 28.53% against GPT-4-Turbo on AlpacaEval 2.0. It also 041 outperforms the (iterative) DPO and IPO on MT-Bench and the Open LLM Leaderboard. No-043 tably, the strong performance of SPPO is achieved without additional external supervision (e.g., re-045 sponses, preferences, etc.) from GPT-4 or other 046 stronger language models. 047

1 Introduction

Large Language Models (LLMs) have demonstrated impressive capabilities, yet they face challenges in ensuring reliability, safety, and ethical alignment. Reinforcement Learning from Human Feedback (RLHF) offers a solution by fine-tuning models to align with human preferences. Traditional RLHF methods (Christiano et al., 2017; Ouyang et al., 2022) rely on reward models to guide this process, but they often fall short of capturing the complexities of human behavior.

Recent research highlights the limitations of parametric preference models like Bradley & Terry (1952), which assume consistent and transitive human preferences. Instead, studies suggest that human preferences can be inconsistent and influenced by various factors, challenging the effectiveness of these models(Tversky, 1969).

To address these issues, researchers have begun exploring more flexible algorithms that directly handle preference probabilities. Emerging approaches, such as Self-play Preference Optimization (SPO, Swamy et al., 2024), aim to identify optimal policies through self-play mechanisms. These methods offer potential improvements but require significant adaptation for large-scale LLM fine-tuning.

In this paper, we introduce Self-Play Preference Optimization (SPPO), a new self-play algorithm designed to solve the two-player constant-sum game for LLM alignment. SPPO utilizes an exponential weight update algorithm within a selfplay framework, where policies are fine-tuned on synthetic data generated by the model itself. Our contributions include a provably convergent SPPO algorithm for LLM alignment, optimizing a simple loss function. Comparisons with state-of-the-art methods like DPO, IPO, and KTO, demonstrate SPPO's superior performance on various benchmarks. Empirical evidence shows that SPPO enhances the Mistral-7B-Instruct-v0.2 model, achieving significant improvements without external supervision from stronger models like GPT-4. Our findings suggest that SPPO provides a robust and scalable solution for aligning large language models with human preferences.

2 Preliminaries

We consider the preference learning scenario as follows. Given a text sequence (commonly referred to as prompt) $\mathbf{x} = [x_1, x_2, ...]$, two text sequences $\mathbf{y} = [y_1, y_2, ...]$ and

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 \mathbf{y}' are generated as responses to the prompt \mathbf{x} . An autoregressive language model π given the prompt \mathbf{x} can generate responses \mathbf{y} following the probability decomposition

$$\pi(\mathbf{y}|\mathbf{x}) = \prod_{i=1}^{N} \pi(y_i|\mathbf{x}, \mathbf{y}_{< i})$$

Given the prompt **x** and two responses **y** and **y**', a preference oracle (either a human annotator or a language model) will provide preference feedback $o(\mathbf{y} \succ \mathbf{y}' | \mathbf{x}) \in \{0, 1\}$ indicating whether **y** is preferred over \mathbf{y}' . We denote $\mathbb{P}(\mathbf{y} \succ \mathbf{y}' | \mathbf{x}) = \mathbb{E}[o(\mathbf{y} \succ \mathbf{y}' | \mathbf{x})]$ as the probability of **y** "winning the duel" over \mathbf{y}' . The KL divergence of two probability distributions of density p and q is defined as $\mathrm{KL}(p || q) = \mathbb{E}_{\mathbf{y} \sim p(\mathbf{y})} \left[\log \frac{p(\mathbf{y})}{q(\mathbf{y})} \right]$.

2.1 RLHF with General Preference

Following Wang et al. (2024); Munos et al. (2023), we aim to establish RLHF methods without a reward model, as the human preference can be non-transitive (Tversky, 1969). Under a general preference oracle $\mathbb{P}(\mathbf{y} \succ \mathbf{y}' | \mathbf{x})$, we follow Dudík et al. (2015) and aim to identify the *von Neumann winner*. More specifically, the von Neumann winner π^* is the (symmetric) Nash equilibrium of the following twoplayer constant-sum game:

$$(\pi^*, \pi^*) = \arg \max_{\pi} \min_{\pi'} \mathbb{E}_{\mathbf{x} \sim \mathcal{X}} \Big[\mathbb{E}_{\mathbf{y} \sim \pi(\cdot | \mathbf{x}), \mathbf{y}' \sim \pi'(\cdot | \mathbf{x})} \big[\mathbb{P}(\mathbf{y} \succ \mathbf{y}' | \mathbf{x}) \big] \Big]. \quad (2.1)$$

In addition, we define the winning probability of one response y against a distribution of responses π as

$$\mathbb{P}(\mathbf{y} \succ \pi | \mathbf{x}) = \mathbb{E}_{\mathbf{y}' \sim \pi(\cdot | \mathbf{x})}[\mathbb{P}(\mathbf{y} \succ \mathbf{y}' | \mathbf{x})]$$

and the winning probability of one policy π against another policy π' as

$$\mathbb{P}(\pi \succ \pi' | \mathbf{x}) = \mathbb{E}_{\mathbf{y} \sim \pi(\cdot | \mathbf{x})} \mathbb{E}_{\mathbf{y}' \sim \pi'(\cdot | \mathbf{x})} [\mathbb{P}(\mathbf{y} \succ \mathbf{y}' | \mathbf{x})].$$

Furthermore, we define $\mathbb{P}(\pi \succ \pi') = \mathbb{E}_{\mathbf{x} \sim \mathcal{X}}[\mathbb{P}(\pi \succ \pi' | \mathbf{x})]$, where \mathbf{x} is a prompt drawn from the prompt distribution \mathcal{X} . The two-player constant-sum game (2.1) can be simplified as

$$(\pi^*, \pi^*) = \arg\max_{\pi} \min_{\pi'} \mathbb{P}(\pi \succ \pi').$$

3 Self-Play Preference Optimization (SPPO)

In this section, we introduce the Self-Play Preference Optimization (SPPO) algorithm, derived from the following theoretical framework.

3.1 Theoretical Framework

There are well-known algorithms to approximately solve the Nash equilibrium in a constant-sum two-player game. In this work, we follow Freund & Schapire (1999) to establish an iterative framework that can asymptotically converge to the optimal policy on average. We start with a theoretical framework that conceptually solves the two-player game for t = 1, 2, ... as follows:

$$\pi_{t+1}(\mathbf{y}|\mathbf{x}) \propto \pi_t(\mathbf{y}|\mathbf{x}) \exp(\eta \mathbb{P}(\mathbf{y} \succ \pi_t|\mathbf{x})).$$
(3.2)

(3.2) is an iterative framework that relies on the multiplicative weight update in each round t and enjoys a clear structure. Initially, we have a base policy π_1 usually from some supervised fine-tuned model. In each round, the updated policy π_{t+1} is obtained from the reference policy π_t following the multiplicative weight update. More specifically, a response y should have a higher probability weight if it has a higher average advantage over the current policy π_t . Equivalently, (3.2) can be written as

$$\pi_{t+1}(\mathbf{y}|\mathbf{x}) = \frac{\pi_t(\mathbf{y}|\mathbf{x}) \exp\left(\eta \mathbb{P}(\mathbf{y} \succ \pi_t | \mathbf{x})\right)}{Z_{\pi_t}(\mathbf{x})}, \quad (3.3)$$

where $Z_{\pi_t}(\mathbf{x}) = \sum_{\mathbf{y}} \pi_t(\mathbf{y}|\mathbf{x}) \exp(\eta \mathbb{P}(\mathbf{y} \succ \pi_t|\mathbf{x}))$ is the normalizing factor (a.k.a., the partition function). For any fixed \mathbf{x} and \mathbf{y} , the ideal update policy π_{t+1} should satisfy the following equation:

$$\log\left(\frac{\pi_{t+1}(\mathbf{y}|\mathbf{x})}{\pi_t(\mathbf{y}|\mathbf{x})}\right) = \eta \cdot \mathbb{P}(\mathbf{y} \succ \pi_t|\mathbf{x}) - \log Z_{\pi_t}(\mathbf{x}).$$
(3.4)

Unlike the pair-wise design in DPO or IPO that cancels the log normalizing factor $\log Z_{\pi_t}(\mathbf{x})$ by differentiating (3.4) between \mathbf{y} and \mathbf{y}' , we choose to approximate (3.4) directly in terms of L_2 distance:

$$\pi_{t+1} = \underset{\pi}{\operatorname{argmin}} \mathbb{E}_{\mathbf{x} \sim \mathcal{X}, \mathbf{y} \sim \pi_t(\cdot | \mathbf{x})} \\ \left(\log \left(\frac{\pi(\mathbf{y} | \mathbf{x})}{\pi_t(\mathbf{y} | \mathbf{x})} \right) - \left(\eta \mathbb{P}(\mathbf{y} \succ \pi_t | \mathbf{x}) - \log Z_{\pi_t}(\mathbf{x}) \right) \right)^2.$$
(3.5)

Estimation of the Probability The optimization objective (3.5) can be approximated with finite samples. We choose to sample *K* responses $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_K \sim \pi_t(\cdot | \mathbf{x})$ for each prompt \mathbf{x} , and denote the empirical distribution by $\widehat{\pi}_t^K$. The finite-sample optimization problem can be approximated as

$$\pi_{t+1} = \underset{\pi}{\operatorname{argmin}} \mathbb{E}_{\mathbf{x} \sim \mathcal{X}, \mathbf{y} \sim \pi_t(\cdot | \mathbf{x})} \left(\log \left(\frac{\pi(\mathbf{y} | \mathbf{x})}{\pi_t(\mathbf{y} | \mathbf{x})} \right) - \left(\eta \mathbb{P}(\mathbf{y} \succ \widehat{\pi}_t^K | \mathbf{x}) - \log Z_{\widehat{\pi}_t^K}(\mathbf{x}) \right) \right)^2. \quad (3.6)$$

Specifically, $\mathbb{P}(\mathbf{y} \succ \widehat{\pi}_t^K | \mathbf{x}) = \sum_{k=1}^K \mathbb{P}(\mathbf{y} \succ \mathbf{y}_k | \mathbf{x})/K$ and $Z_{\widehat{\pi}_t^K}(\mathbf{x}) = \mathbb{E}_{\mathbf{y} \sim \pi_t(\cdot | \mathbf{x})} [\exp(\eta \mathbb{P}(\mathbf{y} \succ \widehat{\pi}_t^K | \mathbf{x}))]. Z_{\widehat{\pi}_t^K}(\mathbf{x})$, treated as an expectation, can be further estimated by B Algorithm 1 Self-Play Preference Optimization (SPPO)1: input: base policy π_{θ_1} , preference oracle \mathbb{P} , learning rate η , number of generated samples K.2: for t = 1, 2, ... do3: Generate synthetic responses by sampling $\mathbf{x} \sim \mathcal{X}$ and $\mathbf{y}_{1:K} \sim \pi_t(\cdot|\mathbf{x})$.4: Annotate the win-rate $\mathbb{P}(\mathbf{y}_k \succ \mathbf{y}_{k'}|\mathbf{x}), \forall k, k' \in [K]$.5: Select responses from $\mathbf{y}_{1:K}$ to form dataset $\mathcal{D}_t = \{(\mathbf{x}_i, \mathbf{y}_i, \widehat{P}(\mathbf{y}_i \succ \pi_t | \mathbf{x}_i))\}_{i \in [N]}$.6: Optimize $\pi_{\theta_{t+1}}$ according to (3.7):

$$\boldsymbol{\theta}_{t+1} \leftarrow \operatorname*{argmin}_{\boldsymbol{\theta}} \mathbb{E}_{(\mathbf{x}, \mathbf{y}, \widehat{P}(\mathbf{y} \succ \pi_t | \mathbf{x})) \sim \mathcal{D}_t} \left(\log \left(\frac{\pi_{\boldsymbol{\theta}}(\mathbf{y} | \mathbf{x})}{\pi_t(\mathbf{y} | \mathbf{x})} \right) - \eta \left(\widehat{P}(\mathbf{y} \succ \pi_t | \mathbf{x}) - \frac{1}{2} \right) \right)^2.$$
(3.1)

7: end for

new samples with in total O(KB) queries of the preference oracle \mathbb{P} . (3.6) is an efficiently tractable optimization problem. Informally speaking, when $K \to \infty$, (3.6) will recover (3.5). We have the following guarantee on the convergence of (3.5):

Theorem 3.1. Assume the optimization problem (3.5) is realizable. Denote π_t as the policy obtained via (3.5) and the mixture policy $\bar{\pi}_T = \frac{1}{T} \sum_{t=1}^T \pi_t$. By setting $\eta = \Theta(1/\sqrt{T})$, we have that

$$\max_{\pi} \left[\mathbb{P}(\pi \succ \bar{\pi}_T) \right] - \min_{\pi} \left[\mathbb{P}(\pi \prec \bar{\pi}_T) \right] = O(1/\sqrt{T}).$$

Theorem 3.1 characterizes the convergence rate of the average policy across the time horizon T towards the Nash equilibrium, in terms of the duality gap. The proof is based on Theorem 1 in Freund & Schapire (1999) with slight modification. For completeness, we include the proof in Appendix E.

Alternatively, we can avoid estimating $\log Z_{\hat{\pi}_t^K}(\mathbf{x})$ by replacing it simply with $\eta/2^1$ in (3.6) to obtain a more clear objective:

$$\pi_{t+1} = \underset{\pi}{\operatorname{argmin}} \mathbb{E}_{\mathbf{x} \sim \mathcal{X}, \mathbf{y} \sim \pi_t(\cdot | \mathbf{x})} \left(\log\left(\frac{\pi(\mathbf{y} | \mathbf{x})}{\pi_t(\mathbf{y} | \mathbf{x})}\right) - \eta \left(\mathbb{P}(\mathbf{y} \succ \widehat{\pi}_t^K | \mathbf{x}) - \frac{1}{2}\right) \right)^2.$$
(3.7)

Intuitively, if a tie occurs (i.e., $\mathbb{P}(\mathbf{y} \succ \widehat{\pi}_t^K | \mathbf{x}) = 1/2$), we prefer the model does not update weight at \mathbf{y} . If \mathbf{y} wins over $\widehat{\pi}_t^K$ on average (i.e., $\mathbb{P}(\mathbf{y} \succ \widehat{\pi}_t^K | \mathbf{x}) > 1/2$), then we increase the probability density at \mathbf{y} to employ the advantage of \mathbf{y} over $\widehat{\pi}_t^K$. In our experiments, we choose to minimize the objective (3.7).

3.2 The SPPO Algorithm

Based on the aforementioned theoretical framework, we propose the *Self-Play Preference Optimization* algorithm in

Algorithm 1.

In each round t, Algorithm 1 will first generate K responses $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_K$ according to $\pi_t(\cdot|\mathbf{x})$ for each prompt \mathbf{x} (Line 3). Then, the preference oracle \mathbb{P} will be queried to calculate the win rate among the K responses (Line 4). At Line 5, certain criteria can be applied to determine which response should be kept in the constructed dataset \mathcal{D}_t and construct the prompt-response-probability triplet $(\mathbf{x}, \mathbf{y}, \hat{P}(\mathbf{y} \succ \pi_t | \mathbf{x}))$. We will discuss the design choices later in Section 4. One straightforward design choice is to include all K responses into \mathcal{D}_t and each $\hat{P}(\mathbf{y}_i \succ \pi_t | \mathbf{x})$ is estimated by comparing \mathbf{y}_i to all K responses. In total, $O(K^2)$ queries will be made. Then the algorithm will optimize (3.7) on the dataset \mathcal{D}_t (Line 6).

4 **Experiments**

We conduct extensive experiments to show the performance of our method and compare it with other baselines.

4.1 Experiment Setup

We briefly summarize our experiment setup as below. For a full description of our experiment setup, see Section C.

Base Model and Datasets: We follow Snorkel's experimental setup, using Mistral-7B-Instruct-v0.2 as our base model and Ultrafeedback for prompts. We split the dataset into three portions to avoid overfitting and ensure fair comparison with Snorkel.

Preference Model: We use PairRM, a 0.4B pair-wise preference model based on DeBERTA-V3, trained on highquality human-preference datasets. PairRM outputs a "relative reward" to balance accuracy and efficiency, following Snorkel's methodology.

Response Generation and Selection: We sample K = 5 responses per prompt with top p = 1.0 and temperature 1.0. We select the responses with the highest and lowest PairRM scores as the winning and losing responses respectively.

Baselines and Benchmarks: We evaluate Mistral-7B-Instruct-v0.2, Snorkel, iterative DPO and IPO, and Selfrewarding LM. Benchmarks include AlpacaEval 2.0, MT-

¹⁰¹ ¹Assuming the winning probability between any pair is a fair ¹⁶² coin toss, when $K \to \infty$, we can show that indeed $Z_{\widehat{\pi}_t^K}(\mathbf{x}) \to e^{\eta/2}$.

Table 1: AlpacaEval 2.0 evaluation of various models (de-165 tailed in Baselines) in terms of both normal and length-167 controlled (LC) win rates in percentage (%). Mistral-7B stands for Mistral-7B-instruct-v0.2; Snorkel stands for 168 169 Snorkel (Mistral-PairRM-DPO); bo16 stands for best-of-16. SPPO demonstrates steady performance gains across 170 171 iterations and outperforms other baselines which show a ten-172 dency to produce longer responses. Additionally, re-ranking 173 with the PairRM reward model (best-of-16) at test time con-174 sistently enhances the performance across all models.

Model	AlpacaEval 2.0			
Widdei	LC Win Rate	Win Rate	Avg. Len	
Mistral-7B	17.11	14.72	1676	
Mistral-7B (bo16)	22.45	17.94	1529	
Snorkel	26.39	30.22	2736	
Snorkel (bo16)	29.97	34.86	2616	
Self-Rewarding Iter1	-	9.94	1092	
Self-Rewarding Iter2	-	15.38	1552	
Self-Rewarding Iter3	-	20.44	2552	
DPO Iter1	23.81	20.44	1723	
DPO Iter2	24.23	24.46	2028	
DPO Iter3	22.30	23.39	2189	
IPO Iter1	23.78	20.77	1693	
IPO Iter2	21.08	23.38	2660	
IPO Iter3	20.06	22.47	2760	
SPPO Iter1	24.79 _(+7.69)	23.51 _(+8.79)	1855	
SPPO Iter2	26.89 _(+2.10)	27.62 _(+4.11)	2019	
SPPO Iter3	28.53 _(+1.64)	31.02 _(+3.40)	2163	
SPPO Iter1 (bo16)	28.71 _(+6.26)	27.77 _(+9.83)	1901	
SPPO Iter2 (bo16)	31.23 _(+2.52)	32.12 _(+4.35)	2035	
SPPO Iter3 (bo16)	32.13 _(+0.9)	34.94 _(+2.82)	2174	

Bench, and the Open LLM Leaderboard, covering variousaspects of language model evaluation.

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200**4.2 Experimental Results**

In the assessment of AI chatbots, human evaluation remains the benchmark for quality and accuracy (Askell et al., 2021; Ouyang et al., 2022). However, due to its limitations in 203 scalability and reproducibility, we explore the alternative ap-204 proach of using the advanced capabilities of GPT-4 (OpenAI et al., 2023) as an automatic evaluation tool. We conduct 206 GPT-4-based automatic evaluation on AlpacaEval 2.0 (Li et al., 2023b) and MT-Bench (Zheng et al., 2023) to measure 208 the chatbot capability of our model. Due to the space limit, 209 we only report the results on AlpacaEval 2.0 in the follow-210 ing and postpone other results including ablation studies to 211 the appendix. 212

Table 1 (AlpacaEval 2.0) shows the win rate over the GPT4-Turbo baseline of different models on 805 prompts. We
also include one column indicating the length-controlled
win rate, and one column on the average length of each
model, to account for the tendency of the LLM-based judge
to favor longer sequence outputs — an issue colloquially

Table 2: AlpacaEval 2.0 leaderboard results of both normal and length-controlled (LC) win rates in percentage (%). Snorkel stands for Snorkel (Mistral-PairRM-DPO). Our SPPO model outperforms many competing models trained on proprietary alignment data (e.g., Claude 2, Gemini Pro, & Llama 3 8B Instruct). With test-time reranking, SPPO Iter3 (best-of-16) is even competitive to GPT-4 0613 and Llama 3 70B Instruct.

Madal	AlpacaEval 2.0				
Model	LC. Win Rate	Win Rate			
GPT-4 Turbo	50.0	50.0			
Claude 3 Opus	40.5	29.1			
GPT-4 0314	35.3	22.1			
Llama 3 70B Instruct	34.4	33.2			
SPPO Iter3 (best-of-16)	32.1	34.9			
GPT-4 0613	30.2	15.8			
Snorkel (best-of-16)	30.0	34.9			
Mistral Medium	28.6	21.9			
SPPO Iter3	28.5	31.0			
Claude 2	28.2	17.2			
Snorkel	26.4	30.2			
Gemini Pro	24.4	18.2			
Mistral 8×7B v0.1	23.7	18.1			
Llama 3 8B Instruct	22.9	22.6			
GPT-3.5 Turbo 0613	22.7	14.1			
Vicuna 33B v1.3	17.6	12.7			

termed the "reward hacking" phenomenon. According to the table, SPPO Iter3 has the highest win rate, 28.52% for the length-controlled version, and 31.02% for the overall win rate. The performance gains over previous iterations are 7.69% (Mistral-7B-Instruct \rightarrow Iter1), 2.10% (Iter1 \rightarrow Iter2), and 1.64% (Iter2 \rightarrow Iter3), respectively, indicating steady improvements across iterations. Additionally, the data indicates that SPPO achieves superior performance compared to the iterative variants of DPO and IPO. The length-controlled win rate for SPPO reaches 28.53%, outperforming the DPO's best rate of 26.39% (by Snorkel) and IPO's rate of 25.45% . Notably, while DPO and IPO training tend to significantly increase the average output length-2736 and 2654, respectively-SPPO shows a more moderate length increase, moving from 1676 in the base model to 2163 at the third iteration. We find that re-ranking with the preference model at test time can consistently improve the performance of base models (Mistral-7B-Instructv0.2), DPO (Snorkel), and SPPO (Iter3) by 5.34%, 3.57%, and 3.6%, respectively. Notably, this shows that while SPPO significantly enhances model alignment using PairRM-0.4B as the sole external supervision, it has not resulted in overoptimization against the preference model (Gao et al., 2023). Future work will explore further improvements in model alignment, potentially through additional iterations beyond the current three (following Snorkel's methodology).

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330 A Related Work

RLHF with Explicit/Implicit Reward Model Originally, reinforcement learning from human feedback (RLHF) was proposed by Christiano et al. (2017) as a methodology that first learns a reward model reflecting human preferences and then uses reinforcement learning algorithms to maximize the reward. This methodology is applied by Ouyang et al. (2022) to fine-tune instruction-following large language models and leads to the popular ChatGPT.

The reward model in the works mentioned above assumes a parametric model such as the Bradley-Terry model (Bradley & 336 Terry, 1952), which assigns a "score" representing how preferred a given response is. More recently, Rafailov et al. (2024) 337 proposed to instead directly solve the closed-form solution of such a score implied by the Bradley-Terry model. The Direct 338 Policy Optimization (DPO) method is claimed to be more efficient and stable, yet, still implicitly assumes such a reward 339 model that specifies the "score". In a similar spirit, Zhao et al. (2023) proposed to calibrate the score so that the score of the 340 winner in comparison has a margin over the score of the loser, and induces a different SLic loss. Similarly, Ethayarajh et al. 341 (2024) derived a different loss function (called KTO) from the Kahneman-Tversky human utility function, which implicitly 342 denotes a score of the given response. Liu et al. (2023) proposed Rejection Sampling Optimization (RSO) which utilizes a 343 preference model to generate preference pairs with candidates sampled from the optimal policy; then preference optimization is applied on the sampled preference pairs. Hong et al. (2024) proposed Odds Ratio Preference Optimization (ORPO) 345 algorithm that can perform supervised fine-tuning and preference alignment in one training session without maintaining an 346 intermediate reference policy. 347

RLHF with General Preference Model Often, the human preference is not strictly transitive, and cannot be sufficiently 349 represented by a single numerical score. Azar et al. (2023) proposed a general preference optimization objective based 350 on the preference probability between a pair of responses instead of a score of a single response. They further propose a 351 learning objective based on identity mapping of the preference probability called IPO (Preference Optimization with Identity 352 mapping), which aims to maximize the current policy's expected winning probability over a given reference policy. Munos 353 et al. (2023) formulated the RLHF problem with general preference as a two-player, constant-sum game, where each player 354 is one policy that aims to maximize the probability of its response being preferred against its opponent. They aim to identify 355 the Nash equilibrium policy of this game and propose a mirror-descent algorithm that guarantees the last-iterate convergence 356 of a policy with tabular representations². Wang et al. (2024) proposed to identify the Nash equilibrium policy for multi-step 357 MDPs when a general preference model is present and shows that the problem can be reduced to a two-player zero-sum 358 Markov game. 359

360 **Theory of RLHF** There is also a line of research to analyze RLHF and provide its theoretical guarantees. Zhu et al. (2023) 361 studied the standard RLHF with separate reward-learning and model-tuning and proposed a pessimistic reward-learning 362 process that provably learns a linear reward model. Wang et al. (2024) proposed a framework to reduce any RLHF problem 363 with a reward model to a reward-based standard RL problem. Additionally, they proposed to identify the Nash equilibrium 364 policy when a general preference model is present and show that the problem can be reduced to a two-player zero-sum 365 Markov game. Xiong et al. (2023) studied the reverse-KL regularized contextual bandit for RLHF in different settings and 366 proposed efficient algorithms with finite-sample theoretical guarantees. Ye et al. (2024) studied the theoretical learnability 367 of the KL-regularized Nash-Learning from Human Feedback (NLHF) by considering both offline and online settings 368 and proposed provably efficient algorithms. Ji et al. (2024) proposed an active-query-based proximal policy optimization 369 algorithm with regret bounds and query complexity based on the problem dimension and the sub-optimality gap. 370

Self-Play Fine-Tuning Most works mentioned above (Rafailov et al., 2024; Zhao et al., 2023; Azar et al., 2023; Ethayarajh et al., 2024) consider one single optimization procedure starting from some reference policy. The same procedure may be applied repeatedly for multiple rounds in a self-play manner. In each round, new data are generated by the policy obtained in the last round; these new data are then used for training a new policy that can outperform the old policy.

The self-play fine-tuning can be applied to both scenarios with or without human preference data. For example, Singh et al. (2023) proposed an Expectation-Maximization (EM) framework where in each round, new data are generated and annotated with a reward score; the new policy is obtained by fine-tuning the policy on the data with a high reward. Chen et al. (2024) proposed a self-play framework to fine-tune the model in a supervised way. In each round, new preference pairs are synthesized by labeling the policy-generated responses as losers and the human-generated responses as winners. Then DPO is applied in each round to fine-tune another policy based on these synthesized preference data. Yuan et al. (2024) proposed Self-Rewarding Language Models, where the language model itself is used to annotate preference on its

 $[\]frac{^{2}\text{Due to the tabular representation, computing the normalizing factor is prohibitive and the algorithm is approximately executed by sampling one token instead of a full response.}$

- 385 own responses. Iterative DPO is applied to fine-tune language models on these annotated data. These works show iterative
- 386 fine-tuning can significantly improve the performance.

387 Swamy et al. (2024) considered a more general multi-step Markov Decision Process (MDP) setting and proposed Self-play

- 388 Preference Optimization (SPO), an RLHF framework that can utilize any no-regret online learning algorithm for preference-
- 389 based policy optimization. They then instantiated their framework with the Soft Policy Iteration as an idealized variant of 390
- their algorithm, which reduces to the exponential weight update rule (3.2) when constrained to the bandit setting. The main
- difference is that they focus on the multi-round Markov decision process (MDP) in robotic or game tasks rather than on 392 fine-tuning large language models and approximating the update using policy optimization methods such as PPO.
- Concurrent to our work, Rosset et al. (2024) proposed the Direct Nash Optimization (DNO) algorithm based on the 394 cross-entropy between true and predicted win rate gaps, and provided theoretical guarantees on the error of finite-sample 395 approximations. However, their practical version still utilizes the iterative-DPO framework as in Xu et al. (2023) with the 396 DPO loss instead of their own DNO loss. Notably, in their experiments, they added the GPT-4 generated responses as 397 their "gold sample" into their fine-tuning data, and used GPT-4 as a judge to assign a numerical score to each response for 398 preference pair construction. In sharp contrast, our work does not require use any strong external supervision besides a 399 small-sized reward model. Another concurrent work (Gao et al., 2024) proposed REBEL, an iterative self-play framework 400 via regressing the relative reward. When applied to the preference setting, it results a similar algorithm to our algorithm 401 SPPO, except that SPPO approximate the log-partition factor $\log Z_{\pi_t}(\mathbf{x})$ with $\eta/2$ while REBEL regresses on the win rate 402 difference (so that $\log Z_{\pi_t}(\mathbf{x})$ is cancelled). Additionally, Calandriello et al. (2024) pointed out that optimising the IPO loss 403 (Azar et al., 2023) iteratively with self-play generated data is equivalent to finding the Nash equilibrium of the two-player 404 game, and they proposed the IPO-MD algorithm based on this observation which generates data with a mixture policy 405 similarly as the Nash-MD algorithm.

406 Comparison with DPO, IPO, and KTO B 407

408 In practice, we utilize mini-batches of more than 2 responses to estimate the win rate of a given response, while the DPO and 409 IPO loss focus on a single pair of responses. When only a pair of responses y_w and y_l is available, we have the pair-wise 410 symmetric loss based on the preference triplet $(\mathbf{x}, \mathbf{y}_w, \mathbf{y}_l)$ defined as: 411

$$\ell_{\text{SPPO}}(\mathbf{x}, \mathbf{y}_w, \mathbf{y}_l; \boldsymbol{\theta}; \pi_{\text{ref}}) := \left(\log \left(\frac{\pi_{\boldsymbol{\theta}}(\mathbf{y}_w | \mathbf{x})}{\pi_{\text{ref}}(\mathbf{y}_w | \mathbf{x})} \right) - \eta \left(\mathbb{P}(\mathbf{y}_w \succ \mathbf{y}_l | \mathbf{x}) - \frac{1}{2} \right) \right)^2 + \left(\log \left(\frac{\pi_{\boldsymbol{\theta}}(\mathbf{y}_l | \mathbf{x})}{\pi_{\text{ref}}(\mathbf{y}_l | \mathbf{x})} \right) - \eta \left(\mathbb{P}(\mathbf{y}_w \prec \mathbf{y}_l | \mathbf{x}) - \frac{1}{2} \right) \right)^2, \tag{B.1}$$

where $\mathbb{P}(\mathbf{y}_w \succ \mathbf{y}_l | \mathbf{x})$ can be either a soft probability within [0,1] or a hard label 1 indicating $\mathbf{y}_w \succ \mathbf{y}_l$. We now compare the SPPO loss to other baselines assuming a hard label $\mathbf{y}_w \succ \mathbf{y}_l$ is given. For the ease of comparison, let

$$a = \beta \log\left(\frac{\pi_{\boldsymbol{\theta}}(\mathbf{y}_w | \mathbf{x})}{\pi_{\text{ref}}(\mathbf{y}_w | \mathbf{x})}\right), b = \beta \log\left(\frac{\pi_{\boldsymbol{\theta}}(\mathbf{y}_l | \mathbf{x})}{\pi_{\text{ref}}(\mathbf{y}_l | \mathbf{x})}\right), c = \beta \text{KL}(\pi_{\boldsymbol{\theta}} \| \pi_{\text{ref}}),$$

then we have

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$$\ell_{\text{DPO}}(\mathbf{y}_w, \mathbf{y}_l, \mathbf{x}) = -\log \sigma(a-b), \tag{B.2}$$

$$\ell_{\rm IPO}(\mathbf{y}_w, \mathbf{y}_l, \mathbf{x}) = [(a-b)-1]^2, \tag{B.3}$$

$$\ell_{\text{KTO}}(\mathbf{y}_w, \mathbf{y}_l, \mathbf{x}) = \sigma(-a+c) + \sigma(b-c) \text{ (simplified)}, \tag{B.4}$$

where $\sigma(x) = e^x/(e^x + 1)$ and the SPPO loss can be written as

$$\ell_{\text{SPPO}}(\mathbf{y}_w, \mathbf{y}_l, \mathbf{x}) = (a - 1/2)^2 + (b + 1/2)^2$$

433 It can be seen that SPPO not only pushes the gap between a and b to be 1, but also attempts to push value of a to be close to 434 1/2 and the value of b to be close to -1/2 such that $\pi_{\theta}(\mathbf{y}_w|\mathbf{x}) > \pi_{\text{ref}}(\mathbf{y}_w|\mathbf{x})$ and $\pi_{\theta}(\mathbf{y}_l|\mathbf{x}) < \pi_{\text{ref}}(\mathbf{y}_l|\mathbf{x})$. We believe this is 435 particularly important: when there are plenty of preference pairs, DPO and IPO can ensure the policy will converge to the 436 target policy, but when the preference pairs are scarce (e.g., one pair for each prompt), there is no guarantee that the estimated 437 reward of the winner a will increase and the estimated reward of the loser b will decrease. Instead, only the reward gap 438 between the winner and the loser (i.e., a - b) will increase. This phenomenon is observed by Pal et al. (2024) that DPO only 439

drives the loser's likelihood to be small, but the winner's likelihood barely changes. We believe that fitting $\beta \log \left(\frac{\pi_{t+1}(\mathbf{y}|\mathbf{x})}{\pi_t(\mathbf{y}|\mathbf{x})}\right)$ directly to $\mathbb{P}(\mathbf{y} \succ \pi_t | \mathbf{x}) - 1/2$ is more effective than IPO which attempts to fit $\beta \log \left(\frac{\pi_{t+1}(\mathbf{y}_w | \mathbf{x})}{\pi_t(\mathbf{y}_w | \mathbf{x})}\right) - \beta \log \left(\frac{\pi_{t+1}(\mathbf{y}|\mathbf{x})}{\pi_t(\mathbf{y}_t | \mathbf{x})}\right)$ to $\mathbb{P}(\mathbf{y}_w \succ \pi_t | \mathbf{x}) - \mathbb{P}(\mathbf{y}_l \succ \pi_t | \mathbf{x})$. In addition, SPPO shares a similar spirit as KTO. The KTO loss pushes *a* to be large by minimizing $\sigma(-a+c)$ and pushes *b* to be small by minimizing $\sigma(b-c)$. In contrast, SPPO pushes *a* to be as large as 1/2and *b* to be as small as -1/2.

On the other hand, we would like to comment that although DPO and KTO can be extended to their iterative variants, they are not by nature iterative algorithms and do not have provable guarantees that they can reach the Nash equilibrium. In contrast, SPPO and IPO are by design capable to solve the Nash equilibrium iteratively. SPPO is superior to IPO because its design explicitly alleviates the data sparsity issue, as discussed above and detailed in Pal et al. (2024).

451 C Experiment Setup

Base Model and Datasets We follow the experimental setup of Snorkel³, a model that utilizes iterative DPO to achieve state-of-the-art performance on AlpacaEval benchmarks. Specifically, we use Mistral-7B-Instruct-v0.2 as our base model⁴. Mistral-7B-Instruct-v0.2 is an instruction fine-tuned version of Mistral-7B-v0.2 model (Jiang et al., 2023a). We also adopt Ultrafeedback (Cui et al., 2023) as our source of prompts which includes around 60k prompts from diverse resources. During generation, we follow the standard chat template of Mistral-7B. In order to avoid overfitting during the fine-tuning, we split the dataset into three portions and use only one portion per iteration. These settings were also adopted by training the model Snorkel-Mistral-PairRM-DPO⁵ (Snorkel). We follow the splitting in Snorkel for a fair comparison.

Preference Model We employ PairRM (Jiang et al., 2023b), an efficient pair-wise preference model of size 0.4B. PairRM is based on DeBERTA-V3 (He et al., 2021) and trained on high-quality human-preference datasets. Results on benchmarks like Auto-J Pairwise dataset (Li et al., 2023a) show that it outperforms most of the language-model-based reward models and performs comparably with larger reward models like UltraRM-13B (Cui et al., 2023). We refer the readers to the homepage on Huggingface⁶ for detailed benchmark results. We therefore keep PairRM as our ranking model following Snorkel for a balance between accuracy and efficiency.

466 Specifically, PairRM will output a "relative reward" $s(\mathbf{y}, \mathbf{y}'; \mathbf{x})$ that reflects the strength difference between \mathbf{y} and \mathbf{y}' , i.e., 467 $\mathbb{P}(\mathbf{y} \succ \mathbf{y}' | \mathbf{x}) = \frac{\exp(s(\mathbf{y}, \mathbf{y}'; \mathbf{x}))}{1 + \exp(s(\mathbf{y}, \mathbf{y}'; \mathbf{x}))}$. Unlike the Bradley-Terry-based reward model, PairRM only assigns the relative reward 468 which is not guaranteed to be transitive (i.e., $s(\mathbf{y}_1, \mathbf{y}_2; \mathbf{x}) + s(\mathbf{y}_2, \mathbf{y}_3; \mathbf{x}) \neq s(\mathbf{y}_1, \mathbf{y}_3; \mathbf{x})$). So it indeed models the general 469 preference.

Response Generation and Selection During the generation phase in each iteration, we use top p = 1.0 and temperature 1.0 to sample from the current policy. We sample with different random seeds to get K = 5 different responses for each prompt. Previous works utilizing Iterative DPO choose 2 responses to form a pair for each prompt. For a fair comparison, we do not include all K = 5 responses in the preference data but choose two responses among them. Following Snorkel, we choose the winner \mathbf{y}_w and loser \mathbf{y}_l to be the response with the *highest* and *lowest* PairRM score, which is defined for each response \mathbf{y}_i as:

$$s_{\text{PairRM}}(\mathbf{y}_i; \mathbf{x}) := \frac{1}{K} \sum_{k=1}^{K} s(\mathbf{y}_i, \mathbf{y}_k; \mathbf{x})$$

481 Probability Estimation We then estimate the win rate over the distribution by the average win rate over all the sampled 482 responses as explained in (3.6):

$$\widehat{P}(\mathbf{y}_i \succ \pi_t | \mathbf{x}_i) = \frac{1}{K} \sum_{k=1}^{K} \mathbb{P}(\mathbf{y}_i \succ \mathbf{y}_k | \mathbf{x}), \forall i \in [K].$$

487 **Hyperparameter Tuning** The experiments are conducted on $8 \times$ Nvidia A100 GPUs. For SPPO, we trained three 488 iterations in total. In each iteration, we selected the model that was trained on the first epoch of the 20k prompts from 489 UltraFeedback to proceed to the next iteration. The global training batch size is set to 64 and η is set to 1*e*3. The learning 490

^{491 &}lt;sup>3</sup>https://huggingface.co/snorkelai/Snorkel-Mistral-PairRM-DPO

^{492 &}lt;sup>4</sup>https://huggingface.co/mistralai/Mistral-7B-Instruct-v0.2

⁴⁹² Shttps://huggingface.co/snorkelai/Snorkel-Mistral-PairRM-DPO

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- 495 rate schedule is determined by the following hyperparameters: learning rate=5.0e-7, number of total training epochs=18,
- 496 warmup ratio=0.1, linear schedule. The best hyper-parameters for each model is selected by the average win-rate (judged 497 by PairRM-0.4B) on a hold-out subset of Ultrafeedback as the metric. For more details on the win-rate comparison using 498 DairRM-0.4B) on a hold-out subset of Ultrafeedback as the metric. For more details on the win-rate comparison using 499 DairRM-0.4B) on a hold-out subset of Ultrafeedback as the metric. For more details on the win-rate comparison using 490 DairRM-0.4B) on a hold-out subset of Ultrafeedback as the metric.
- 498 PairRM as a judge, please refer to Section 4.2 and Figure 3.
- Baselines We evaluate the following base models as well as baseline methods for fine-tuning LLMs:
- Mistral-7B-Instruct-v0.2: Mistral-7B-Instruct-v0.2 is an instruction fine-tuned version of Mistral-7B-v0.2 model (Jiang et al., 2023a). It is the starting point of our algorithm.
- Snorkel (Mistral-PairRM-DPO): We directly evaluate the uploaded checkpoint on HuggingFace⁷. This model is obtained by three rounds of iterative DPO from Mistral-7B-Instruct-v0.2.
- (Iterative) DPO: We also implement the iterative DPO algorithm by ourselves. The experimental settings and model selection schemes align with those used for SPPO, except for the adoption of the DPO loss function as defined in (B.2). Hyperparameters are optimized to maximize the average win-rate assessed by PairRM at each iteration. Note that the practical algorithm in Rosset et al. (2024) is essentially the same as iterative DPO.
- (Iterative) IPO: We implement the iterative IPO algorithm by ourselves. The experimental setting and the model selection scheme is the same as iterative DPO, except that the loss function is the IPO loss (B.3). For fair comparison, hyperparameters for IPO is also selected by evaluation using the average PairRM win-rate on the hold-out subset of Ultrafeedback.
- Self-rewarding LM: Yuan et al. (2024) proposed to prompt the LLM itself as a preference judge to construct new preference pairs and iteratively fine-tune the LLM with the DPO algorithm. We use the AlpacaEval 2.0 win rate reported by Yuan et al. (2024) for comparison. Note that Self-rewarding LM is a trained from Llama 2 70B.
- Benchmarks Following previous works, we use AlpacaEval 2.0 (Dubois et al., 2024a), MT-Bench (Zheng et al., 2024), and Open LLM Leaderboard (Beeching et al., 2023b) as our evaluation benchmarks.
- AlpacaEval 2.0 is an LLM-based automatic evaluation benchmark. It employs AlpacaFarm (Dubois et al., 2024b) as its prompts set composed of general human instructions. The model responses and the reference response generated by GPT-4-Turbo are fed into a GPT-4-Turbo-based annotator to be judged. We follow the standard approach and report the win rate over the reference responses.
- MT-Bench (Zheng et al., 2024) is a collection of 80 high-quality multi-turn open-ended questions. The questions cover topics like writing, role-playing, math, coding, etc.. The generated answer is judged by GPT-4 and given a score directly without pairwise comparison.
- Open LLM Leaderboard (Beeching et al., 2023b) consists of six datasets, each of which focuses on a facet of language model evaluation. In detail, the evaluation rubric includes math problem-solving, language understanding, human falsehood mimicking, and reasoning. We follow the standard evaluation process and use in-context learning to prompt the language model and compute the average score over six datasets to measure the performance.

535 536 **D** Additional Results

537 **D.1 MT-Bench results**

We also provide a radar chart analyzing the MT-Bench results in Figure 1 (right). We found that the performance of SPPO models consistently improve along with the iterative alignment iterations.

In Figure 1 (left), we evaluate the performance of SPPO on MT-Bench. We can see that SPPO Iter3 outperforms all baseline models, achieving an average score of 7.59. While we are not certain why the MT-Bench performance drops at the first two iterations, the performance of SPPO at the final iteration still improves over the base model. Since the length-controlled AlpacaEval 2.0 has a 98% Pearson correlation with human evaluations and 10× more evaluation prompts, it likely provides a more reliable evaluation than MT-Bench. To gain deeper understanding on MT-Bench performance, we plot the improvement in Figure 1 (right), broken down by question prompt category. SPPO Iter3 demonstrates notable gains in RolePlay, Reasoning, Math, and Coding tasks.

⁵⁴⁸ ⁷https://huggingface.co/snorkelai/Snorkel-Mistral-PairRM-DPO

Self-Play Preference Optimization for Language Model Alignment

				Writing
Model	 1st Turn	MT-Bench 2nd Turn	Average	Humanities Roleplay SPPO Iter1 SPPO Iter2
Mistral-7B-Instruct-v0.2	7.78	7.25	7.51	SPPO Iter3
Snorkel (Mistral-PairRM-DPO)	7.83	7.33	7.58	
DPO Iter1	7.45	6.58	7.02	STEM 0 2 4 6 8 10 Reasoning
DPO Iter2	7.57	6.56	7.06	
DPO Iter3	7.49	6.69	7.09	
SPPO Iter1	7.63	6.79	7.21	
SPPO Iter2	7.90	7.08	7.49	Extraction Math
SPPO Iter3	7.84	7.34	7.59	
				- Coging

Figure 1: **MT-Bench Evaluation.** Left: SPPO Iter3 outperforms all baseline models by achieving an average score of 7.59. Despite initial drops in performance in the first two iterations, SPPO Iter3 improves upon the base model by the final iteration. Right: Radar chart of MT-Bench results. SPPO Iter3's improves across different MT-Bench categories, showing significant gains in RolePlay, Reasoning, Math, and Coding tasks.

568 569 **D.2 Open LLM Leaderboard results**

570 Table 3: **Open LLM Leaderboard Evaluation**. SPPO fine-tuning improves the base model's performance on Arc, 571 TruthfulQA, and GSM8k, reaching a state-of-the-art average score of 66.75. However, subsequent iterations of DPO, IPO, 572 and SPPO see a decline in performance. It is possible that aligning with human preferences (simulated by the PairRM 573 preference model in our study) may not always enhance, and can even detract from, overall performance.

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Models	Arc	TruthfulQA	WinoGrande	GSM8k	HellaSwag	MMLU	Average
Mistral-7B-Instruct-v0.2	63.65	66.85	77.98	41.93	84.89	59.15	65.74
Snorkel	66.04	70.86	77.74	36.77	85.64	60.83	66.31
DPO Iter1	63.14	68.39	77.19	40.33	85.25	59.41	65.62
DPO Iter2	64.16	67.84	76.09	39.95	85.23	59.03	65.38
DPO Iter3	65.19	67.89	77.27	32.30	85.49	59.00	64.52
IPO Iter1	64.68	68.60	77.98	43.75	85.08	59.04	66.52
IPO Iter2	62.12	66.30	77.51	39.20	83.15	59.70	64.66
IPO Iter3	62.97	67.12	77.51	37.45	83.69	59.57	64.72
SPPO Iter1	65.02	69.40	77.82	43.82	85.11	58.84	66.67
SPPO Iter2	65.53	69.55	77.03	44.35	85.29	58.72	66.75
SPPO Iter3	65.36	69.97	76.80	42.68	85.16	58.45	66.40

590 **Open LLM Leaderboard** We further evaluate the capabilities of SPPO models using Huggingface Open LLM Leader-591 board (Beeching et al., 2023a). This leaderboard encompasses 6 different datasets, each focusing on a a specific capability of 592 LLMs: Arc (Clark et al., 2018), HellaSwag (Zellers et al., 2019), Winogrande (Sakaguchi et al., 2021), MMLU (Hendrycks 593 et al., 2020), TruthfulQA (Lin et al., 2021), and GSM8k (Cobbe et al., 2021). The models are prompted with zero or few-shot 594 exemplars. The results, presented in Table 3, demonstrate that SPPO can enhance the performance of the base model on Arc, 595 TruthfulQA, and GSM8k, and achieve the state-of-the-art performance with an averagte score of 66.75. However, these 596 improvements do not hold in subsequent alignment iterations: DPO, IPO, and SPPO's performance declines after the first 597 or second iterations. This limitation may be attributed to the "alignment tax" phenomenon (Askell et al., 2021), which 598 suggests that aligning with human preferences (simulated by PairRM preference in our study) might not improve or even 599 hurt the general performance. Improving language model capabilities through alignment iterations remains a topic for future 600 research, and we posit that incorporating high-quality SFT annotations (Chen et al., 2024) could play a significant role in 601 this endeavor.

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605 D.3 Comparing RLHF algorithms over iterations

In Figure 2, we plot the win rate against GPT-4-Turbo on AlpacaEval 2.0 of different RLHF algorithms. We can see that the performance gains of SPPO over previous iterations are 7.69% (Mistral-7B-Instruct \rightarrow Iter1), 2.10% (Iter1 \rightarrow Iter2), and 1.64% (Iter2 \rightarrow Iter3), respectively, indicating steady improvements across iterations.



Figure 2: Win Rate against GPT-4-Turbo with (a) and without (b) Length Controlling (LC) on AlpacaEval 2.0. SPPO
 demonstrates steady improvements on both LC and raw win rates.

D.4 Evaluation using PairRM as a judge

As SPPO identifies the von Neumann winner (see (2.1)) in a two-player constant-sum game, we examine the pairwise preferences among SPPO models and other baselines. The pairwise win rates, measured by PairRM, are depicted in Figure 3. We observe that in all algorithms—namely DPO, IPO, and SPPO—the newer model iterations surpass the previous ones. For example, SPPO Iteration 3 outperforms SPPO Iteration 2. Both SPPO and IPO consistently outperform DPO across all iterations. While SPPO is superior to IPO in the first two iterations, IPO exceeds SPPO in performance during the final iteration. Considering the superior performance of SPPO in standard benchmarks evaluated by GPT-4 or against ground-truth answers (e.g., AlpacaEval 2.0, MT-Bench, and Open LLM Leaderboard), along with IPO's tendency to produce longer sequence outputs (see Avg. Len in Table 1), we believe this is due to IPO exploiting the length bias in PairRM that favors longer sequences. Conversely, SPPO models benefit from a more robust regularization within a multiplicative weight update framework.

D.5 Ablation Study

We study the effect of mini-batch size when estimating the win rate $\mathbb{P}(\mathbf{y} \succ \pi_t | \mathbf{x})$. Specifically, for each prompt, we still generate 5 responses and choose the winner \mathbf{y}_w and loser \mathbf{y}_l according to the PairRM score. When estimating the probability, we varies the batch size to be K = 2, 3, 5. For K = 2, we estimate $\mathbb{P}(\mathbf{y} \succ \pi_t | \mathbf{x})$ with only 2 samples \mathbf{y}_w and \mathbf{y}_l :

$$\widehat{P}(\mathbf{y}_w \succ \pi_t | \mathbf{x}) = \frac{\mathbb{P}(\mathbf{y}_w \succ \mathbf{y}_w | \mathbf{x}) + \mathbb{P}(\mathbf{y}_w \succ \mathbf{y}_l | \mathbf{x})}{2} = \frac{1/2 + \mathbb{P}(\mathbf{y}_w \succ \mathbf{y}_l | \mathbf{x})}{2},$$

and $\widehat{P}(\mathbf{y}_l \succ \pi_t | \mathbf{x})$ similarly. K = 5 indicates the original setting we use.

We compare the results on AlpacaEval 2.0, as shown in Figure 4. We find that the performance of SPPO is robust to the noise in estimating $\mathbb{P}(\mathbf{y} \succ \pi_t | \mathbf{x})$. While K = 5 initially outperforms K = 2 in the first iteration, the difference in their performance diminishes in subsequent iterations. Additionally, we observe that K = 2 exhibits a reduced tendency to increase output length.

E Proof of Theorem 3.1

Proof of Theorem 3.1. Suppose the optimization problem is realizable, we have exactly that

$$\pi_{t+1}(\mathbf{y}|\mathbf{x}) \propto \pi_t(\mathbf{y}|\mathbf{x}) \exp(\eta \mathbb{P}(\mathbf{y} \succ \pi_t|\mathbf{x})), \text{ for } t = 1, 2, \dots$$
(E.1)

To prove that the exponential weight update can induce the optimal policy, we directly invoke a restated version of Theorem 1 in Freund & Schapire (1999):





Figure 3: Pairwise win rates among base model (Mistral-7B-Instruct-v0.2), DPO models, IPO models, and SPPO models using **PairRM-0.4B** as a judge, which may favor models with longer outputs. On benchmarks with more powerful judge models (e.g., GPT-4), such as AlpacaEval 2.0 and MT-Bench, SPPO outperforms other baseline algorithms by a large margin.

					28				
Mini Datah		AlpacaEval 2.0		20					
Nillii-Balcii	Iteration	Win	Rate	Avg. Len	_ 26				
Size		LC.	Raw	(chars)	%) %)				
	Iter1	23.85	23.53	1948	Rate	•			
K = 2	Iter2	26.91	27.24	1999	^{بل} 22				
	Iter3	28.26	28.22	1961	Ú.		Snorkel (Mistra	l-PairRM-DPO)	
	Iter1	24.79	23.51	1855	- 20		Mistral-7B-Instr	uct-v0.2	
K = 5	Iter2	26.89	27.62	2019	18	_•_	SPPO $(K=2)$ SPPO $(K=5)$		
	Iter3	28.53	31.02	2163	-	tor1			ltor?
						Leit	ILE	12	iter:

Figure 4: AlpacaEval 2.0 evaluation on SPPO of different mini-batch size in terms of both normal and length-controlled (LC) win rates in percentage (%). K = 2,5 denote different mini-batch sizes when estimating the win rate $\mathbb{P}(\mathbf{y} \succ \pi_t | \mathbf{x})$.

Lemma E.1 (Theorem 1 in Freund & Schapire (1999), restated). For any oracle \mathbb{P} and for any sequence of mixed policies $\mu_1, \mu_2, \ldots, \mu_T$, the sequence of policies $\pi_1, \pi_2, \ldots, \pi_T$ produced by (E.1) satisfies:

$$\sum_{t=1}^{T} \mathbb{P}(\pi_t \prec \mu_t) \leq \min_{\pi} \left[\frac{\eta}{1 - e^{-\eta}} \sum_{t=1}^{T} \mathbb{P}(\pi \prec \mu_t) + \frac{\mathrm{KL}(\pi \| \pi_0)}{1 - e^{-\eta}} \right]$$

715 By setting $\mu_t = \pi_t$, we have that

$$\frac{T}{2} \le \min_{\pi} \left[\frac{\eta T}{1 - e^{-\eta}} \mathbb{P}(\pi \prec \bar{\pi}_T) + \frac{\mathrm{KL}(\pi \| \pi_0)}{1 - e^{-\eta}} \right],$$

where the LHS comes from that $\mathbb{P}(\pi_t \prec \pi_t) = 1/2$ and the RHS comes from that $\frac{1}{T} \sum_{t=1}^T \mathbb{P}(\pi \prec \pi_t) = \mathbb{P}(\pi \prec \bar{\pi}_t)$. Now rearranging terms gives

$$\frac{1-e^{-\eta}}{2\eta} \le \min_{\pi} \left[\mathbb{P}(\pi \prec \bar{\pi}_T) + \frac{\mathrm{KL}(\pi \| \pi_0)}{\eta T} \right].$$

We can naively bound the KL-divergence $\operatorname{KL}(\pi \| \pi_0) \leq \|\log \pi_0(\cdot)\|_{\infty}$, which can be seen as a (large) constant. By choosing $\eta = \frac{\|\log \pi_0(\cdot)\|_{\infty}}{\sqrt{T}}$, we have

$$\frac{1}{2} - \frac{\|\log \pi_0(\cdot)\|_{\infty}}{4\sqrt{T}} + O(T^{-1}) \le \min_{\pi} \left[\mathbb{P}(\pi \prec \bar{\pi}_T) \right] + \sqrt{\frac{\|\log \pi_0(\cdot)\|_{\infty}}{T}}$$

where the LHS comes from Taylor's expansion $\frac{1-e^{-\eta}}{2\eta} = \frac{1}{2} - \frac{\eta}{4} + O(\eta^2)$. Notice that 1/2 at the LHS is already the value of the symmetric two-player constant-sum game. This shows that for appropriately chosen η and T, the mixture policy $\bar{\pi}_T$ is close to the minimax optimal policy (Nash equilibrium).

⁵ The optimality gap is thus bounded by

$$\begin{aligned} \max_{\pi} \left[\mathbb{P}(\pi \succ \bar{\pi}_T) \right] &- \min_{\pi} \left[\mathbb{P}(\pi \prec \bar{\pi}_T) \right] \\ &= \max_{\pi} \left[1 - \mathbb{P}(\pi \prec \bar{\pi}_T) \right] - \min_{\pi} \left[\mathbb{P}(\pi \prec \bar{\pi}_T) \right] \\ &= 2 \left(\frac{1}{2} - \min_{\pi} \left[\mathbb{P}(\pi \prec \bar{\pi}_T) \right] \right) \\ &= O\left(\frac{1}{\sqrt{T}} \right). \end{aligned}$$

F Response Examples in Different Iterations

PromptYou will be given a definition of a task first, then some input between 2 or more individuals. The dialog will include informa of the participants. At the end, you will be asked to provide an 2 participants. In this scenario, '0' will represent a spousal rel and '2' will represent a child/parent relationship. Speaker 1: I Wendy. Speaker 2: Oh my God! How cute is the on-call docto thinking about jamming this pen in my eye. Speaker 4: Dr. Bur no-no-no, not Dr. Burke. Dr. Burke is out of town. The-the on-c Dr. Richard Burke is out of town. Dr. Timothy Burke, his son, What is the relationship between Speaker 5 and Richard Burke?Mistral-7BThe relationship between Speaker 5 and Richard Burke is that of is identified as the son of another character in the dialog.Iteration 1The relationship between Speaker 5 and Richard Burke is that of is identified as the son of another character in the dialog.Iteration 2The relationship between Speaker 5 and Richard Burke is that of reveals that Dr. Timothy Burke is the on-call Burke.Iteration 3Speaker 5 is the individual asking about the relationship, so they Burke. The information provided in the dialog reveals that Dr. and the son of Dr. Richard Burke. Therefore, the answer is: The Dr. Richard Burke is that of a divid (Dr. Timothy Burke) and participants.	of the task. You are given a dialog tion as to the relationship between 2 inswer as to the relationship of those itionship, '1' will represent siblings Il be right with you. Okay? Thanks ? Speaker 3: Ooh, so cute, that I'n the will see you know. Speaker 2: Of Il doctor will see me now. Speaker 4 vill see you now. Speaker 5: Ready Output: a parent and child, as Richard Burker of a father and child. Based on the I doctor and the son of Dr. Richard
Mistral-7BThe relationship between Speaker 5 and Richard Burke is that of is identified as the son of another character in the dialog.Iteration 1The relationship between Speaker 5 and Richard Burke is that dialogue, it was revealed that Dr. Timothy Burke is the on-ca Burke.Iteration 2The relationship between Speaker 5 and Richard Burke is that or reveals that Dr. Timothy Burke is the on-call doctor and he is Burke.Iteration 3Speaker 5 is the individual asking about the relationship, so they Burke. The information provided in the dialog reveals that Dr. and the son of Dr. Richard Burke. Therefore, the answer is: The Dr. Richard Burke is that of a shild (Dr. Timothy Burke) and point	a parent and child, as Richard Burko of a father and child. Based on the l doctor and the son of Dr. Richard
Iteration 1The relationship between Speaker 5 and Richard Burke is that dialogue, it was revealed that Dr. Timothy Burke is the on-ca Burke.Iteration 2The relationship between Speaker 5 and Richard Burke is that or reveals that Dr. Timothy Burke is the on-call doctor and he is Burke.Iteration 3Speaker 5 is the individual asking about the relationship, so they Burke. The information provided in the dialog reveals that Dr. and the son of Dr. Richard Burke. Therefore, the answer is: The Dr. Richard Burke is that of a shild (Dr. Timothy Burke) and po	of a father and child. Based on the l doctor and the son of Dr. Richard
Iteration 2The relationship between Speaker 5 and Richard Burke is that o reveals that Dr. Timothy Burke is the on-call doctor and he is Burke.Iteration 3Speaker 5 is the individual asking about the relationship, so they Burke. The information provided in the dialog reveals that Dr. and the son of Dr. Richard Burke. Therefore, the answer is: The Dr. Bighard Burke is that of a shild (Dr. Timothy Burke) and part	
Iteration 3 Speaker 5 is the individual asking about the relationship, so they Burke. The information provided in the dialog reveals that Dr. and the son of Dr. Richard Burke. Therefore, the answer is: The Dr. Bishard Burke is that of a shild (Dr. Timothy Burke) and pa	a father and child. The conversation identified as the son of Dr. Richard
relationship, but they are not themselves a part of it. The specific for sibling, 2 for child/parent) align with this description: Speake (2) connect as a parent-child duo. Output: 2 (child/parent relati role is to determine the relationship between herself and Dr. R related (she is an outside inquirer), the correct answer pertains on the dialog: Dr. Richard Burke (father) and Dr. Timothy Burke (st	re not directly related to Dr. Richard Timothy Burke is the on-call doctor relationship between Speaker 5 and ent. Speaker 5 is inquiring about the d relationship codes (0 for spousal, 1 c 5 (0, 1, or 2) and Dr. Richard Burke onship) In this scenario, Speaker 5's ichard Burke, but since they are not y to the relationship identified within on).

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835	Tab	le 5: Another generation example of our fine-tuned model by SPPO at different iterations.
836 837 838 839 840 841	Prompt	Q: Context: Roman Brady is a fictional character from the long running NBC soap opera, Days of Our Lives. The role was originated in 1981 by Wayne Northrop who played the role until 1984, was filled by Drake Hogestyn from 1986 – 1991, again by Northrop from 1991 – 1994, and is currently being portrayed by series veteran Josh Taylor, who stepped into the role in 1997. Question: who is roman brady on days of our lives? Let's give stream of consciousness below
841 842 843 844 845	Mistral-7B	Roman Brady is a fictional character on the NBC soap opera "Days of Our Lives." He was first portrayed by Wayne Northrop from 1981 to 1984. Later, Drake Hogestyn took over the role from 1986 to 1991. Northrop returned to the role from 1991 to 1994. Since 1997, the character is being portrayed by Josh Taylor. Roman Brady is a significant character in the show's long-running storylines.
846 847 848 849 850 851	Iteration 1	Roman Brady is a fictional character on the NBC soap opera "Days of Our Lives." He was first portrayed by Wayne Northrop from 1981 to 1984. Drake Hogestyn took over the role from 1986 to 1991. Northrop returned to play Roman again from 1991 to 1994. Since 1997, the character has been portrayed by Josh Taylor. So, in summary, Roman Brady is a long-standing character on "Days of Our Lives" who has been played by three different actors over the years: Wayne Northrop (1981-1984, 1991-1994), Drake Hogestyn (1986-1991), and currently by Josh Taylor (1997-present).
852 853 854 855 856 856	Iteration 2	Roman Brady is a fictional character on the NBC soap opera "Days of Our Lives." He was first portrayed by Wayne Northrop from 1981 to 1984. Drake Hogestyn took over the role from 1986 to 1991. Northrop returned to play Roman again from 1991 to 1994. Since 1997, the character has been portrayed by Josh Taylor. Overall, Roman Brady is a long-standing and complex figure in the show's history, with multiple actors bringing their unique interpretations to the role.
858 859 860 861 862 863 864 865 866 866 866 867 868	Iteration 3	Roman Brady is a fictional character on the NBC soap opera "Days of Our Lives." He was originally played by Wayne Northrop from 1981 to 1984. Drake Hogestyn took over the role from 1986 to 1991. Northrop returned to portray Roman once more from 1991 to 1994. Since 1997, the character has been portrayed by Josh Taylor.Roman Brady is a complex and prominent figure in the long-running daytime drama. Initially played by Northrop in the early 1980s, his tenure included involvement in various storylines, such as romantic relationships and business dealings. Hogestyn's portrayal during the late 1980s and early 1990s introduced new dimensions to the character. Northrop's second stint, from 1991 to 1994, further developed Roman's narrative. Since 1997, Josh Taylor has assumed the role, continuing to contribute to the evolving story of Roman Brady on "Days of Our Lives." Throughout these different portrayals, Roman has remained a central character, known for his intricate relationships, business ventures, and personal struggles.
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Self-Play Preference Optimization for Language Model Alignment