# Triple Preference Optimization: Achieving Better Alignment with Less Data in a Single Step Optimization

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#### Abstract

 Large Language Models (LLMs) perform well across diverse tasks, but aligning them with hu- man demonstrations is challenging. Recently, Reinforcement Learning (RL)-free methods like Direct Preference Optimization (DPO) have emerged, offering improved stability and scalability while retaining competitive perfor- mance relative to RL-based methods. However, while RL-free methods deliver satisfactory per- formance, *they require significant data to de- velop a robust Supervised Fine-Tuned (SFT) model* and *an additional step to fine-tune this model on a preference dataset*, which con- strains their utility and scalability. In this paper, we introduce Triple Preference Optimization **(TPO)**, a new preference learning method de-017 signed to align an LLM with three preferences without requiring a separate SFT step and using considerably less data. Through a combination of practical experiments and theoretical analy- sis, we show the efficacy of TPO as a single-022 step alignment strategy. Specifically, we fine- tuned the Phi-2 (2.7B) and Mistral (7B) mod- els using TPO directly on the UltraFeedback dataset, achieving superior results compared to models aligned through other methods such as SFT, DPO, KTO, IPO, CPO, and ORPO. More- over, the performance of TPO without the SFT component led to notable improvements in the **MT-Bench score, with increases of +1.27 and +0.63** over SFT and DPO, respectively. Addi- tionally, TPO showed higher average accuracy, **Surpassing DPO and SFT by 4.2% and 4.97%** on the Open LLM Leaderboard benchmarks.

#### **035** 1 Introduction

 LLMs are trained across a wide array of tasks, demonstrating their remarkable versatility in solv- [i](#page-9-0)ng diverse tasks [\(Brown et al.,](#page-8-0) [2020;](#page-8-0) [Narayanan](#page-9-0) [et al.,](#page-9-0) [2021;](#page-9-0) [Bubeck et al.,](#page-8-1) [2023\)](#page-8-1). However, their training on data of varying quality can lead to many issues, such as the generation of toxic or harmful [t](#page-9-2)ext under certain contexts [\(Perez et al.,](#page-9-1) [2022;](#page-9-1) [Gan-](#page-9-2)[guli et al.,](#page-9-2) [2022\)](#page-9-2), and in general, the generation of

<span id="page-0-0"></span>

Figure 1: Comparison of the loss functions of TPO and DPO. TPO's loss function incorporates two main objectives. Its first term optimizes the log probability of preferences ( $\mathcal{L}_{\text{preference}}(\pi_{\theta})$ ), which demonstrates that optimizing preferences doesn't necessitate a reference model (See Section [3\)](#page-2-0). Through its second term, TPO aims to learn the gold standard response ( $\mathcal{L}_{\text{reference}}$ ). This aspect of the loss function is regulated by a parameter  $\alpha$ , which serves as a parameter controlling the extent to which the policy model learns the gold standard response.

outputs that are not desired by humans. Hence, it **044** is crucial to align LLMs with human expectations **045** and preferences that prioritize their helpfulness, **046** honesty, and harmlessness [\(Bai et al.,](#page-8-2) [2022\)](#page-8-2). **047**

Supervised Fine-Tuning (SFT) is a direct align- **048** ment method that involves fitting a model to human- **049** written data [\(Sanh et al.,](#page-10-0) [2022\)](#page-10-0). However, this ap- 050 proach fails to fully impart the human perspective **051** to the model. During training, the model only re- **052** ceives a reference response for each input, thus **053** lacking exposure to incorrect answers and prefer- **054** ences, which ultimately constrains its performance **055** on downstream tasks [\(Touvron et al.,](#page-10-1) [2023\)](#page-10-1). **056**

A prominent method in AI alignment for LLMs **057**

 is Reinforcement Learning with Human Feedback (RLHF) [\(Ouyang et al.,](#page-9-3) [2022\)](#page-9-3). Despite its impres- sive performance relative to SFT, RLHF faces limi- tations such as instability and susceptibility to re- ward hacking [\(Liu et al.,](#page-9-4) [2024\)](#page-9-4). Consequently, a recent approach called Direct Preference Optimiza- tion (DPO) [\(Rafailov et al.,](#page-9-5) [2023\)](#page-9-5) has emerged. DPO is an RL-free method that directly optimizes human preferences by shifting from RL to simple binary cross-entropy. However, DPO encounters several limitations: 1) high dependency on the SFT part [\(Tunstall et al.,](#page-10-2) [2023\)](#page-10-2), 2) tendency to overfit beyond a single epoch [\(Azar et al.,](#page-8-3) [2023\)](#page-8-3), and 3) in- efficient learning and memory utilization [\(Xu et al.,](#page-10-3) **072** [2024\)](#page-10-3).

 To address these limitations, various alignment methods have been proposed for dialogue systems [\(Tunstall et al.,](#page-10-2) [2023\)](#page-10-2), harmful and helpfulness **question answering [\(Wu et al.,](#page-10-4) [2023\)](#page-10-4), summariza-** tion [\(Zhao et al.,](#page-10-5) [2023\)](#page-10-5), and translation [\(Xu et al.,](#page-10-3) [2024\)](#page-10-3) and all these studies include a separate SFT component. During SFT, models are fine-tuned to generate appropriate responses to the correspond- ing input prompts. Meanwhile, in DPO, models are fine-tuned to enhance the likelihood of generating preferred responses over less desirable ones and [n](#page-9-5)ot to stray far away from the SFT model [\(Rafailov](#page-9-5) [et al.,](#page-9-5) [2023\)](#page-9-5).

 In this paper, we introduce the Triple Pref-**erence Optimization (TPO), a new preference**  learning approach. In TPO, we combine the two separate optimization steps (supervised fine-tuning and preference learning) into a single [s](#page-9-6)tep based on Pareto Front concept [\(Lotov and](#page-9-6) [Miettinen,](#page-9-6) [2008\)](#page-9-6), with the training data having both the gold standard response (as in SFT) and the preferences (as in PPO/DPO) in a consolidated format. Thus, our training data will be of the form *(input prompt, gold standard response* (yref )*, preferred response* (yw)*, less-preferred response* 098 (y<sub>l</sub>)). Specifically, we jointly optimize a policy **model** with  $-\mathbb{E}_{(x,y_{ref})\sim\mathcal{D}}[\log \pi_{\theta}(y_{ref} | x)]$  and  $-\mathbb{E}_{(x,y_w,y_l)\sim\mathcal{D}}\left[\log \sigma\left(\beta \log \pi_\theta\left(y_w \mid x\right) - \beta \log \pi_\theta\left(y_l \mid x\right)\right)\right]$ in one step (See Figure [1\)](#page-0-0).

 Our results show that TPO exhibits impres- sive performance compared to SFT across vari- ous benchmarks and outperforms other alignment methods such as DPO. Specifically, Mistral (7B), fine-tuned by TPO and trained with six times less **data** than other alignment techniques, outperforms SFT, DPO, KTO, IPO, CPO, and ORPO across nine

benchmarks on the Open LLM Leaderboard. No- **109** tably, Mistral aligned with TPO achieved a +0.72 **110** increase in the MT-Bench score over SFT. **111**

Overall, TPO addresses two key shortcomings in **112** alignment tasks. Firstly, by removing  $\pi_{ref}$  justified 113 in Section [3,](#page-2-0) TPO mitigates the inefficient learning **114** and memory utilization issues observed in DPO, **115** IPO, and KTO, allowing for more computational **116** efficiency with less memory usage. Secondly, TPO **117** enhances performance over SFT and other align- **118** ment methods by maximizing the likelihood of **119** gold response, regularized by parameter  $\alpha$ . and si- **120** multaneously optimizing between two preferences **121** (preferred and less-preferred responses). Despite **122** TPO's need for three preferences and its higher cost **123** relative to other methods, our findings reveal that **124** it's possible to considerably lessen the training data **125** required and still achieve superior outcomes (See **126** Table [1\)](#page-5-0). **127** 

Our findings suggest that a separate SFT step **128** is not necessary for TPO and, in certain scenarios, **129** having one may even hinder TPO's performance **130** (See Tables [1](#page-5-0) and [2\)](#page-5-1). **131**

We summarize our primary contributions as fol**lows:** 133

- 1. We propose a new preference learning method **134** called Triple Preferences Optimization (TPO) **135** that simplifies the alignment process and re- **136** duces two stages to one stage. **137**
- 2. Theoretically, we derive the TPO objective **138** and show that combining the human expec- **139** tation data and preference dataset achieves **140 better performance.** 141
- 3. Comprehensive experiments reveal that the **142** TPO method, applied to two distinct base- **143** line models—Mistral (7 B) and Phi-2 (2.7 **144** B)—outperforms SFT, KTO, IPO, DPO, CPO, 145 and ORPO in terms of performance across ten **146** different benchmarks (refer to Tables [1,](#page-5-0) [2,](#page-5-1) and **147** [3\)](#page-7-0). **148**
- 4. Integrating the SFT step with the preference **149** alignment step and moderating it with a regu- **150** larization parameter  $(\alpha)$  enhances the model's 151 performance while reducing the data required **152** for training (See Figure [3\)](#page-17-0). **153**

# 2 Related Works **<sup>154</sup>**

The performance of Large Language Models **155** [\(](#page-8-4)LLMs) on a variety of tasks are remarkable [\(Anil](#page-8-4) **156** [et al.,](#page-8-4) [2023\)](#page-8-4). Nonetheless, effectively aligning **157** LLMs remains a significant challenge. Current **158**

**224** . **238**

(1) **<sup>250</sup>**

 studies have fine-tuned LLMs using datasets of human preferences, leading to improvements in translation [\(Kreutzer et al.,](#page-9-7) [2018\)](#page-9-7), summarization [\(Stiennon et al.,](#page-10-6) [2022\)](#page-10-6), story-telling [\(Ziegler et al.,](#page-10-7) [2019\)](#page-10-7), instruction-following [\(Ramamurthy et al.,](#page-9-8) [2023\)](#page-9-8), and dialogue systems.

 RLHF [\(Christiano et al.,](#page-9-9) [2023\)](#page-9-9) aims to optimize for maximizing the expected reward by interacting with a reward model trained using the Bradley- Terry (BT) model [\(Bong and Rinaldo,](#page-8-5) [2022\)](#page-8-5), typi- cally through RL-algorithms like Proximal Policy Optimization [\(Schulman et al.,](#page-10-8) [2017\)](#page-10-8). While RLHF enhances model performance, it faces challenges such as instability, reward hacking, and scalability inherent in RL-settings.

 Recent works [\(Zhao et al.,](#page-10-5) [2023;](#page-10-5) [Yuan et al.,](#page-10-9) [2023\)](#page-10-9) have presented techniques to overcome these challenges by optimizing relative preferences with- out relying on reinforcement learning. In partic- ular, DPO [\(Rafailov et al.,](#page-9-5) [2023\)](#page-9-5) offers a method to directly fit an SFT model to human preferences using the Bradley-Terry (BT) model, providing the- oretical insights into the alignment process. How- ever, IPO [\(Azar et al.,](#page-8-3) [2023\)](#page-8-3) has mathematically revealed the limitations of the DPO approach con- cerning overfitting and generalization. It proposes a comprehensive objective for learning from hu- man preferences. Zephyr [\(Tunstall et al.,](#page-10-2) [2023\)](#page-10-2) has improved DPO by utilizing the distillation method.

 KTO [\(Ethayarajh et al.,](#page-9-10) [2023\)](#page-9-10), drawing inspi- ration from Kahneman and Tversky's influential [w](#page-10-10)ork on prospect theory [\(Tversky and Kahne-](#page-10-10) [man,](#page-10-10) [1992\)](#page-10-10), seeks to maximize the utility of LLM outputs directly rather than optimizing the log- likelihood of preferences. By prioritizing the de- termination of whether a preference is desirable or undesirable, this method eliminates the require-ment for two preferences for the same input.

**Recently, CPO [\(Xu et al.,](#page-10-3) [2024\)](#page-10-3) introduced an**  efficient method for learning preferences by com- bining maximum-likelihood loss with the DPO loss function, aiming to improve memory usage and [l](#page-9-11)earning efficiency. Additionally, ORPO [\(Hong](#page-9-11) [et al.,](#page-9-11) [2024\)](#page-9-11) proposed a novel approach by incor- porating a penalty term to prevent the learning of unpreferred responses while enhancing the likeli-hood of learning preferred responses.

 We observe two primary challenges in the alignment process addressed in mentioned stud- ies. *Firstly*, alignment methods like DPO require an SFT component or perform better with one. *Secondly*, there are concerns regarding inefficient **210** learning and memory usage. Although the CPO **211** approach has shown effectiveness in learning, con- **212** flicts between its objectives may limit the policy **213** model's performance. In this research, we explore **214** these limitations and propose a new algorithm to **215** address them. **216** 

## <span id="page-2-0"></span>3 Triple Preference Optimization **<sup>217</sup>**

In this section, we introduce Triple Preference **218** Optimization (TPO), a new approach to prefer- **219** ence learning. This method optimizes a policy **220** model  $(\pi_{\theta})$  by maximizing the likelihood of the 221 gold response and optimizing for the preferences **222** simultaneously. 223

Typically, in NLP tasks, we utilize a dataset **225**  $D_{reference} = \{x^i, y^i_{ref}\}_{i=1}^N$ , where x is the input 226 and  $y_{ref}$  is the gold standard response, crafted 227 by humans or large models like GPT-4 and **228** validated by humans. Additionally, for applying **229** preference optimization methods, a dataset **230**  $D_{preference} = \{x^i, y_w^i, y_l^i\}_{i=1}^N$  is needed, where 231  $y_w$  and  $y_l$  are the preferred and unpreferred re-  $232$ sponses respectively, generated by smaller models **233** such as LLaMA-3. The aim of TPO is to optimize **234** three preferences concurrently. To achieve this, we **235** merge the reference and preference datasets **236** into one dataset  $D_{TPO} = \{x^i, y_{ref}^i, y_w^i, y_l^i\}_{i=1}^N$ , es-<br>237 tablishing a response hierarchy of  $y_{ref} \succ y_w \succ y_l$ . Further details on the TPO objective will be **239** discussed in the following subsection. **240**

#### <span id="page-2-2"></span>3.1 Deriving the TPO objective **241**

Motivated by the goal of simplifying the alignment **242** process to a single step and enhancing the learn- **243** ing mechanisms of the DPO, we derive the TPO **244** objective. We start with a simple RL objective **245** for aligning an LLM parameterized with  $\theta$ , repre- 246 sented as  $\pi_{\theta}$  with preferences. The RL objective is 247 just maximizing the expected reward [\(Ziegler et al.,](#page-10-7) **248** [2019\)](#page-10-7) as shown in Equation [1:](#page-2-1) **249**

$$
\max_{\pi_{\theta}} \left[ \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(y|x)} [r_{\phi}(x, y)] \right] \tag{1}
$$

<span id="page-2-1"></span>where  $r_{\phi}$  represents the expected reward that the **251** model receives for a given input x and output  $252$ y. However, maximizing the reward without con- **253** straints can lead to distribution collapse in an **254** LLM. Drawing inspiration from the Maximum **255** Entropy Reinforcement Learning (MERL) frame- **256** work [\(Hejna et al.,](#page-9-12) [2023\)](#page-9-12), we have modified the **257**

(9) **310**

 RLHF objective, as detailed in Equation [4.](#page-3-0) The MERL framework aims to maximize causal entropy alongside the expected reward. This objective is formally defined in Equation [2.](#page-3-1)

<span id="page-3-1"></span>
$$
\max_{\pi_{\theta}} \mathbb{E}_{x \sim \mathcal{D}} \left[ \mathbb{E}_{y \sim \pi_{\theta}(y|x)} [r_{\phi}(x, y)] + \beta \mathcal{H}_{\pi_{\theta}}(y|x) \right]
$$
\n(2)

**263** By definition of Entropy,

**262**

**266**

$$
\mathcal{H}_{\pi_{\theta}}(y|x) = -\sum_{y} \pi_{\theta}(y|x)log(\pi_{\theta}(y|x)) \tag{3}
$$

**265** The objective becomes,

<span id="page-3-0"></span>
$$
\max_{\pi_{\theta}} \mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(y|x)} \left[ r_{\phi}(x, y) - \beta \log \pi_{\theta}(y|x) \right]
$$
\n(4)

 Based on this, the optimal policy model induced 268 by a reward function  $r(x, y)$  could be derived as shown in Equation [5](#page-3-2) (See Appendix [A.1\)](#page-11-0). It takes the following form:

<span id="page-3-2"></span>271 
$$
\pi_r(y|x) = \frac{1}{Z(x)} \exp\left(\frac{1}{\beta}r(x, y)\right) \tag{5}
$$

where  $Z(x) = \sum_{y} \exp\left(\frac{1}{\beta}\right)$ 272 where  $Z(x) = \sum_{y} \exp\left(\frac{1}{\beta}r(x, y)\right)$  is the new par- tition function. Inspired by [\(Rafailov et al.,](#page-9-5) [2023\)](#page-9-5), we show that the reward function, in terms of the optimal policy that it induces, is calculated as per Equation [6](#page-3-3) given below:

<span id="page-3-3"></span>
$$
r(x,y) = \beta \log \pi_r(y|x) + \beta \log Z(x) \quad (6)
$$

**278** Subsequently, we can represent the ground-truth  $279$  reward  $r^*(x, y)$  in the form of its corresponding 280 optimal policy  $\pi^*$  that it induces.

**281** Since the Bradley-Terry model is dependent only **282** on the difference between the two reward functions, 283 i.e.,  $p^*(y_w > y_l|x) = \sigma(r^*(x, y_w) - r^*(x, y_l)),$ **284** where, we can reparameterize it as follows in Equa-**285** tion [7:](#page-3-4)

<span id="page-3-4"></span>
$$
p^*(y_w > y_l \mid x) = \sigma\left(\beta \log \pi^*(y_w \mid x) - \beta \log \pi^*(y_l \mid x)\right)
$$
\n
$$
- \beta \log \pi^*(y_l \mid x)\right)
$$
\n(7)

**287** Similar to the reward modeling approach, we **288** model the human preferences, which is now in terms of a parameterized policy  $\pi_{\theta}$ . Thus, we for- **289** mulate maximum-likelihood objective (*preference* **290** objective) for a dataset  $D = \{x^i, y_w^i, y_l^i\}_{i=1}^N$  as 291 outlined in Equation [8:](#page-3-5) **292**

<span id="page-3-5"></span>
$$
\mathcal{L}_{\text{preference}}\left(\pi_{\theta}\right) = -\mathbb{E}_{(x,y_w,y_l)\sim\mathcal{D}}\n\left[\log \sigma\left(\beta \log \pi_{\theta}(y_w \mid x) \quad (8)\right) \right]
$$
\n
$$
-\beta \log \pi_{\theta}(y_l \mid x)\big)\right]
$$
\n(8)

Looking at the Equation [8,](#page-3-5) the objective is fitting **294** an reward which is reparameterized as  $r(x, y) = 295$  $\beta \log \pi(y|x)$ . In section [3.2,](#page-4-0) we theoretically ex- **296** plain that fitting this reward would ultimately re- **297** cover the optimal policy. **298**

The comparison between the loss function in **299** Equation [8](#page-3-5) and the DPO loss function indicates **300** that the new function is more efficient because it **301** requires only one model during training. How- **302** ever, even though maximizing the objective under **303** the MERL setting prevents distribution collapse, it **304** trains a pessimistic model, which also limits the **305** model from learning the preferred responses effec- **306** tively. To counteract this limitation, we maximize **307** the likelihood of the gold response. The adjustment **308** is specified in Equation [9.](#page-3-6) **309** 

<span id="page-3-6"></span>
$$
\mathcal{L}_{\text{reference}} = -\mathbb{E}_{(x, y_{ref}) \sim \mathcal{D}} \left[ \log \pi_{\theta} \left( y_{ref} \mid x \right) \right] \tag{9}
$$

Based on Equations [8,](#page-3-5) and [9,](#page-3-6) the TPO is de- **311** fined as a multi-objective (bi-objective) optimiza- **312** tion problem as supported by Pareto Front con- **313** cept [\(Lotov and Miettinen,](#page-9-6) [2008\)](#page-9-6). The TPO loss **314** function is framed as follows: **315**

$$
\mathcal{L}_{\text{TPO}} = \mathcal{L}_{\text{preference}} + \alpha \mathcal{L}_{\text{reference}} \qquad (10) \qquad 316
$$

where hyper-parameter  $(\alpha)$  plays a crucial role in  $\beta$ 17 moderating the model's learning of the gold re- **318** sponse. The impact of the  $\alpha$  on the model's perfor-  $319$ mance is detailed in Section [4.3.](#page-7-1)

Insights into the TPO update. A deeper mech- **321** anistic understanding of TPO can be achieved by **322** analyzing the gradient of the  $\mathcal{L}_{TPO}$  loss function.  $323$ The expression of this gradient in relation to the **324**  $parameters \theta$  is as follows:  $325$ 

$$
\begin{array}{l} 370 \\ 371 \\ 372 \\ 373 \\ 374 \\ 375 \\ 376 \\ 377 \\ 378 \\ 379 \\ 380 \\ 381 \\ 382 \\ 383 \\ 384 \\ 385 \\ 386 \\ 399 \\ 391 \\ 392 \\ 393 \\ 394 \\ 395 \\ 396 \\ 399 \\ 400 \\ 401 \\ 402 \\ 403 \\ 404 \\ 405 \\ 406 \\ 407 \\ 408 \\ \end{array}
$$

$$
326 \t \nabla_{\theta} \mathcal{L}_{\text{TPO}} =
$$

$$
\nabla_{\theta} \mathcal{L}_{\text{TPO}} = - \mathbb{E}_{(x, y_{ref}, y_w, y_l) \sim \mathcal{D}} \left[ \alpha \nabla_{\theta} \log \pi(y_{ref} | x) \right]
$$

$$
\overbrace{\text{increase likelihood of } y_{ref}}
$$

$$
+ \beta \sigma (\beta \log \pi_{\theta}(y_l|x) - \beta \log \pi_{\theta}(y_w|x))
$$
  
increase weight when reward estimate is wrong

328 
$$
\times \left[ \frac{\nabla_{\theta} \log \pi(y_w | x)}{\text{increase likelihood of } y_w} - \frac{\nabla_{\theta} \log \pi(y_l | x)}{\text{decrease likelihood of } y_l} \right] \tag{11}
$$

329 where  $r(x, y) = \beta \log \pi_{\theta}(y | x)$  is the reward in-**herently determined by the policy model**  $\pi_{\theta}$ **. In-** tuitively, the gradient of the TPO loss function works to increase the likelihood of the gold com- pletions  $y_{ref}$ , simultaneously enhancing the pref- erence aspect by amplifying the likelihood of pre-**ferred completions**  $y_w$  **and reducing the likelihood**  of the less-preferred completions  $y_l$ , which are weighed by how incorrectly the implicit reward model orders the preferences. (more details on Ap- **pendix [A.2\)](#page-12-0). Notably, the hyper-parameters**  $\beta$  **and**  $\alpha$  significantly influence the performance of the policy model, as discussed further in Section [4.3.](#page-7-1)

#### <span id="page-4-0"></span>**342** 3.2 Theory behind TPO

 In this section, we provide a theoretical founda- tion for the TPO algorithm, drawing inspiration from [\(Rafailov et al.,](#page-9-5) [2023\)](#page-9-5). We observe that the preference optimization objective aligns with the principles of a Bradley-Terry model, where the reward parameterization is defined as  $r(x, y)$  =  $\beta \log \pi_{\theta}(y|x)$ . Consequently, we optimize our para-350 metric model  $\pi_{\theta}$  in a manner similar to reward model optimization, as shown by [\(Ouyang et al.,](#page-9-3) [2022\)](#page-9-3). We expand on the theory underlying this reparameterization of the reward function, illustrat- ing that it does not constrain the range of reward models that can be modeled and ensures accurate retrieval of the optimal policy. We initiate this dis- cussion by following the insights presented in DPO about the equivalent class of reward models.

**359** Definition 3.1 *Two reward functions* r(x, y) *and* 360  $r^{'}(x, y)$  are equivalent iff  $r(x, y) - r^{'}(x, y) = g(x)$ **361** *for some function* g*.*

**362**

 We can state the following two lemmas as it is apparent that there exists an equivalence relation, dividing the set of reward functions into distinct **366** classes.

**367** Lemma 3.1 *Under the Plackett-Luce, and in par-***368** *ticular the Bradley-Terry preference framework,* **369** *two reward functions from the same class induce*

*the same preference distribution. [\(Rafailov et al.,](#page-9-5)* **3300)** *[2023\)](#page-9-5)* **371**

**Lemma 3.2** *Two reward functions from the same* 32 *equivalence class induce the same optimal policy* **373** *under the constrained RL problem. [\(Rafailov et al.,](#page-9-5)*  $\qquad \qquad$ 3 *[2023\)](#page-9-5)* **375**

The proofs are shown in Appendix [A.3.](#page-12-1)

<span id="page-4-2"></span>**Theorem 3.1** *Under mild assumptions, all re-*  $\frac{37}{2}$ *ward classes consistent with Plackett-Luce mod-* **378** *els can be represented with the reparameteriza-* **379** *tion*  $r(x, y) = \beta \log \pi(y|x)$  *for some model*  $\pi(y|x)$ . *[\(Rafailov et al.,](#page-9-5) [2023\)](#page-9-5)* 3

As proposed in DPO, upon imposing certain 3 constraints on the under-constrained Plackett-Luce **383** family of preference models, such that we preserve **344** 3 the class of representable reward model, it possible to explicitly make the optimal policy in Equa- 3 tion [5](#page-3-2) analytically tractable for all prompts  $x$ . The  $\qquad$  3 theorem is elaborated in Appendix [A.4.](#page-13-0) We further elaborate our theoretical basis for defining and 3 optimally addressing the TPO objective within a **390** multi-objective optimization framework.

<span id="page-4-1"></span>**Definition 3.2** Let  $f_i$  denote  $i^{th}$  objective, S 392 *denote the feasible policy space, then in a multi-* **393** *objective optimization setting, a policy*  $\pi^* \in S$  *is* 394 *said to be Pareto optimal if there does not exist* **395**  $\mathcal{L}$  *another policy*  $\pi \in \mathcal{S}$  *such that*  $f_i(\pi) \leq f_i(\pi^*)$  *for* 396  $all \, i = 1, ..., k \, and \, f_j(\pi) < f_j(\pi^*) \, for \, at \, least \, 397$ *one index j.* 3

Looking at the objectives in Equation [8](#page-3-5) and 4 Equation [9,](#page-3-6) it is obvious that optimizing them 401 together is non-trivial; that is, there does not **4** exist a policy that is optimal with respect to both 4 objectives. It can be seen that the objectives **404** are conflicting with each other, especially when  $40$  $y_{ref} \sim y_w$ , as one objective is maximizing the 406<sup>*4*</sup> log probability and the other is minimizing the **407** log probability. This means that the objectives are  $40$ at least partly conflicting. For a multi-objective **409** problem, [\(Miettinen,](#page-9-13) [1999\)](#page-9-13) show that optimizing **410** one objective and converting the other objective/s **411** as a constraint with an upper bound, the solution to **412** this  $\epsilon$  – *constrained* problem is Pareto optimal. 413 This shows that optimizing the TPO objective, **414** which is a bi-objective problem, gives an optimal 415 policy that is Pareto optimal as defined in [3.2.](#page-4-1) **416**

# 4 Experiments and Results **<sup>417</sup>**

In this section, we present a comprehensive em- **418** pirical analysis of TPO, yielding several key find- **419**

<span id="page-5-0"></span>

Model	Align	<b>ARC</b>	<b>TruthfulOA</b>	Winogrande	<b>HellaSwag</b>	<b>MMLU</b>	Average
Mistral	<b>SFT</b>	60.41	43.73	74.19	81.69	60.92	64.18
Mistral+SFT	DPO.	59.04	46.70	76.63	82.10	60	64.91
Mistral+SFT	<b>IPO</b>	59.30	42.22	76.4	81.02	59.93	63.77
Mistral+SFT	KTO	57.84	49.88	76.47	81.61	59.73	65.1
Mistral+SFT	<b>CPO</b>	57.50	53.22	75.92	80.37	58.41	65.08
Mistral	<b>ORPO</b>	58.61	52.77	77.5	82.04	63.26	66.83
Mistral+SFT	TPO (our)	58.02	59.05	76.47	80.6	59.48	66.72
Mistral	TPO (our $\alpha = 1$   $\beta = 0.1$ )	61.34	60	78.21	83.18	63.18	69.18
Mistral	TPO (our $\alpha = 0.9$   $\beta = 0.2$ )	60.23	57.34	78.29	83.01	63.75	68.52

Table 1: Comparing TPO's performance with other alignment methods reveals that the Mistral+TPO model exhibits comparable performance across different benchmarks and, on average, outperforms other methods. In particular, Mistral+TPO performed remarkably on the TruthfulQA benchmark. It's worth noting that the Mistral+TPO model is directly trained with TPO, which contributes to its superior performance. Additionally, for all benchmarks, accuracy is the metric used to gauge performance. More detail about ORPO in Appendix [B.1.](#page-15-0)

<span id="page-5-1"></span>

Model	Align	<b>MT-Bench</b>	<b>BB-causal</b>	<b>BB-sports</b>	<b>BB-formal</b>	<b>OpenBookOA</b>
Mistral	<b>SFT</b>	5.94	51.57	61.76	51.4	43.8
Mistral+SFT	CPO.	6.2	49.47	70.68	51.07	44.6
Mistral+SFT	DPO.	6.64	52.1	71.9	51	46.2
Mistral+SFT	<b>IPO</b>	6.43	51.57	65.01	51.22	44.6
Mistral+SFT	KTO.	6.48	53.68	73.42	51.33	45.8
Mistral	<b>ORPO</b>	5.47	54.21	73.93	50.4	44.4
Mistral+SFT	$TPO$ (our)	6.66	54.21	73.93	50.84	45.6
Mistral	TPO (our $\alpha = 1$   $\beta = 0.1$ )	6.22	55.26	73.63	51.06	48.2
Mistral	TPO (our $\alpha = 0.9 \mid \beta = 0.2$ )	6.66	56.31	73.32	50.5	47.8

Table 2: In our comparison of TPO with other alignment methods across more benchmarks, Mistral+SFT+TPO and Mistral+TPO emerge as the top performer, surpassing other methods in MT-Bench and BB-causal, BB-sports, OpenBookQA. For BB-causal, BB-sports, BB-formal, and OpenBookQA, performance is evaluated based on accuracy, while MT-Bench uses a scoring system generated by GPT-4. More detail about ORPO in Appendix [B.1.](#page-15-0)

 ings: 1) Phi-2+TPO and Mistral+TPO trained on 10K data outperform Phi-2+SFT and Mistral+SFT trained on 200K data by 12.7% and 7.2% on MT- Bench respectively. 2) Phi-2 fine-tuned with TPO surpasses the performance of models aligned with other methods on the MT-Bench. 3) Similarly, Mis- tral fine-tuned with TPO exceeds the performance of other alignment techniques across the majority of Open LLM Benchmarks. 4) Within the TPO method, the hyper-parameters  $\alpha$  and  $\beta$  play a criti- cal role in influencing performance outcomes. 5) An ablation study focusing on batch size adjust- ments reveals that enlarging the batch size leads to improved performance for models optimized with **434** TPO.

# **435** 4.1 Experimental Setup

 Models. All experiments were conducted using zephyr-sft-full and Mistral-7B-v0.1 as Mis- tral (7 B), and Phi-2 (2.7 B) [\(Javaheripi et al.,](#page-9-14) [2023\)](#page-9-14). We utilized the Transformer Reinforcement Learning (TRL) library for fine-tuning [\(von Werra et al.,](#page-10-11) **440** [2020\)](#page-10-11). It's noted that the notation "+" is used to **441** indicate that a model has been fine-tuned with a **442** specific algorithm, such as "+TPO". Further train- **443** ing details for each method are in Appendix [B.](#page-14-0) **444**

**Datasets.** In this study, we employ two dialogue 445 datasets: 1) UltraChat [\(Ding et al.,](#page-9-15) [2023\)](#page-9-15) and **446** 2) UltraFeedback [\(Cui et al.,](#page-9-16) [2023\)](#page-9-16). UltraChat **447** comprises 200k examples generated by GPT-3.5- **448** TURBO across 30 topics and 20 text material types, **449** offering a high-quality dataset utilized for train- **450** ing the SFT model. Meanwhile, UltraFeedback **451** consists of a 64K set of responses generated by **452** state-of-the-art models such as LLaMA-2 evalu- **453** ated by a teacher model such as GPT-4. To train **454** TPO, which requires three preferences, we create **455** a custom dataset from the UltraFeedback dataset. **456** Here, the response with the highest score serves as **457** the reference response, the second-highest score as **458** the chosen response, and the lowest score as the **459**

 [r](#page-10-12)ejected response. In light of findings from [\(Saeidi](#page-10-12) [et al.,](#page-10-12) [2024\)](#page-10-12), which indicate that alignment meth- ods perform better with smaller training sets on one epoch, and due to computational limitations, we re- strict our analysis to 12K (10K for training and 2K for evaluation) data points, randomly selected from the custom UltraFeedback dataset (More details in Appendix [B\)](#page-14-0).

 Evaluation. We evaluate our models in both single-turn and multi-turn scenarios using the MT- Bench benchmark [\(Ding et al.,](#page-9-15) [2023\)](#page-9-15). MT-Bench is composed of 160 questions covering eight dif- ferent knowledge domains, designed to be evalu- ated by GPT-4. To have a comprehensive evalua- tion we assess all alignment methods using five Open LLM Leaderboard benchmarks including ARC [\(Clark et al.,](#page-9-17) [2018\)](#page-9-17), HellaSwag [\(Zellers et al.,](#page-10-13) [2019\)](#page-10-13), MMLU [\(Hendrycks et al.,](#page-9-18) [2021\)](#page-9-18), Truthful [Q](#page-10-14)A [\(Lin et al.,](#page-9-19) [2022\)](#page-9-19), and Winogrande [\(Sakaguchi](#page-10-14) [et al.,](#page-10-14) [2019\)](#page-10-14). We further explore the performance of the models by evaluating them on four benchmarks from Big Bench [\(bench authors,](#page-8-6) [2023\)](#page-8-6), including Causal Judgment (causal reasoning), Sports Under- standing (commonsense reasoning), Formal Falla-cies, and OpenBookQA [\(Mihaylov et al.,](#page-9-20) [2018\)](#page-9-20).

### **485** 4.2 Demonstration of TPO Performance

 We evaluate the TPO approach against other align- ment techniques, such as KTO, IPO, CPO, DPO, and ORPO, using MT-Bench and the Open LLM Leaderboard Benchmarks. Our comparison in- volves two distinct model configurations: 1) the alignment of an SFT model using TPO and vari- ous other alignment methods, and 2) applying TPO directly to fine-tune a pre-trained model. Across all alignment approaches, we utilized Phi-2 (2.7 B) and Mistral (7 B) as the baseline models (More details in Appendix [B\)](#page-14-0). Additionally, we compared the ORPO method with a version that excludes the SFT part, the rationale for which is detailed in Appendix [B.1.](#page-15-0)

 MT-Bench. The data presented in Table [3](#page-7-0) reveals that the Phi-2+TPO method outperforms other alignment techniques, enhancing the MT-Bench score by 12.7% and 7.2% over Phi-2+SFT+DPO and Phi-2+SFT, respectively. Remarkably, Phi- 2+TPO achieves this superior performance even when trained on just 10K data, in stark contrast to Phi-2+SFT's training on 200K data (See Table [3\)](#page-7-0). Additionally, the results in Table [2](#page-5-1) demonstrate that Mistral+TPO surpasses competing alignment

<span id="page-6-0"></span>

Figure 2: The MT-Bench score for various  $\alpha$  and  $\beta$ settings in Mistral+TPO illustrates the influence of  $\alpha$  on performance.

methods in MT-Bench scores. Mistral+TPO **510** trained on 10K data shows a 7.2% improvement **511** over Mistral+SFT, which is trained on 200K data. **512**

**513**

The results in Table [2](#page-5-1) and Table [6](#page-16-0) in the 514 Appendix indicate that TPO exceeds the perfor- **515** mance of other alignment methods, inspite of 516 the SFT step being skipped (See Appendix [C.1\)](#page-15-1). **517** Furthermore, additional experiments show that **518** TPO achieves greater improvements over DPO, **519** KTO, IPO, and CPO by 13.3%, 13.6%, 2.5%, and **520** 13.3% respectively, on SFT trained on 10K data **521** (See Appendix [C.2\)](#page-15-2). **522**

Open LLM Leaderboard Benchmarks. The **523** primary findings, as detailed in Table [1,](#page-5-0) high- **524** light that Mistral+SFT+TPO, on average, sur- **525** passes other alignment methods. This supe- **526** rior performance is largely attributed to its no- **527** table success in the TruthfulQA benchmark de- **528** spite lagging behind Mistral+SFT+DPO in per- **529** formance. An intriguing observation from the **530** data is that Mistral+TPO not only excels on **531** average but also leads in performance across **532** all benchmarks, showcasing the effectiveness of **533** the TPO strategy. Specifically, Mistral+TPO **534** achieved average accuracy improvements over Mis- **535** tral+SFT, Mistral+SFT+DPO, Mistral+SFT+IPO, **536** Mistral+SFT+KTO, Mistral+SFT+CPO, and Mis- **537** tral+ORPO by 4.97%, 4.27%, 5.37%, 4.07%, **538** 4.07%, and 2.35%, respectively. For additional **539** results, readers are directed to Appendix [D.](#page-16-1) **540**

<span id="page-7-0"></span>

		<b>Alignment Method</b>								
Model	$+$ SFT						+SFT+DPO +SFT+IPO +SFT+KTO +SFT+CPO +ORPO +SFT+ORPO +SFT+TPO +TPO			
Phi-2	5.42	6.06	5.91	6.64	6.42	6.06	4.32	6.18	6.69	

Table 3: The comparison of Phi-2's performance when aligned with various methods on MT-Bench shows that Phi-2+TPO surpasses other alignment techniques. More detail about ORPO in Appendix [B.1.](#page-15-0)

 Exploration on More Benchmarks. For a com- prehensive evaluation, we assessed the efficacy of the TPO method against various alignment strategies across different benchmarks: BB-causal, BB-sports, BB-formal, and OpenBookQA. As detailed in Table [2,](#page-5-1) Mistral+SFT+TPO exhib- ited superior performance on BB-causal and BB-sports benchmarks, while it showed less impressive results on BB-formal and Open- BookQA. Notably, Mistral+TPO not only en- hanced the Mistral+SFT+TPO's outcomes on BB- causal and OpenBookQA but also surpassed Mis- tral+SFT, Mistral+SFT+DPO, Mistral+SFT+IPO, Mistral+SFT+KTO, Mistral+SFT+CPO, and Mis- tral+ORPO in accuracy by 4.81%, 1.71%, 3.91%, 1.01%, 3.01%, and 1.3%, respectively. Additional results can be found in Appendix [D.](#page-16-1)

#### <span id="page-7-1"></span>**558** 4.3 Ablation Studies

 In this subsection, we delve into the impact of  $\alpha$  and β values, batch size, and learning rate on the performance of the TPO method. Central to our exploration is the TPO method's ability to bypass the SFT stage, thereby assessing its efficacy with- out this component. Our evaluation focuses on the MT-Bench score and the Open LLM Leaderboard benchmarks to gauge the models' performance.

 Impact of  $\alpha$  and  $\beta$ . Alpha and Beta serve as crucial hyper-parameters that simultaneously en- hance the likelihood of the correct response and refine preference learning. Figure [2](#page-6-0) illustrates that the Mistral+TPO model, when set with  $\alpha$ =0.9 and  $\beta$ =0.2, outperforms alternatives in terms of perfor- mance on the MT-Bench. Additionally, Figure [3](#page-17-0) highlights that Mistral+TPO notably excels in the Open LLM Leaderboard benchmarks, boasting an average accuracy performance increase of 5.12% over the SFT method.

 Other hyper-parameters. We extend our anal- ysis to examine the influence of various hyperpa- rameters on the TPO's efficacy, including differ-ent epochs, learning rates, and batch sizes, specifically with the Mistral+TPO model. We discovered **582** that the learning rate is particularly critical when **583** dealing with smaller datasets; a change by two **584** orders of magnitude prevented the model from con- **585** verging. Additionally, while different batch sizes **586** do affect performance, there's a threshold beyond **587** which performance plateaus and no longer bene-  $588$ fits from increases. Interestingly, we observed that **589** Mistral+TPO, when trained on 10K data, tends to **590** overfit after just one epoch, with additional epochs **591** failing to enhance performance. Nonetheless, we **592** hypothesize that performance improves with larger **593** datasets beyond the initial epoch, as detailed further **594** in Appendix [E.](#page-16-2) **595**

# 5 Conclusions **<sup>596</sup>**

In this paper, we begin by addressing the lim- **597** itations inherent in existing alignment methods. **598** Typically, alignment techniques require an SFT **599** component to achieve notable results. However, **600** incorporating SFT introduces two primary chal- **601** lenges: firstly, fine-tuning a model using SFT de- **602** mands a substantial dataset (for example, complet- **603** ing a chat task may require fine-tuning with 200K 604 data points). Secondly, generating a preferences **605** dataset by sampling from the SFT model poses **606** additional difficulties, including determining the **607** optimal configuration for producing preferred and **608** less preferred responses. To address these short- **609** comings, we introduce TPO, a new alignment ap- **610** proach aimed at concurrently optimizing for hu- **611** man preferences and gold responses. Our findings **612** demonstrate the impressive performance of TPO **613** compared to other alignment methods on ten bench- **614** marks. Particularly, Mistral and Phi-2 fine-tuned **615** by TPO achieve increases in the MT-Bench score **616** of +0.72 and +1.27, respectively, compared to SFT, **617** despite being trained on a dataset six times smaller. **618** Another intriguing insight is the significant influ- **619** ence that the values of  $\alpha$  and  $\beta$  have on the model's 620 performance. **621**

### **<sup>622</sup>** Limitations and Future Works

 While TPO has demonstrated impressive perfor- mance compared to other alignment methods across various benchmarks, the requirement to pre- pare three preferences for each input in a dataset poses challenges. In this section, we outline poten- tial directions for future work. Our evaluation of TPO focused on chat completion tasks, but we are particularly interested in examining its effective- ness in other areas, such as safety and reasoning. Another intriguing aspect for further study is inves- tigating how the quality of reference and preferred responses affects TPO's performance. Notably, our current findings suggest that the reference response is generally better than the preferred response. In- vestigating whether increasing the preferential dif- ference between these responses enhances perfor- mance could yield valuable insights. Additionally, we are interested in exploring TPO's effectiveness in larger models, such as those with 30 B or 70 B, which represents a promising avenue for future work. Drawing inspiration from the new method proposed in [\(Chatterjee et al.,](#page-9-21) [2024\)](#page-9-21) for fine-tuning diffusion models, we are keen to investigate how these models perform when aligned using the TPO **647** method.

# **<sup>648</sup>** Ethics Statement

**649** We have used AI assistants (Grammarly and **650** ChatGPT) to address the grammatical errors and **651** rephrase the sentences.

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# **921 Appendix**

**926**

#### **922 A** Derivation

#### <span id="page-11-0"></span>**923** A.1 Deriving the optimal policy under the Preference Objective

**924** In this section, we derive the optimal policy achieved by optimizing the objective in Equation [4.](#page-3-0) For a 925 given prompt  $x$ , the objective can be analogously written as follows:

$$
\max_{\pi} \mathbb{E}_{y \sim \pi(y|x)} \left[ r(x, y) - \beta \log \pi(y|x) \right] s.t. \sum_{y} \pi(y|x) = 1
$$

**927** Next, we form a lagrangian for the above objective with  $\lambda$  being the lagrangian multiplier.

$$
\mathcal{L} = \sum_{y} \pi(y|x) r(x, y) - \beta \left[ \sum_{y} \pi(y|x) \log \pi(y|x) \right] + \lambda \left[ 1 - \sum_{y} \pi(y|x) \right]
$$

929 **Differentiating L with respect to**  $\pi(y|x)$  **results in,** 

930 
$$
\frac{\partial \mathcal{L}}{\partial_{\pi(y|x)}} = r(x,y) - \beta \left[ \log \pi(y|x) + 1 \right] - \lambda
$$

**931** To obtain the optimal policy, we can set the above equation to zero and solve for  $\pi(y|x)$ .

$$
r(x,y) - \beta \left[ \log \pi(y|x) + 1 \right] - \lambda = 0
$$

$$
\log \pi(y|x) = \frac{1}{\beta}r(x,y) - \frac{\lambda}{\beta} - 1
$$

934 
$$
\pi(y|x) = \exp\left(\frac{1}{\beta}r(x,y)\right).\exp\left(\frac{-\lambda}{\beta} - 1\right)
$$

935 Since  $\sum_{y} \pi(y|x) = 1$ , the second exponent is a partition function that does normalization as shown **936** below:

$$
\left[\sum_{y} \exp\left(\frac{1}{\beta}r(x,y)\right)\right].\exp\left(\frac{-\lambda}{\beta} - 1\right) = 1
$$

938 
$$
\exp\left(\frac{-\lambda}{\beta} - 1\right) = \left[\sum_{y} \exp\left(\frac{1}{\beta}r(x, y)\right)\right]^{-1}
$$

939 **Hence, the partition function**  $Z(x) = \sum_{y} \exp(\frac{1}{\beta}r(x, y))$  and the optimal policy  $\pi_r(y|x)$  induced by 940 **reward function**  $r(x, y)$  is therefore given by,

<span id="page-11-1"></span>941 
$$
\pi_r(y|x) = \frac{1}{Z(x)} \exp\left(\frac{1}{\beta}r(x, y)\right)
$$
 (1)

942 Now, we can express the reward function in terms of an optimal policy  $\pi_r$  by performing some algebraic **943** transformations on Equation [1](#page-11-1) as shown below,

$$
\pi_r(y|x).Z(x) = \exp\left(\frac{1}{\beta}r(x,y)\right)
$$

Taking logarithm and multiplying by  $\beta$  on both sides,

$$
r(x,y) = \beta \log \pi_r(y|x) + \beta \log Z(x) \tag{2}
$$

# <span id="page-12-2"></span><span id="page-12-0"></span>A.2 Deriving the Gradient of the TPO Objective **947 947**

In this section, we derive the gradient of the TPO objective: **948**

$$
\nabla_{\theta} \mathcal{L}_{\text{TPO}} = -\nabla_{\theta} \mathbb{E}_{(x, y_{ref}, y_w, y_l) \sim \mathcal{D}} \left[ \alpha \log \pi_{\theta}(y_{ref}|x) + \log \sigma(\beta \log \pi_{\theta}(y_w|x) - \beta \log \pi_{\theta}(y_l|x)) \right] \tag{1}
$$

We can rewrite the RHS of the Equation [1](#page-11-1) as **950** 

$$
\nabla_{\theta} \mathcal{L}_{\text{TPO}} = -\mathbb{E}_{(x, y_{ref}, y_w, y_l) \sim \mathcal{D}} \left[ \underbrace{\alpha \nabla_{\theta} \log \pi_{\theta}(y_{ref}|x)}_{\text{(a)}} + \underbrace{\nabla_{\theta} \log \sigma(\beta \log \pi_{\theta}(y_w|x) - \beta \log \pi_{\theta}(y_l|x))}_{\text{(b)}} \right]
$$
\n(2)

In equation [2,](#page-12-2) the part (b) can be rewritten with **952**

$$
u = \beta \log \pi_{\theta}(y_w|x) - \beta \log \pi_{\theta}(y_l|x)
$$
\n<sup>(953)</sup>

$$
\nabla_{\theta} \log \sigma(u) = \frac{1}{\sigma(u)} \nabla_{\theta} \sigma(u) \tag{954}
$$

$$
\nabla_{\theta} \log \sigma(u) = \frac{\sigma'(u)}{\sigma(u)} \nabla_{\theta}(u)
$$

Using the properties of sigmoid function function  $\sigma'(u) = \sigma(u)(1 - \sigma(u))$  and  $\sigma(-u) = 1 - \sigma(u)$ , 956

$$
\nabla_{\theta} \log \sigma(u) = \frac{\sigma(u)(1 - \sigma(u))}{\sigma(u)} \nabla_{\theta}(u)
$$

$$
\nabla_{\theta} \log \sigma(u) = (1 - \sigma(u)) \nabla_{\theta}(u) \tag{958}
$$

$$
\nabla_{\theta} \log \sigma(u) = \sigma(-u) \nabla_{\theta}(u) \tag{959}
$$

<span id="page-12-3"></span>
$$
\nabla_{\theta} \log \sigma(u) = \beta \sigma(\beta \log \pi_{\theta}(y_l|x) - \beta \log \pi_{\theta}(y_w|x)) \left[ \nabla_{\theta} \log \pi(y_w|x) - \nabla_{\theta} \log \pi(y_l|x) \right] \tag{3}
$$

Plugging Equation [3](#page-12-3) into Equation [2](#page-12-2) we get, **961**

$$
\nabla_{\theta} \mathcal{L}_{\text{TPO}} = - \mathbb{E}_{(x, y_{ref}, y_w, y_l) \sim \mathcal{D}} \left[ \alpha \nabla_{\theta} \log \pi (y_{ref} | x) \right]
$$

$$
+\beta\sigma(\beta\log\pi_\theta(y_l|x)-\beta\log\pi_\theta(y_w|x))\hspace{2cm}\text{963}
$$

$$
\times \left[ \nabla_{\theta} \log \pi(y_w | x) - \nabla_{\theta} \log \pi(y_l | x) \right] \tag{4}
$$

# <span id="page-12-1"></span>**A.3 Proof of Lemma** 965

In this section, we will prove the lemmas from Section [3.2.](#page-4-0) **966**

**967** Lemma 1 Restated. Under the Plackett-Luce preference framework, and in particular the Bradley-Terry **968** framework, two reward functions from the same equivalence class induce the same preference distribution.

969 Proof. Let's consider two reward functions,  $r(x, y)$  and  $r'(x, y)$ . They are said to be equivalent if they 970 can be related by  $r'(x, y) = r(x, y) + g(x)$  for some function g. We analyze this in the context of the 971 general Plackett-Luce model, which includes the Bradley-Terry model (special case when  $K = 2$ ). Here, 972 we denote the probability distribution over rankings generated by a given reward function  $r(x, y)$  as  $p_r$ . 973 Given any prompt x, responses  $y_1, ..., y_K$ , and a ranking  $\tau$ , we can establish the following:

$$
p_{r'}(\tau \mid y_1, \ldots, y_K, x) = \prod_{k=1}^K \frac{\exp(r'(x, y_{\tau(k)}))}{\sum_{j=k}^K \exp(r'(x, y_{\tau(j)}))}
$$

$$
= \prod_{k=1}^{K} \frac{\exp(r(x, y_{\tau(k)}) + g(x))}{\sum_{j=k}^{K} \exp(r(x, y_{\tau(j)}) + g(x))}
$$

$$
= \prod_{k=1}^{K} \frac{\exp(g(x)) \exp(r(x, y_{\tau(k)}))}{\exp(g(x)) \sum_{j=k}^{K} \exp(r(x, y_{\tau(j)}))}
$$

977  
\n978  
\n978  
\n978  
\n
$$
= \prod_{k=1}^{K} \frac{\exp(r(x, y_{\tau(k)}))}{\sum_{j=k}^{K} \exp(r(x, y_{\tau(j)}))}
$$
\n978

**979** This completes the proof.

**980 Lemma 2 Restated.** Two reward functions from the same equivalence class induce the same optimal **981** policy under the constrained RL problem.

982 Proof. Let's consider two reward functions,  $r(x, y)$  and  $r'(x, y)$ . They are said to be equivalent if they 983 can be related by  $r'(x, y) = r(x, y) + g(x)$  for some function g. Let  $\pi_r$  and  $\pi_{r'}$  be the optimal policies **984** induced by their corresponding reward functions. By Equation [5,](#page-3-2) for all x, y we have,

$$
\pi_{r'}(y \mid x) = \frac{1}{\sum_{y} \exp\left(\frac{1}{\beta}r'(x, y)\right)} \exp\left(\frac{1}{\beta}r'(x, y)\right)
$$
  
\n
$$
= \frac{1}{\sum_{y} \exp\left(\frac{1}{\beta}(r(x, y) + g(x))\right)} \exp\left(\frac{1}{\beta}(r(x, y) + g(x))\right)
$$
  
\n
$$
= \frac{1}{\exp\left(\frac{1}{\beta}g(x)\right)\sum_{y} \exp\left(\frac{1}{\beta}r(x, y)\right)} \exp\left(\frac{1}{\beta}r(x, y)\right) \exp\left(\frac{1}{\beta}g(x)\right)
$$
  
\n
$$
= \frac{1}{\sum_{y} \exp\left(\frac{1}{\beta}r(x, y)\right)} \exp\left(\frac{1}{\beta}r(x, y)\right)
$$
  
\n
$$
= \pi_{r}(y \mid x),
$$

**985**

**990**

**974**

$$
= 3
$$
\n986

\nThis completes the proof.

#### <span id="page-13-0"></span>**987** A.4 Proof of Theorem

**988** Theorem 1 Restated. *For a parameter* β > 0*, all reward equivalence classes can be reparameterized* **989** *as*  $r(x, y) = \beta \log \pi(y|x)$  *for some model*  $\pi(y|x)$ *.* 

**991** Proof. Consider a reward function  $r(x, y)$ , which induces an optimal model  $\pi_r(y|x)$  under the MERL **992** framework, which takes the form as shown in Eq[.5](#page-3-2) in Section [3.1.](#page-2-2) Following, Equation [2](#page-12-2) in Section [A.1](#page-11-0) **993** of Appendix, we have:

$$
r(x,y) = \beta \log \pi_r(y|x) + \beta \log Z(x) \tag{1}
$$

where  $Z(x) = \sum_{y} \exp(\frac{1}{\beta}r(x, y))$  is the partition function of the optimal policy induced by the reward 995 function  $r(x, y)$ . Let  $r'(x, y)$  be a new reward function such that  $r'(x, y) = r(x, y) - \beta \log Z(x)$ . It is **996** obvious that the new reward function is within the equivalence class of  $r$ , and the we have: **997** 

$$
r^{'}(x,y) = r(x,y) - \beta \log Z(x) \tag{99}
$$

From the Equation [1,](#page-11-1) we get **999** 

$$
r'(x,y) = \beta \log \pi_r(y|x) + \beta \log Z(x) - \beta \log Z(x)
$$
\n<sup>1000</sup>

$$
r'(x,y) = \beta \log \pi_r(y|x)
$$

This completes the proof. **1002** 

**Proposition 1.** For a parameter  $\beta > 0$ , every equivalence class of reward functions has a unique reward 1003 function  $r(x, y)$ , which can be reparameterized as  $r(x, y) = \beta \log \pi(y|x)$  for some model  $\pi(y|x)$ .

Proof – by – Contradiction. Let us assume that we have two reward functions from the same class, 1005 such that  $r'(x, y) = r(x, y) + g(x)$ . Assume that  $r'(x, y) = \beta \log \pi'(y|x)$  for some model  $\pi'(y|x)$  and 1006  $r(x, y) = \beta \log \pi(y|x)$  for some model  $\pi(y|x)$ , such that  $\pi' \neq \pi$ . We then have,

$$
r'(x, y) = r(x, y) + g(x)
$$
  
=  $\beta \log \pi(y|x) + g(x)$   
=  $\beta \log \pi(y|x) + \beta \log \exp(\frac{1}{\beta}g(x))$   
=  $\beta \log \pi(y|x) \exp(\frac{1}{\beta}g(x))$   
=  $\beta \log \pi'(y|x)$ 

for all prompts *x* and completions *y*. Then, we must have  $\pi(y|x) \exp(\frac{1}{\beta}g(x)) = \pi'(y|x)$ . Since these are 1009 probability distributions, summing over *y* on both sides, **1010 1010** 

$$
\sum_{y} \left[ \pi(y|x) \exp\left(\frac{1}{\beta}g(x)\right) \right] = \sum_{y} \pi'(y|x)
$$

$$
\exp\left(\frac{1}{\beta}g(x)\right) = 1
$$

Since  $\beta > 0$ ,  $g(x)$  must be 0 for all x. Therefore, we will have  $r(x, y) = r'(x, y)$ , which contradicts 1012 our initial condition of  $\pi'$  $\neq \pi$ . 1013

<span id="page-14-0"></span>Thus, by contradiction, we have shown that every reward class has a unique reward function that can be **1014** represented by the reparameterization in Theorem [3.1.](#page-4-2) **1015** 

<span id="page-15-3"></span>

Table 4: Detailed information of Open LLM Leaderboard and Big Bench benchmarks.

#### B Training and Evaluation Details

 All models were trained using the AdamW optimizer without weight decay. Furthermore, parameter- efficient techniques such as LoRA [\(Hu et al.,](#page-9-22) [2021\)](#page-9-22) were not employed. The experiments were conducted on 4 A100 GPUs, utilizing bfloat16 precision, and typically required 5-8 hours to complete. All models are trained for one epoch, employing a linear learning rate scheduler with a peak learning rate of 5e-07 and 10% warmup steps. Additionally, the global batch size is set to 16, and  $\beta = 0.1$  is used to regulate the deviation from the reference model. For every dataset used in our evaluation, we detail the count of few-shot examples utilized along with the specific metric employed for assessment in Table [4.](#page-15-3)

1024 The custom UltraFeedback dataset includes  $y_{ref}$ ,  $y_w$ , and  $y_l$  for each input x. For a fair comparison, 1025 when training alignment methods based on the SFT model, we utilized  $y_w$  and  $y_l$  under the assumption that the model was trained on yref during supervised fine-tuning. Conversely, in scenarios where we directly trained a model using alignment methods, we used  $y_{ref}$  and  $y_l$ .

<span id="page-15-0"></span>B.1 Detail Evaluation for ORPO

 The central hypothesis of the ORPO method [\(Xu et al.,](#page-10-3) [2024\)](#page-10-3) suggests that skipping the SFT component can achieve performance comparable to that of SFT and DPO methods. Based on this premise, it is essential to compare a model directly fine-tuned using ORPO against other alignment methods. To test this hypothesis, we designed two experiments: 1) Fine-tuning an SFT model using ORPO, and 2) Fine-tuning a pre-trained model using ORPO.

<span id="page-15-4"></span>

Model	Alien	<b>MT-Bench</b>	<b>ARC</b>	TruthfulOA	Winogrande	HellaSwag	MMLU	BB-causal	<b>BB-sports</b>	<b>BB-formal</b>	<b>OpenBookOA</b>
Mistral	ORPO	5.47	58.61	52.77		82.04	63.26	54.21	73.93	50.41	44.4
Mistral+SFT	ORPO.	4.93	53.92	48.03	75.69	79.69	59.62	50.52	71.19	51.07	43.4
Phi-2	ORPO	6.06	61.17	45.68	74.42	74.69	58.33	55.78	50.7	49.01	52.8
$Phi-2+SFT$	<b>ORPO</b>	4.32	55.11	49.15	74.74	70.38	55.36	54.21	50.91	49.27	44.8

Table 5: Comparison OPRO method on different scenarios.

 The results presented in Table [5](#page-15-4) indicate that, consistent with the hypothesis outlined in the paper [\(Xu](#page-10-3) [et al.,](#page-10-3) [2024\)](#page-10-3), ORPO performs better when the SFT component is omitted. Thus, for our comparisons, we utilized the Mistral+ORPO and Phi-2+ORPO models.

#### C More Experiments

 In this section, we assess the performance of alignment methods in two distinct scenarios: 1) skipping the SFT component and 2) aligning an SFT model that has been fine-tuned on a dataset of 10K instances using various alignment techniques.

#### <span id="page-15-1"></span>C.1 Skipping the SFT Component

 The primary benefit of using TPO is the ability to skip the SFT component, which often results in better performance for TPO without SFT. In this experiment, we also investigate the effectiveness of other alignment methods without the SFT part. For this purpose, we directly trained a Mistral-7B-v0.1 model using various alignment techniques like DPO, KTO, IPO, CPO, and ORPO.

<span id="page-15-2"></span> The results in Table [6](#page-16-0) indicate that without the SFT component, both DPO and IPO fail to match the performance levels of Mistral+SFT. Additionally, the results for KTO and CPO show negligible differences when compared with SFT. Although ORPO recommends bypassing the SFT phase in the alignment process, it seems that a policy model fine-tuned with ORPO underperforms when only one epoch is used. A comparison between the results in Tables [2](#page-5-1) and [6](#page-16-0) reveals that most of the alignment methods perform better when the SFT part is retained.

<span id="page-16-0"></span>

Table 6: Comparison of the performance of various alignment methods on skipping the SFT part using MT-Bench.

#### C.2 Aligning an SFT Model with Less Data **1052**

<span id="page-16-3"></span>In this experiment, we investigate how alignment methods perform when applied to an SFT model trained **1053** on significantly less data. TPO utilizes the dataset  $D = \{x^i, y_{ref}^i, y_w^i, y_l^i\}_{i=1}^N$ . Initially, we fine-tune a 1054 Mistral-7B-v0.1 model on 10K data, which are designated as  $y_{ref}$  for TPO. Subsequently, we applied 1055 various alignment methods to this fine-tuned model. **1056** 1056



Table 7: Comparison of the performance of various alignment methods on different SFT models using the MT-Bench. Notably, the score for Mistral+SFT trained on 10K data is 4.2, while the score for Mistral+SFT trained on 200K data is 5.94.

The findings presented in Table [7](#page-16-3) suggest that alignment methods yield superior results when applied to **1057** an SFT model trained on a larger dataset. It is evident that, when using the same data as for Mistral+TPO, **1058** other models perform significantly worse. These results confirm our hypothesis that TPO surpasses other **1059** methods with considerably less data. **1060** 1060

#### <span id="page-16-1"></span>D More results on Open LLM Leaderboard and Big Bench Benchmarks **<sup>1061</sup>**

Our assessment of Phi-2 through the Open LLM Leaderboard benchmarks, in comparison with various **1062** alignment methods, showed that Phi-2+TPO, trained on a dataset of 10K, achieved performance on par **1063** with other alignment strategies across the ARC, TruthfulQA, and MMLU benchmarks. Also, The results **1064** showed that this model performs better on BB-causal and OpenBookQA. **1065** 



Table 8: Comparison between TPO and other alignment methods on Open LLM Leaderboard and Big Bench benchmarks based on Phi-2 model.

### <span id="page-16-2"></span>E More results on Ablation Studies **<sup>1066</sup>**

This section presents the performance of Mistral+TPO across various learning rate, epoch, and batch size **1067** utilizing the MT-Bench score as the benchmark for assessment. **1068**

In Figure [3](#page-17-0) we compared TPO with SFT on different value of  $\alpha$  and  $\beta$  on Open LLM Leaderboard 1069 **benchmarks.** 1070

Model Align		<b>Learning Rate</b>	Epoch	<b>Batch Size</b>	<b>First Turn</b> (Score)	<b>Second Turn</b> (Score)	Average (Score)	
Mistral Mistral	TPO $(\alpha=1 \beta=0.1)$ TPO $(\alpha=1 \beta=0.1)$	5e-07 $2e-05$		16 16	6.78	5.66	6.22	
Mistral Mistral Mistral	TPO $(\alpha=0.9 \beta=0.2)$ TPO $(\alpha=0.9 \beta=0.2)$ TPO $(\alpha=0.9 \beta=0.2)$	5e-07 5e-07 5e-07		16 32 16	7.12 6.98 7.2	6.2 6.1 6	6.66 6.54 6.61	

Table 9: Performance of the Mistral+TPO on different values of hyper-parameters.

<span id="page-17-0"></span>

Figure 3: This figure displays the performance of Mistral+TPO across various settings of  $\alpha$  and  $\beta$ . In several configurations, Mistral+TPO outperforms SFT on the Open LLM Leaderboard benchmarks. Further discussion is provided in Section [4.3.](#page-7-1)