SOFT PREFERENCE OPTIMIZATION: ALIGNING LAN GUAGE MODELS TO EXPERT DISTRIBUTIONS

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Abstract

We propose Soft Preference Optimization (SPO), a method for aligning generative models, such as Large Language Models (LLMs), with human preferences, without the need for a reward model. SPO optimizes model outputs directly over a preference dataset through a natural loss function that integrates preference loss with a regularization term across the model's entire output distribution rather than limiting it to the preference dataset. Although SPO does not require the assumption of an existing underlying reward model, we demonstrate that, under the Bradley-Terry (BT) model assumption, it converges to a softmax of scaled rewards, with the distribution's "softness" adjustable via the softmax exponent, an algorithm parameter. We showcase SPO's methodology, its theoretical foundation, and its comparative advantages in simplicity and alignment precision.

1 INTRODUCTION

The alignment problem focuses on adjusting a generative model (e.g., Large Language Models 025 (LLMs)) to align its outputs with human preferences and ethical standards or to tailor the model for 026 specific tasks; and is especially important after supervised fine-tuning on datasets with mixed-quality 027 samples. A widely embraced approach involves refining these models based on expert (i.e., human) preferences, typically expert-provided comparisons of pairs of model-generated outputs (Christiano 029 et al., 2017). Given a preference dataset \mathcal{D} and a pre-trained model π_{ref} , preference alignment seeks to train a new model, π_{θ} , whose outputs are better aligned with the preference in \mathcal{D} (Radford et al., 031 2018; Ramachandran et al., 2016). A notable advancement in this field has been the application of Reinforcement Learning from Human Feedback (RLHF), which involves training a reward-model 033 based of actions preferred by humans and then optimizing π_{θ} to maximize these learned rewards while 034 ensuring closeness to the initial model behaviors (Ouyang et al., 2022). Despite the effectiveness of RLHF in addressing the alignment problem, RLHF involves a relatively complex pipeline, susceptible 035 to propagation of reward-model's biases over to the policy optimization. 036

037 Recently, several studies have introduced methods for the direct optimization of preferences, including 038 Direct Preference Optimization (DPO) among others (Rafailov et al., 2023; Amini et al., 2024; Chowdhury et al., 2024; Xu et al., 2024; Yin et al., 2024; Xu et al., 2023; Tunstall et al., 2023). 040 These approaches eliminate the need for a separate reward model training phase, instead adjusting the model directly using preference data, and often outperform RLHF-based approaches. These 041 reward-model-free methods enjoy advantages over RLHF-based approaches, such as simplified 042 pipelines, reduced computational complexity, and avoidance of the bias transfer from the reward 043 model to policy optimization. Indeed, the rationale for incorporating an additional component, the 044 reward model, into a supervised learning context with a supervised dataset, is debatable. 045

In this work, we propose a simple and effective reward-model-free alignment method, termed *Soft Preference Optimization* (SPO). SPO seeks to align the model's *preference estimates* (detailed in Section 3) with expert preferences \mathcal{D} , through minimizing a loss function of the form

AlignmentLoss $(\pi_{\theta}, \pi_{ref}, \mathcal{D}) = PreferenceLoss(\pi_{\theta}, \mathcal{D}) + Regularizer(\pi_{\theta}, \pi_{ref}),$ (1)

where the Regularizer may be chosen as the KL divergence. We discuss natural choices for the model's preference estimates and the preference loss function in Sections 3 and 4.

Unlike RLHF and DPO, the development of SPO does not rely on assumptions regarding the existence of underlying rewards, such as the Bradley-Terry (BT) model (Bradley & Terry, 1952). Nevertheless,

we demonstrate that if the BT model is applicable and given an asymptotically large preference dataset, SPO is theoretically guaranteed to converge to a softmax of the rewards, which inspires the designation "*Soft* Preference Optimization". Unlike DPO, which tends toward a deterministic model even with an extremely large dataset if the regularization coefficient is nearly zero (Azar et al., 2023), SPO allows for the adjustment of the softmax's exponent through an input parameter, thereby offering flexibility in modulating the "softness" of the output distribution.

060 SPO has two main distinctions from its successor reward-model-free alignment methods. The first 061 distinction involves the choice of a preference loss that aligns model's preference estimates with 062 expert's preferences, resulting in a favorable fixed point as discussed in the previous paragraph. The 063 other distinction of SPO with DPO and similar algorithms lies in the application of regularization. 064 DPO restricts regularization to the preference dataset, which is counter-intuitive since the dataset already provides specific data points for the model to fit; thus, additional regularization within 065 this limited scope is unnecessary. More critically, since the preference dataset represents a tiny 066 subset of the potential outputs of the model, focusing regularization solely within this subset can 067 lead to undesirable, extensive shift in the model's distribution outside of the dataset, resulting in a 068 non-coherent behaviours. Acknowledging this limitation, SPO applies regularization across the entire 069 output distribution of the model, not just within the confines of the preference dataset. 070

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2 BACKGROUND

Consider a finite context (or query) space \mathcal{X} and a finite action (or response) space \mathcal{Y} . For a given 074 query $x \in \mathcal{X}$, a behavior policy (such as a pre-trained model) is employed to generate responses 075 $y_1, y_2 \in \mathcal{Y}$. These responses are subsequently evaluated by expert raters (e.g., humans) to determine 076 which of y_1 or y_2 constitutes a more appropriate response to the query x. We adopt the notation 077 $y_1 \succ y_2$ to denote that y_1 is preferred over y_2 in a specific context. The true expert preferences are typically represented by a probability, $p^*(y_1 \succ y_2 | x)$, reflecting the inherent randomness due to the 079 variable nature of the experts, who may be a group of humans with slightly differing preferences. A preference dataset, \mathcal{D} , is compiled by collecting expert preferences for multiple $(x; y_1, y_2)$ tuples. 081 In detail, \mathcal{D} comprises tuples $(x; y_w, y_l)$, where $y_w \succ y_l$ indicates the preferred (winner) and less 082 preferred (loser) responses based on expert evaluations.

RLHF comprises two main phases: reward modeling and reinforcement learning (RL) fine-tuning. The initial phase, reward modeling, operates under the assumption that there exist latent rewards r(y|x) that form the basis of expert preferences. This phase aims to develop a model capable of closely approximating these underlying rewards. A widely accepted method for defining these latent rewards is through the Bradley-Terry (BT) model (Bradley & Terry, 1952), alongside the Plackett-Luce (PL) ranking models (Luce, 2005; Plackett, 1975). The BT model posits that the distribution of expert preferences, p^* , is characterized by

$$p^{\text{BT}}(y_1 \succ y_2|x) \stackrel{\text{def}}{=} \sigma\left(r(y_1|x) - r(y_2|x)\right) = \frac{\exp\left(r(y_1|x)\right)}{\exp\left(r(y_1|x)\right) + \exp\left(r(y_2|x)\right)},\tag{2}$$

where $\sigma(\cdot)$ represents the sigmoid function. Subsequently, the reward model $r_{\phi}(y|x)$ is trained to minimize the negative log-likelihood loss, $-\mathbb{E}_{(x;y_w,y_l)\sim\mathcal{D}}[\sigma(r(y_w|x) - r(y_l|x))]$. The PL model generalizes the BT model for data involving rankings, modeling the expert distribution as

$$p^{\mathrm{PL}}(y_1 \succ \dots \succ y_n \,|\, x) \stackrel{\text{def}}{=} \prod_{k=1}^{n-1} \frac{\exp\left(r(y_k|x)\right)}{\sum_{i=k}^n \exp\left(r(y_i|x)\right)},\tag{3}$$

for all $(x; y_1, \ldots, y_n) \in \mathcal{X} \times \mathcal{Y}^n$.

The RL fine-tuning phase aims to train a model, π_{θ} , to maximize a loss function of the form

$$\mathcal{L}_{\mathrm{RLHF}}(\pi_{\theta}, \pi_{\mathrm{ref}}, r_{\phi}) = -\mathbb{E}_{x \sim \mathcal{D}, y \sim \pi_{\theta}(\cdot | x)} [r_{\phi}(y | x)] + \beta \mathcal{D}_{\mathrm{KL}}(\pi_{\theta} \parallel \pi_{\mathrm{ref}}), \tag{4}$$

104 where β is a non-negative constant, r_{ϕ} is the trained reward function, and π_{ref} is a reference policy 105 often acquired through supervised fine-tuning on high-quality data and is typically identical to the 106 behavior policy. The D_{KL} term in the loss function acts as a regularizer, ensuring the model does not 107 significantly deviate from the distribution where the reward model is most accurate. RL fine-tuning 108 employs reinforcement learning algorithms, like PPO (Schulman et al., 2017), to optimize the above loss function (Ouyang et al., 2022), introducing significant complexity into the RLHF pipeline.
Additionally, the RLHF framework allows for the propagation of any generalization errors from the reward model to the RL fine-tuned model. The DPO framework (Rafailov et al., 2023) addresses these challenges by simplifying the problem into a single-phase supervised learning approach, thus avoiding the pitfalls associated with separate reward modeling and RL fine-tuning phases.

DPO circumvents the need for a reward model by directly optimizing the following loss function:

$$\mathcal{L}_{\rm DPO}(\pi_{\theta}, \pi_{\rm ref}, \mathcal{D}) = -\mathbb{E}\left[\log \sigma \left(\beta \log \frac{\pi_{\theta}(y_w|x)}{\pi_{\rm ref}(y_w|x)} - \beta \log \frac{\pi_{\theta}(y_l|x)}{\pi_{\rm ref}(y_l|x)}\right)\right].$$
(5)

117 It was demonstrated in (Rafailov et al., 2023) that \mathcal{L}_{DPO} has the same minimizer as \mathcal{L}_{RLHF} , under the 118 conditions of the BT model, an asymptotically large dataset, and a sufficiently large model capacity (i.e., a *tabular model* that encodes the probability of $\pi_{\theta}(y|x)$ for all $x \in \mathcal{X}$ and $y \in \mathcal{Y}$ into a vector). 120 The DPO framework was further extended in (Azar et al., 2023), aiming to directly maximize the 121 *win-rate* of π_{θ} against π_{ref} .

3 SPO - BASIC

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156 157 Following (1), we consider a loss function of the form:

$$\mathcal{L}_{\text{SPO}}(\pi_{\theta}, \pi_{\text{ref}}, \mathcal{D}) = \mathcal{L}_{\text{pref}}(\pi_{\theta}, \mathcal{D}) + \text{Reg}(\pi_{\theta}, \pi_{\text{ref}}),$$
(6)

where \mathcal{L}_{pref} and Reg stand for *preference loss* and *regularizer*, respectively. We proceed to further detail these components.

131 The regularization term, $\operatorname{Reg}(\pi_{\theta}, \pi_{ref})$, aims to ensure that π_{θ} avoids producing outputs that are highly improbable under π_{ref} . A common and effective choice is the KL divergence, $\mathcal{D}_{KL}(\pi_{\theta} \parallel \pi_{ref})$, 132 although other regularization options are viable (Zhao et al., 2022). Importantly, $\text{Reg}(\pi_{\theta}, \pi_{\text{ref}})$ does 133 not incorporate the preference dataset \mathcal{D} as an input. This is because within \mathcal{D} , the model aims to 134 fit to the target preferences, making additional regularization within \mathcal{D} unnecessary. In fact, the 135 regularization term primarily aims to regularize π_{θ} outside \mathcal{D} . This approach diverges from the DPO 136 and several other existing loss functions (detailed in Section 8), which only consider the divergence 137 of π_{θ} from π_{ref} within the preference dataset. 138

We now turn our attention to the preference loss. Given a query x, let $\pi_{\theta}(y|x)$ denote the probability that model π_{θ} generates output y. When presented with a query x and two responses, y_1 and y_2 , we define the probability that π_{θ} prefers y_1 over y_2 as

$$\mathcal{P}_{\pi_{\theta}}(y_{1} \succ y_{2} \mid x) \stackrel{\text{def}}{=} P\left(\text{output of } \pi_{\theta}(\cdot \mid x) \text{ is } y_{1} \mid \text{output of } \pi_{\theta}(\cdot \mid x) \text{ is in } \{y_{1}, y_{2}\}\right)$$

$$= \frac{\pi_{\theta}(y_{1} \mid x)}{\pi_{\theta}(y_{1} \mid x) + \pi_{\theta}(y_{2} \mid x)},$$
(7)

where the last equality follows from the definition of conditional probability. We can then employ
log-likelihood loss to measure the alignment of preference-probabilities' with the preference-dataset
labels,

$$-\mathbb{E}_{(x;y_w,y_l)\sim\mathcal{D}}\Big[\log \mathcal{P}_{\pi_\theta}(y_w \succ y_l \mid x)\Big].$$
(8)

We consider a preference loss $\mathcal{L}_{\text{pref}}^{\alpha}(\pi_{\theta}, \mathcal{D})$ that extends the above cross entropy loss by employing arbitrary exponents for π_{θ} . Specifically, we let for any $\alpha > 0$,

$$\mathcal{L}_{\text{pref}}^{\alpha}(\pi_{\theta}, \mathcal{D}) \stackrel{\text{def}}{=} -\frac{1}{\alpha} \mathbb{E}_{(x; y_w, y_l) \sim \mathcal{D}} \left[\log \frac{\pi_{\theta}(y_w \mid x)^{\alpha}}{\pi_{\theta}(y_w \mid x)^{\alpha} + \pi_{\theta}(y_l \mid x)^{\alpha}} \right],\tag{9}$$

and for $\alpha = 0$,

$$\mathcal{L}_{\text{pref}}^{0}(\pi_{\theta}, \mathcal{D}) \stackrel{\text{def}}{=} -\frac{1}{2} \mathbb{E}_{(x; y_{w}, y_{l}) \sim \mathcal{D}} \left[\log \frac{\pi_{\theta}(y_{w} \mid x)}{\pi_{\theta}(y_{l} \mid x)} \right].$$
(10)

The $\mathcal{L}_{\text{pref}}^{\alpha}$ takes the specific form (10) because the gradient of (9) approaches the gradient of (10) when $\alpha \to 0$, as can be easily verified from the following closed form expression for any $\alpha \ge 0$,

$$-\nabla_{\theta} \mathcal{L}_{\text{pref}}^{\alpha}(\pi_{\theta}, \mathcal{D}) = \mathbb{E}_{(x; y_w, y_l) \sim \mathcal{D}} \left[\frac{\pi_{\theta}(y_l | x)^{\alpha}}{\pi_{\theta}(y_w | x)^{\alpha} + \pi_{\theta}(y_l | x)^{\alpha}} \left(\nabla_{\theta} \log \pi_{\theta}(y_w | x) - \nabla_{\theta} \log \pi_{\theta}(y_l | x) \right) \right].$$

Here, $\pi_{\theta}(y_l|x)^{\alpha}/(\pi_{\theta}(y_w|x)^{\alpha} + \pi_{\theta}(y_l|x)^{\alpha})$ serves as a measure of the model's error in preferring y_w over y_l . Consequently, the magnitude of this preference error proportionally scales the adjustment $\nabla_{\theta} \log \pi_{\theta}(y_w|x) - \nabla_{\theta} \log \pi_{\theta}(y_l|x)$, leading to larger updates when the error is large.

The loss function $\mathcal{L}_{\text{pref}}^{\alpha}(\pi_{\theta}, \mathcal{D})$ contains the cross-entropy loss in (8) as a special case when $\alpha = 1$. The α parameter allows for tailoring the model to exhibit different entropies; models minimized under $\mathcal{L}_{\text{pref}}^{\alpha}$ will display higher entropy for larger α values, gradually moving towards a deterministic model akin to DPO as α approaches zero; as established in the next theorem.

Although the SPO framework does not rely on existence of underlying reward functions, and in particular the BT assumption, it is insightful to study the preference loss $\mathcal{L}_{\text{pref}}^{\alpha}$ under the conditions where the BT model assumption is valid. Intuitively, for a *BT expert model*, defined as $\pi(y|x) = \exp(r(y|x))/Z(x)$ with Z(x) being the partition function, the preference probability in (7) would be identical to the BT preference formula (2). In the next theorem, we further study the landscape of $\mathcal{L}_{\text{pref}}^{\alpha}$ under the BT model assumption. To eliminate local minima and saddle points that arise from nonlinear model spaces such as neural networks, in the theorems we consider a *tabular model* that encodes the probability of $\pi_{\theta}(y|x)$ for all $x \in \mathcal{X}$ and $y \in \mathcal{Y}$ into a large vector.

Theorem 1. Suppose that the BT model holds with rewards $r(\cdot|x)$, and fix any probability distribution D over $\mathcal{X} \times \mathcal{Y} \times \mathcal{Y}$ that has full support¹ and is consistent with the BT assumption.² Then, for any $\alpha \ge 0$, in the tabular model, $\mathcal{L}_{pref}^{\alpha}$ has a unique minimizer Softmax $(r(\cdot|x)/\alpha)$ (reducing to argmax $r(\cdot|x)$ for $\alpha = 0$). Furthermore, this minimizer is globally absorbing, and the landscape of $\mathcal{L}_{pref}^{\alpha}$ contains no other first-order stationary point (i.e., no other local minima, local maxima, or saddle points).

The proof is provided in Appendix A. According to Theorem 1, minimizer of $\mathcal{L}_{\text{pref}}^{\alpha}$ is the softmax of BT rewards divided by α , where α controls the entropy of the final model. Specifically, in the the asymptotically large dataset regime, when $\alpha = 1$, the preference loss reaches its minimum at the hypothetical *BT expert model* that generates the preference dataset's labels, defined as Softmax $(r(\cdot|x))$.

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4 THE GENERAL SPO ALGORITHM

191 192 We further expand the preference loss of SPO by considering a weighting over different samples, 193 where the weights can depend on π_{θ} . This weighting only affects (improves) the optimization process 194 without changing the fixed point, as we show in this section.

195 We call a function $\mu : \mathcal{Y} \times \mathcal{Y} \times \mathcal{X} \to \mathbb{R}^+$ symmetric positive if $\mu(y_1, y_2 \mid x) = \mu(y_2, y_1 \mid x) > 0$, 196 for all $x \in \mathcal{X}$ and all $y_1, y_2 \in \mathcal{Y}$. Given a symmetric positive function μ and an $\alpha \ge 0$, we define 197 weighted preference loss as

$$\mathcal{L}_{\text{pref}}^{\alpha,\mu}(\pi_{\theta},\mathcal{D}) \stackrel{\text{def}}{=} -\frac{1}{\alpha} \mathbb{E}_{(x;y_w,y_l)\sim\mathcal{D}} \left[\mu(y_w,y_l \mid x) \log \frac{\pi_{\theta}(y_w \mid x)^{\alpha}}{\pi_{\theta}(y_w \mid x)^{\alpha} + \pi_{\theta}(y_l \mid x)^{\alpha}} \right]$$
(11)

if $\alpha > 0$, and for $\alpha = 0$ we let

$$\mathcal{L}_{\text{pref}}^{0,\mu}(\pi_{\theta},\mathcal{D}) \stackrel{\text{def}}{=} -\frac{1}{2} \mathbb{E}_{(x;y_w,y_l)\sim\mathcal{D}} \left[\mu(y_w,y_l \mid x) \log \frac{\pi_{\theta}(y_w \mid x)}{\pi_{\theta}(y_l \mid x)} \right].$$
(12)

The weight-function μ controls the impact of individual samples within the loss calculation. The utility of μ emerges from the observation that not all sample pairs in the preference dataset hold equivalent significance. For instance, diminishing the weights of dataset samples $(x; y_w, y_l)$ where both responses y_w and y_l are of low quality (e.g., low probability) can be particularly advantageous. This can be achieved for example by setting

$$\mu(y_1, y_2 \mid x) = 2\sigma \left(\left(\pi_{\theta}(y_1 \mid x) + \pi_{\theta}(y_2 \mid x) \right)^{\gamma} - \hat{\mathbb{E}}_{(y_1', y_2' \mid x') \sim \mathcal{D}} \left[\left(\pi_{\theta}(y_1' \mid x') + \pi_{\theta}(y_2' \mid x') \right)^{\gamma} \right] \right),$$
(13)

²¹¹ ¹Full support in this context means that the probability distribution assigns a non-zero sampling probability to all $(x; y_w, y_l) \in \mathcal{X} \times \mathcal{Y} \times \mathcal{Y}$.

^{213 &}lt;sup>2</sup>Consistency with the BT holds if the relative probability of outcomes is determined by a logistic function of 214 the reward differences. More specifically, $\mathcal{D}(x; y_1, y_2)/\mathcal{D}(x; y_2, y_1) = p^{\mathrm{BT}}(y_1 \succ y_2|x)/p^{\mathrm{BT}}(y_2 \succ y_1|x) =$ 215 $\exp(r(y_1 \mid x) - r(y_2 \mid x))$, for all $(x; y_1, y_2) \in \mathcal{X} \times \mathcal{Y} \times \mathcal{Y}$, where p^{BT} is defined in (2) and $r(\cdot|\cdot)$ is the reward function in the BT model.

A	lgorithm 1 SPO
_	for $t = 0, 1, 2, \dots$ do
	if t is a multiple of T : # once every T iterations
	Generate a batch \mathcal{B} of online samples $y \sim \pi_{\theta}(\cdot x)$, for a set of recently observed $x \sim \mathcal{D}$.
	Compute $\mathcal{L}_{\text{pref}}^{\alpha,\mu}(\pi_{\theta},\mathcal{D})$ from (11), using the μ function given in (13).
	Compute token-wise regularizer $\widehat{\mathcal{D}_{KL}}(\pi_{\theta} \parallel \pi_{ref})$ from (15), using the online samples batch \mathcal{B} .
	Form the SPO loss function $\mathcal{L}_{\text{SPO}}(\pi_{\theta}, \pi_{\text{ref}}, \mathcal{D}) = \mathcal{L}_{\text{pref}}^{\alpha, \mu}(\pi_{\theta}, \mathcal{D}) + \widehat{\mathcal{D}_{\text{KL}}}(\pi_{\theta} \parallel \pi_{\text{ref}}).$
	Update the network using an optimizer of interest for the loss function $\mathcal{L}_{SPO}(\pi_{\theta}, \pi_{ref}, \mathcal{D})$.
	end for

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where σ is the sigmoid function, $\gamma \ge 0$ is a hyperparameter (e.g., 0.01) to dampen the influence of exponentially shrinking probabilities, and $\hat{\mathbb{E}}$ aims to ensure that the significance of a pair is measured relative to other pairs and can be obtained by averaging over the current batch. The μ function boils down to uniform weights if $\gamma = 0$ or if all pairs in the batch have similar sum-probabilities.

While μ may depend on π_{θ} , it is important to note that gradient propagation through μ is not permitted. Specifically, the gradient $\nabla_{\theta} \mathcal{L}_{\text{pref}}^{\alpha,\mu}(\pi_{\theta}, \mathcal{D})$ is given by

$$-\mathbb{E}_{(x;y_w,y_l)\sim\mathcal{D}}\left[\mu(y_w,y_l|x)\frac{\pi_{\theta}(y_l|x)^{\alpha}}{\pi_{\theta}(y_w|x)^{\alpha}+\pi_{\theta}(y_l|x)^{\alpha}}\left(\nabla_{\theta}\log\pi_{\theta}(y_w|x)-\nabla_{\theta}\log\pi_{\theta}(y_l|x)\right)\right].$$
(14)

Interestingly, the weight function, μ , mainly influences the optimization process, not the ultimate fixed point, in the tabular setting and under asymptotically large preference dataset, as we show in the next theorem. The proof is given in Appendix A.

Theorem 2. Suppose that the conditions of Theorem 1 hold. Then for any $\alpha \ge 0$ and any symmetric positive function μ , the softmax of the BT rewards divided by α , Softmax $(r(\cdot|x)/\alpha)$ (reducing to argmax $r(\cdot|x)$ for $\alpha = 0$), is the unique globally absorbing fixed point of the differential equation $\pi = \prod (-\nabla_{\theta} \mathcal{L}_{pref}^{\alpha,\mu}(\pi_{\theta}, \mathcal{D}))$, where $\prod(\cdot)$ stands for projection onto the probability simplex, and the gradient is given in (14).

We now proceed to discuss the computation of \mathcal{D}_{KL} regularizer in (6). In order to estimate $\mathcal{D}_{\text{KL}}(\pi_{\theta} \| \pi_{\text{ref}}) = \mathbb{E}_x \mathbb{E}_{y \sim \pi_{\theta}(\cdot | x)} \left[\log \left(\pi_{\theta}(y | x) / \pi_{\text{ref}}(y | x) \right) \right]$, we generate online samples from the current model π_{θ} . This is however costly for sequential models, where sequence generation necessitates sequential calls to the model. To mitigate this problem, we generate a batch of samples from π_{θ} intermittently, for example once every T steps, and keep using samples from this batch for approximating \mathcal{D}_{KL} , until the next batch of samples is generated.

Given a batch of samples (x, y) with $y \sim \pi_{\theta}(\cdot|x)$, in order to we obtain a reduced variance approximation of \mathcal{D}_{KL} , we employ the following token-wise \mathcal{D}_{KL} formula:

$$\widehat{\mathcal{D}_{\mathrm{KL}}}(\pi_{\theta} \parallel \pi_{\mathrm{ref}}) \stackrel{\text{def}}{=} \mathbb{E}_{(x;y)\in\mathrm{batch}} \left[\sum_{\tau=1}^{|y|} \mathcal{D}_{\mathrm{KL}} \Big(\pi_{\theta}(Y_{\tau} \mid x, y_{:\tau}) \parallel \pi_{\mathrm{ref}}(Y_{\tau} \mid x, y_{1:\tau}) \Big) \right]
= \mathbb{E}_{(x;y)\in\mathrm{batch}} \left[\sum_{\tau=1}^{|y|} \sum_{s\in\mathcal{S}} \pi_{\theta}(Y_{\tau} = s \mid x, y_{1:\tau}) \log \frac{\pi_{\theta}(Y_{\tau} = s \mid x, y_{1:\tau})}{\pi_{\mathrm{ref}}(Y_{\tau} = s \mid x, y_{1:\tau})} \right],$$
(15)

where S is the set of all possible tokens. Note that $\pi(Y_{\tau} = s \mid x, y_{1:\tau})$ is readily available from the softmax of the logits, in the network's output. Therefore, the sum in (15) can be computed with negligible computational overhead (excluding the initial forward path). Note that $\widehat{\mathcal{D}_{KL}}$ is a biased estimate of the sequence- \mathcal{D}_{KL} . However, we empirically found that the benefit of reduced variance brought by the token-wise approximation out-weights the potential negative impact of the resulting bias. Moreover, similar to sequence- \mathcal{D}_{KL} , the token-wise \mathcal{D}_{KL} is a proximity measure for π_{θ} and π_{ref} , and is therefore a conceptually sound choice of regularizer. Algorithm 1 summarized the SPO algorithm.

5 SPO FOR OTHER DATA-TYPES: BEST-OF-*n* PREFERENCE AND RANKED PREFERENCE

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In this section, we generalize the SPO algorithm for other types of preference data: best-of-*n* preference data and ranked-data. We extend the definition of a symmetric function to *n*-responses by calling a function $\mu : \mathcal{Y}^n \times \mathcal{X} \to \mathbb{R}^+$ symmetric positive if $\mu(y_{\tau(1)}, \ldots, y_{\tau(n)} | x) = \mu(y_1, \ldots, y_n | x) > 0$, for all $x \in \mathcal{X}$ all $y_1, \ldots, y_n \in \mathcal{Y}$, and all permutations τ of $(1, \ldots, n)$.

Best-of-*n* **preference data:** Given an $n \ge 2$, a sample $(x; y_1, \ldots, y_n; i^*)$ of a best-of-*n* preference dataset consists of a query *x* along with *n* responses y_1, \ldots, y_n , one of which (i.e., y_{i^*}) is labeled by the expert as the best response. Given a symmetric positive function μ and an $\alpha > 0$, we propose the following preference loss for a best-of-*n* preference dataset \mathcal{D} :

$$\mathcal{L}_{\text{pref-}n}^{\alpha,\mu}(\pi_{\theta},\mathcal{D}) \stackrel{\text{def}}{=} -\frac{1}{\alpha} \mathbb{E}_{(x;y_1,\dots,y_n;i^*)\sim\mathcal{D}} \left[\mu(y_1,\dots,y_n \mid x) \log \frac{\pi_{\theta}(y_{i^*} \mid x)^{\alpha}}{\sum_{i=1}^n \pi_{\theta}(y_i \mid x)^{\alpha}} \right].$$
(16)

285 As before, we stop the gradient from propagating through μ , even though μ may depend on π_{θ} . 286 Similar to the case of pairwise preferences, we show in the following theorem that the loss in (16) is 287 minimized at the softmax of rewards, if we assume existence of an underlying reward function. In 288 particular, given a reward function $r(\cdot|x): \mathcal{X} \to \mathcal{Y}$ and a distribution \mathcal{D} over $\mathcal{X} \times \mathcal{Y}^n \times \{1, \dots, n\}$, 289 we say that \mathcal{D} is *consistent with n-ary BT model* if for any $(x; y_1, \ldots, y_n) \in \mathcal{X} \times \mathcal{Y}^n$ and any 290 $i, j \in \{1, \dots, n\}, \mathcal{D}(x; y_1, \dots, y_n; i) / \mathcal{D}(x; y_1, \dots, y_n; j) = \exp(r(y_i \mid x) - r(y_i \mid x)).$ Note that 291 this definition boils down to the definition of consistency with BT model for n = 2 in Section 3. 292 Proof of the following theorem is given in Appendix B.

Theorem 3. Consider a reward function $r(\cdot \mid x)$ and a probability distribution \mathcal{D} with full support over $\mathcal{X} \times \mathcal{Y}^n \times \{1, ..., n\}$ that is consistent with the *n*-ary BT model. Then, for any $\alpha > 0$ and any symmetric positive function μ , in the tabular model, $\operatorname{Softmax}(r(\cdot \mid x) / \alpha)$ is the unique globally absorbing fixed point of the differential equation $\dot{\pi} = \prod \left(-\nabla_{\theta} \mathcal{L}_{\operatorname{pref-}n}^{\alpha,\mu}(\pi_{\theta}, \mathcal{D}) \right)$, where $\prod(\cdot)$ stands for projection onto the probability simplex.

Ranked Preference Data: A ranked preference dataset consists of samples of the form $(x; y_1, \ldots, y_n; \tau)$, where x is a query, y_1, \ldots, y_n are n responses, and τ is a permutation representing the relative preference $y_{\tau(1)} \succ \cdots \succ y_{\tau(n)}$ of the expert over these responses. Given an $\alpha > 0$ and a sequence of symmetric positive function $\mu_k : \mathcal{X} \times \mathcal{Y}^k \to \mathbb{R}$ for $k = 2, \ldots, n$, we propose the following preference loss for a ranked preference dataset \mathcal{D} :

$$\mathcal{L}_{\mathrm{rank}}^{\alpha,[\mu]}(\pi_{\theta},\mathcal{D}) \stackrel{\mathrm{def}}{=} -\frac{1}{\alpha} \mathbb{E}_{(x;y_1,\dots,y_n;\tau)\sim\mathcal{D}} \left[\sum_{k=1}^{n-1} \mu_k(y_{\tau(k)},\dots,y_{\tau(n)}|x) \log \frac{\pi_{\theta}(y_{\tau(k)}|x)^{\alpha}}{\sum_{j=k}^n \pi_{\theta}(y_{\tau(j)}|x)^{\alpha}} \right].$$
(17)

We can control the importance weight of responses in different ranks through appropriate adjustment of weight functions μ^1, \ldots, μ^{n-1} . For example, by setting $\mu_k = 0$ for $k = 2, \ldots, n-1, \mathcal{L}_{rank}^{\alpha,[\mu]}$ boils down to $\mathcal{L}_{pref-n}^{\alpha,\mu^1}$. Here again, the gradient is not allowed to propagate through μ^1, \ldots, μ^{n-1} , even though these functions may depend on π_{θ} . The following theorem shows that, assuming existence of underlying rewards under the PL model (3), the softmax of these rewards is the unique minimizer of $\mathcal{L}_{rank}^{\alpha,\mu}$. The proof relies on Theorem 3, and is given in Appendix C.

Theorem 4. Suppose that the PL model holds with rewards $r(\cdot|x)$, and a probability distribution \mathcal{D} with full support over $\mathcal{X} \times \mathcal{Y}^n \times \{\text{Identity permutation}\}$ that is consistent with the PL model.³ Then, for any $\alpha > 0$ and any sequence $[\mu] = \mu^1, \ldots, \mu^{n-1}$ of symmetric positive functions, in the tabular model, Softmax $(r(\cdot|x)/\alpha)$ is the unique globally absorbing fixed point of the differential equation $\dot{\pi} = \prod (-\nabla_{\theta} \mathcal{L}_{\text{rank}}^{\alpha,[\mu]}(\pi_{\theta}, \mathcal{D}))$, where $\prod(\cdot)$ stands for projection onto the probability simplex.

³²¹ 322 ³Consistency with the PL model holds if $\mathcal{D}(x; y_1, \ldots, y_n; \tau) / \mathcal{D}(x; y_1, \ldots, y_n; \tau') = p^{\mathrm{PL}}(y_{\tau(1)} \succ \cdots \succ y_{\tau(n)}|x) / p^{\mathrm{PL}}(y_{\tau'(1)} \succ \cdots \succ y_{\tau'(n)}|x)$, for all $(x; y_1, \ldots, y_n) \in \mathcal{X} \times \mathcal{Y}^n$ and all permutations τ and τ' , where p^{PL} is defined in (3).

324 COMPARATIVE ANALYSIS: SPO VERSUS DPO 6 325

326 This section contrasts the SPO method with the DPO algorithm conceptually. A detailed empirical 327 comparison follows in Section 7. 328

A key difference between SPO and DPO lies in how regularization (\mathcal{D}_{KL}) is applied. In RLHF and SPO, \mathcal{D}_{KL} is used to prevent π_{θ} from straying too far from π_{ref} in unexplored regions, reducing the risk 330 of distribution shifts. In contrast, the DPO loss function (5) applies regularization only to preference 331 dataset samples, which is suboptimal because 1) it fails to prevent distribution shifts in unexplored 332 regions, and 2) regularizing within the dataset can hinder alignment with the preferences. In contrast, 333 SPO incorporates a global regularizer to prevent undesired out-of-dataset distribution shifts. In the 334 context of a question-answering task, the term "out-of-dataset region" refers to query-response pairs 335 where the response is not part of the preference dataset. The query in these pairs may or may not be 336 included in the dataset, but it should, in either case, be relevant to the test domain. 337

Moreover, SPO has an advantage over DPO and RLHF in avoiding determinism. In cases where the 338 preference dataset is comparable to pre-training data size, regularization (\mathcal{D}_{KL}) becomes unnecessary 339 (and we can set $\beta \simeq 0$), in which case RLHF and DPO loss functions tend to produce deterministic 340 models; that is they tend to return a single high-quality response per query. This reduced diversity 341 makes DPO prone to mode collapse (Azar et al., 2023). SPO, however, controls entropy via the α 342 parameter in (9), even without the use of regularizer (see Theorem 1), preserving response diversity. 343 This makes SPO more adaptable for continual learning and future alignments. 344

It is noteworthy that unlike RLHF and DPO, the SPO framework does not assume the existence of an 345 underlying reward model or rely on assumptions like the BT model. Instead, SPO's preference loss 346 directly aligns π_{θ} with the preferences in the dataset, making it potentially more adaptable to broader 347 alignment contexts. Additionally, SPO is not limited to using \mathcal{D}_{KL} for regularization, unlike DPO and 348 IPO, which depend on \mathcal{D}_{KL} for derivations of their loss functions. 349

We also note that the DPO loss cannot be separated into components like (6), where the preference 350 loss is independent of π_{ref} and paired with a regularizer like \mathcal{D}_{KL} . As a short proof, consider a case 351 where $\pi_{\theta}(y_w|x) = \pi_{\theta}(y_l|x)$ for a sample $(x; y_w, y_l) \in \mathcal{D}$. Here, the alignment loss in (6) remains 352 symmetrical with respect to $\pi_{ref}(y_w|x)$ and $\pi_{ref}(y_l|x)$; swapping their values wouldn't affect either 353 the preference loss or \mathcal{D}_{KL} . This symmetry doesn't hold in the DPO framework, as seen in the DPO 354 loss in (5). Therefore, the DPO loss cannot be represented in the separable form of (6). 355

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EXPERIMENTS 7

359 This section presents empirical evaluations of SPO. All codes and datasets are available online at (Anonymous, 2024).

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7.1 ALIGNMENT TO PAIRWISE PREFERENCE DATA

364 Experiment setting: To evaluate the performance of SPO, we trained a Llama2-7B model (Touvron et al., 2023) on a pairwise preference dataset for question-answering available in AlpacaFarm (Dubois 366 et al., 2023), and computed the win-rates against the Llama2-7B SFT model on AlpacaEval 2 (Li et al., 367 2023), using GPT4-Turbo API. More specifically, we used the following pipeline. We downloaded 368 the pretrained Llama2-7B model and performed supervised fine-tuning on the AlpacaFarm SFT 369 dataset available at Dubois et al. (2023), to obtain the SFT model. Initializing the weights on the 370 SFT model, we then performed alignment to the preference dataset from AlpacaFarm that contains 371 pairs of question-answering samples and preference labels provided by GPT-4. We compared the 372 performance of SPO with several reward-model-free alignment algorithms, namely DPO (Rafailov 373 et al., 2023), IPO (Azar et al., 2023), KTO (Ethayarajh et al., 2024), CPO (Xu et al., 2024), R-DPO 374 (Park et al., 2024), and SimPO (Meng et al., 2024). For SPO, the experiment includes both the basic 375 and weighted versions of SPO, with the weight function μ given in (13). We trained each algorithm for a few epochs, used GPT4-Turbo to compute its win-rate against the SFT model at the end of each 376 epoch, and reported the maximum win-rate for each algorithm. Additional details about setting of 377 this experiment is provided in Appendix D.1.

Results: Table 1 presents the win-rates and length-controlled (LC) win-rates (Dubois et al., 2023)
of different algorithms against the SFT model. The SPO algorithm outperforms the other tested
algorithms in both conventional win-rate and LC win-rate. Furthermore, the weighted version of
SPO performs better than the basic version, demonstrating the advantage of incorporating the weight
function. Standard deviation of the reported win-rates is 1.5%. Moreover, LC win-rates in Table 1
are evaluated on models with hyperparameters optimized for win-rates. Notably, SPO shows better
generalization to LC win-rates compared to other baselines, some of which show less than 50% LC
winrate against the SFT model.

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Table 1: Alignment of the Llama2-7B model on AlpacaFarm dataset.

Alignment method	Win-rate(%)	LC Win-rate(%)
SFT	50.00	50.00
R-DPO	52.50	41.49
CPO	54.10	39.38
SimPO	58.48	49.73
КТО	58.50	51.94
IPO	58.59	49.60
DPO	59.16	51.26
SPO-basic (unweighted)	60.83	53.17
SPO	61.63	56.25

7.2 ALIGNMENT TO RANKING AND BEST-OF-*n* PREFERENCE DATA

401 Experiment setting: Dataset: Alignment research has largely focused on pairwise preferences, and 402 publicly available datasets for other preference types are rather scarce. To address this, we generated 403 an *n*-ary ranked preference dataset (n = 4) using GPT40 API as the labeler. Building on TinyStories (Eldan & Li, 2023) –a synthetic collection of short stories aimed at children aged 3 to 4- we created 404 a preference dataset to align the stories to an older audience. The dataset contains around 5,000 405 samples, each with four stories generated by the TinyStories pre-trained 110M model, ranked by 406 GPT40-2024-08-06 based on coherence and engagement for older students. The best-of-n dataset 407 was then derived by removing the rank labels for the 2nd, 3rd, and 4th responses. Further details are 408 in Appendix E, and the datasets are available online at (Anonymous, 2024). 409

Training: Using the implementation from (Karpathy, 2024) and the supervised fine-tuned model
from (Karpathy, 2023), we aligned a 110M parameter model with ranking and best-of-*n* versions of
SPO. We compared this with three baselines: the ranking version of DPO (AppendixA3 of (Rafailov
et al., 2023)), S-DPO (Chen et al., 2024), and Best-response-SFT. Best-response-SFT is derived by
all performing supervised fine-tuning on all top-rank responses. See Appendix D.2 for further details.

Results: Tables 2 and 3 present peak win rates against the Best-response-SFT model for aligning the
110M TinyStories SFT model to ranking and best-of-*n* datasets using different algorithms. The SPO
algorithm outperforms all baselines for both types of alignment. Standard deviation of the reported
win-rates is 1.4%.

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Table 2: Alignment of TinyStories SFT model to the ranking dataset.

Alignment method	Win-rate (%)
Best-response-SFT	50.0
DPO (ranking version)	67.0
S-DPO (ranking)	55.1
SPO (ranking)	68.5

Table 3: Alignment of TinyStories SFT model to the best-of-*n* dataset.

Alignment method	Win-rate (%)
Best-response-SFT	50.0
S-DPO (best-of- <i>n</i>)	66.0
SPO-basic (best-of- <i>n</i>)	67.8
SPO (best-of- <i>n</i>)	70.5

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7.3 Ablation Study

Global regularization vs in-dataset regularization: To evaluate the significance of global regularization, we trained a Llama2-7B SFT model the SPO-basic algorithm while replacing the global \mathcal{D}_{KL} regularizer of (15) with in-dataset regularizers. In particular, we tested three different in-dataset regularizers, including the popular $-\log \pi(y_w|x)$ regularizer that is used in several alignment algorithm like CPO, SLiC-HF (Zhao et al., 2023), and RRHF (Yuan et al., 2024). Other experiment settings are similar to the setting discussed in Section 7.1. Table 4 provides the list of these in-dataset regularizers, as well as the peak win-rates of SPO-basic using these regularizers against the Llama2-7B SFT model. As it can be seen from the table, the global \mathcal{D}_{KL} regularizer of (15) achieved better performance compared to in-dataset regularizers.

439 Weight function μ : As observed in the experiment of Section 7.1 on the alignment to AlpacaFarm 440 preferences dataset, the weighted version of SPO achieved win-rate 61.63% compared to the win-rate 441 of 60.83% for SPO-basic. In the experiment of Section 7.2 on the alignment to best-of-*n* preferences 442 dataset, the weighted version of SPO improved the win-rate to 70.5%, up from 67.8% for SPO-443 basic. In the ranking experiment, use of non-uniform μ did not improve the win-rate. In all of 444 these experiments, the μ function in the weighted SPO algorithm is of the form (13) with parameter 445 $\gamma = 0.01$. We performed no sweeping on the parameter $\gamma = 0.01$.

Table 4: Ablation of SPO regularizer (model: Llama2-7B, dataset:	AlpacaFarm)
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Regularizer type	Regularizer formula	Win-rate vs. SFT
in-dataset (log probability)	$-\mathbb{E}_{(x;y_w,y_l)\in\mathcal{D}}[\log \pi_{\theta}(y_w x)]$	54.1
in-dataset (tokenwise)	$\mathbb{E}_{(x;y)\in D}\left[\sum_{\tau=0}^{ y -1}\mathbb{E}_{Y\sim\pi_{\theta}}(\cdot x,y_{1:\tau})\log\frac{\pi_{\theta}(Y x,y_{1:\tau})}{\pi_{\mathrm{ref}}(Y x,y_{1:\tau})}\right]$	59.7
in-dataset (importance sampling)	$\mathbb{E}_{(x;y)\in D} \left[\frac{\pi_{\theta}(y x)}{\pi_{\mathrm{ref}}(y x)} \log \frac{\pi_{\theta}(y x)}{\pi_{\mathrm{ref}}(y x)} \right]$	59.9
global	Eq. (15)	60.8

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8 RELATED WORKS

459 RLHF aims to align AI systems with human preferences, relying on human judgments rather than 460 manual rewards or demonstrations. This method has been successfully applied in fine-tuning large 461 language models (LLMs) (Achiam et al., 2023; Touvron et al., 2023; Ouyang et al., 2022), but 462 faces challenges including data quality issues, reward misgeneralization, and policy optimization 463 complexities. Research to enhance RLHF includes methods such as rejection sampling for response 464 generation (Dong et al., 2023; Touvron et al., 2023), where the highest-reward response from a 465 fixed number is selected for fine-tuning. Zhang et al. (2023) simplified instruction alignment with language models into a goal-oriented reinforcement learning task, utilizing a two-phase approach 466 of high-temperature online sampling and supervised learning with relabeled data during offline 467 training. A two-loop learning algorithm, Grow and Improve, has also been proposed for iterative 468 model alignment and training on a fixed dataset (Gulcehre et al., 2023). The Grow loop leverages the 469 existing model to create and sample a dataset while the Improve loop iteratively trains the model on a 470 fixed dataset. 471

Given the challenges of RLHF, reward-model-free alignment methods emerged fairly recently and 472 have gained a lot of popularity. Reward-model-free approach to alignment was popularized specif-473 ically after introduction of DPO in (Rafailov et al., 2023), which is breifly outlined in Section 2. 474 Recently, several works have been proposed methods to improve DPO. Building on DPO, Ji et al. 475 (2024) proposed Efficient Exact Optimization (EXO) method, which aligns language models by 476 minimizing reverse KL divergence, offering a more stable and efficient alternative to RL-based 477 methods. Azar et al. (2023) proposed an objective called ΨPO for learning from human preferences 478 that is expressed in terms of pairwise preferences, with no need for assumption of the BT model. 479 The authors focused on a specific instance, IPO, of Ψ PO by setting Ψ as the identity, aiming to 480 mitigate the overfitting and tendency-towards-deterministic-policies issues observed in DPO. Munos 481 et al. (2023) formulated the alignment problem as finding the Nash equilibrium (NE) of a maximin 482 game with two policies π and π' as two players where each policy receives pay off of probability 483 of winning over the other policy. The authors showed that the NE point can be approximated by running a mirror-descent-like algorithm. Rosset et al. (2024) and Swamy et al. (2024) proposed other 484 approaches to approximate the NE point based on no-regret algorithms (Freund & Schapire, 1997). 485 Chowdhury et al. (2024) proposed a loss function which is an unbiased estimate of the original DPO

486 loss, and aims to alleviate sensitivity to flipped labels due to labeling noise. Amini et al. (2024) 487 added an offset term within the sigmoid function in the DPO loss. In this manner, the model puts 488 more weight on the winning response. To control the length of the output, R-DPO (Park et al., 2024) 489 modified the DPO loss by adding a regularization term that penalizes lengthy responses. To achieve 490 the same goal, SimPO (Meng et al., 2024) replaced the log-likelihood ratio between the current policy and the baseline model with the average log probability of the sequence under the current policy. 491 In (Rafailov et al., 2024), a token-level formulation of DPO has been proposed which enables a 492 likelihood search over a DPO model by classical search-based algorithms, such as MCTS. Inspired 493 by cringe loss previously proposed for binary feedback, Xu et al. (2023) adapted cringe loss for the 494 pairwise preference context. Recently, in (Ethayarajh et al., 2024), KTO loss has been proposed for 495 alignment from non-paired preference datasets. Sessa et al. (2024) introduced BOND, which replaces 496 a reward model with a win-rate model that predicts the likelihood of a response being better than a 497 randomly sampled reference response. This win-rate model is then used to train the policy towards a 498 best-of-n policy, effectively aligning it with human preferences. In the same vein, Gui et al. (2024) 499 proposed BoNBoN Alignment, which directly integrates best-of-n sampling into the training process, 500

In practice, the performance of an alignment technique highly depends on the quality of the human 501 preference dataset. Noisy preference pairs could potentially limit the language models from capturing 502 human intention. In (Liu et al., 2023), DPO was used in conjunction with an improved preference dataset via a rejection sampling technique, arguing that DPO suffers from a mismatch between the 504 sampling distribution and the policy corresponding to true expert preferences. (Tunstall et al., 2023) 505 formed a dataset of conservative pairs by collecting AI feedback through an ensemble of chat model 506 completions, followed by GPT-4 scoring. Then, they employed DPO for alignment to this improved 507 dataset. The work in (Yin et al., 2024) leveraged semantic correlations of prompts in the dataset to 508 form more conservative response pairs. For a given prompt $(x; y_w, y_l)$, a prompt x' with a similar semantic to a tuple $(x'; y'_w, y'_l)$ is used to form more conservative pairs. 509

510 Zhao et al. (2022) proposed a separable alignment technique called SLiC, where, similar to SPO, the 511 alignment loss is the sum of two terms: a calibration loss that contrasts winner and loser responses, 512 encouraging the model π_{θ} to assign more probability to the winner, and a regularizer term. SLiC 513 was further developed in (Zhao et al., 2023) for alignment to preference data, where they proposed 514 the SLiC-HF algorithm. SLiC-HF involves a rectified contrastive loss as its calibration loss and a 515 log-likelihood term as the regularization. Unlike SPO, SLiC-HF's regularization is limited to the 516 preference or pre-training datasets, not using online samples from π_{θ} as in the \mathcal{D}_{KL} regularizer.

517 Concurrent to our work, CPO (Xu et al., 2024) motivated the preference loss in (9) as a heuristic 518 approximation of DPO to reduce its complexity by removing π_{ref} from the DPO loss. This results in 519 a contrastive loss similar to SPO-basic (9). In contrast, we derived (9) and its extension in (11) as 520 what should be truly minimized, regardless of complexity considerations. Other major differences include CPO's use of in-dataset regularization versus SPO's global regularization, the incorporation 521 of a weighting mechanism in SPO, the generalization of SPO to other data types, and theoretical 522 guarantees proposed in this work. As we demonstrated in experiments (see Table 4), the choice of 523 regularizer significantly impacts performance. 524

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9 LIMITATIONS

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This paper introduced SPO, a class of algorithms designed for alignment to the expert's distribution, with controlled softness. The paper also presents theoretical results demonstrating favorable landscape and convergence properties of SPO. Below, we discuss some limitations of this work.

Limitations of the SPO Algorithm: The main limitation of the SPO framework is the computational complexity of the regularizer, which requires online sampling from π_{θ} . This limitation was discussed in Section 4, when intermittent batch generation of samples was proposed to mitigate the computational overhead.

Limitations of the Current Study: The "softness" of the model's output, controlled by the parameter α , allows SPO to excel in applications requiring exploration and diversity, such as LLM reasoning. Since current alignment benchmarks prioritize win rates over diversity, our experiments may underestimate SPO's potential, exploration of which remains a subject for future research.

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Appendices

A PROOF OF THEOREMS 1 AND 2

In this appendix, we present the proof of Theorems 1 and 2. The high-level proof idea is to show that moving along the projected⁴ negative gradient of the preference loss (i.e., the ODE direction) results in an absolute reduction of the Euclidean distance of π_{θ} from Softmax $(r(\cdot|x)/\alpha)$.

710 Without loss of generality, we prove the theorem for a single fixed $x \in \mathcal{X}$, and remove x from the 711 notations, for the sake of notation simplicity.

712 Given the rewards $r(\cdot)$ in the Bradley-Terry model, let

$$\pi^*(\cdot) \stackrel{\text{def}}{=} \text{Softmax}\left(r(\cdot)\right). \tag{18}$$

For any $\alpha \in [0, 1)$, let 716

$$\tau_{\alpha}^{*}(\cdot) \stackrel{\text{def}}{=} \operatorname{Softmax}\left(r(\cdot)/\alpha\right),\tag{19}$$

and let π^{α} be its vector representation. Therefore, for any $\alpha \in [0, 1]$, and for any y,

$$\pi^*(y) = z_{\alpha} \times \left(\pi^*_{\alpha}(y)\right)^{\alpha}, \quad \text{where } z_{\alpha} \stackrel{\text{def}}{=} \frac{\left(\sum_{y'} e^{r(y')/\alpha}\right)^{\alpha}}{\sum_{y'} e^{r(y')}}.$$
 (20)

Moreover, it follows from the consistency of distribution \mathcal{D} with the Bradley-Terry model that for any pair (y_1, y_2) ,

$$\frac{\mathcal{D}(y_1, y_2)}{\mathcal{D}(y_1, y_2) + \mathcal{D}(y_2, y_1)} = \mathcal{P}_{\mathcal{D}}(y_1 \succ y_2) = \frac{\exp r(y_1)}{\exp r(y_1) + \exp r(y_2)} = \frac{\pi^*(y_1)}{\pi^*(y_1) + \pi^*(y_2)}.$$
 (21)

For any $y_1, y_2 \in \mathcal{Y}$ let

$$\tilde{\mu}(y_1, y_2) \stackrel{\text{def}}{=} \mu(y_1, y_2) \big(\mathcal{D}(y_1, y_2) + \mathcal{D}(y_2, y_1) \big).$$
(22)

Note that the symmetry of μ implies symmetry of $\tilde{\mu}$ with respect to its first and second arguments. Then,

$$\mu(y_1, y_2) \mathcal{D}(y_1, y_2) = \tilde{\mu}(y_1, y_2) \frac{\mathcal{D}(y_1, y_2)}{\mathcal{D}(y_1, y_2) + \mathcal{D}(y_2, y_1)} = \tilde{\mu}(y_1, y_2) \frac{\pi^*(y_1)}{\pi^*(y_1) + \pi^*(y_2)}, \quad (23)$$

where the last equality follows from (21).

⁷³⁶ Consider a π_{θ} in the relative interior of the probability simplex and let v be the negative gradient of the preference loss

$$\mathbf{v} \stackrel{\text{def}}{=} -\nabla_{\pi_{\theta}} \mathcal{L}_{\text{pref}}^{\alpha,\mu}(\pi_{\theta}, \mathcal{D}), \tag{24}$$

where $\mathcal{L}_{\text{pref}}^{\alpha,\mu}$ is defined in (14). For any $y \in \mathcal{Y}$, let v(y) be the entry of v that corresponds to y. Then,

$$v(y) = \sum_{y' \in \mathcal{Y}} \mathcal{D}(y, y') \mu(y, y') \frac{\pi_{\theta}(y')^{\alpha}}{\pi_{\theta}(y)^{\alpha} + \pi_{\theta}(y')^{\alpha}} \left(\frac{d}{d\pi_{\theta}(y)} \log \pi_{\theta}(y) - \frac{d}{d\pi_{\theta}(y)} \log \pi_{\theta}(y')\right)$$

$$+ \sum_{y' \in \mathcal{Y}} \mathcal{D}(y', y) \mu(y', y) \frac{\pi_{\theta}(y)^{\alpha}}{\pi_{\theta}(y)^{\alpha} + \pi_{\theta}(y')^{\alpha}} \left(\frac{d}{d\pi_{\theta}(y)} \log \pi_{\theta}(y') - \frac{d}{d\pi_{\theta}(y)} \log \pi_{\theta}(y)\right)$$

$$= \sum_{y' \in \mathcal{Y}} \tilde{\mu}(y, y') \frac{\pi^{*}(y)}{\pi^{*}(y) + \pi^{*}(y')} \frac{\pi_{\theta}(y')^{\alpha}}{\pi_{\theta}(y)^{\alpha} + \pi_{\theta}(y')^{\alpha}} \frac{1}{\pi_{\theta}(y)}$$

$$- \sum_{y' \in \mathcal{Y}} \tilde{\mu}(y, y') \frac{\pi^{*}(y')}{\pi^{*}(y) + \pi^{*}(y')} \frac{\pi_{\theta}(y)^{\alpha}}{\pi_{\theta}(y)^{\alpha} + \pi_{\theta}(y')^{\alpha}} \frac{1}{\pi_{\theta}(y)}$$

$$= \sum_{y' \in \mathcal{Y}} \frac{\tilde{\mu}(y, y') \left(\pi^{*}(y)\pi_{\theta}(y')^{\alpha} - \pi^{*}(y')\pi_{\theta}(y)^{\alpha}\right)}{\pi_{\theta}(y) \left(\pi^{*}(y) + \pi^{*}(y')\right) \left(\pi_{\theta}(y)^{\alpha} + \pi_{\theta}(y')^{\alpha}\right)},$$
(25)

⁴Projection on the probability simplex.

where the first equality follows from (14) and by considering all the terms that include y either as winner (the first sum) or loser (the second sum); the second equality is due to (23) and the fact that $\tilde{\mu}$ is symmetric. To simplify the notation, for any y and y', let

$$h(y,y') \stackrel{\text{def}}{=} \frac{\tilde{\mu}(y,y')}{\pi_{\theta}(y) \pi_{\theta}(y') \left(\pi^*(y) + \pi^*(y')\right) \left(\pi_{\theta}(y)^{\alpha} + \pi_{\theta}(y')^{\alpha}\right)}.$$
(26)

Then, (25) simplifies to

$$v(y) = \sum_{y' \in \mathcal{Y}} h(y, y') \,\pi_{\theta}(y') \, \big(\pi_{\theta}(y')^{\alpha} \pi^{*}(y) - \pi_{\theta}(y)^{\alpha} \pi^{*}(y') \big).$$
(27)

⁷⁶⁵ Consequently,

$$\begin{aligned} \mathbf{v}^{T}(\pi_{\theta} - \pi_{\alpha}^{*}) &= \sum_{y \in \mathcal{Y}} v(y) \left(\pi_{\theta}(y) - \pi_{\alpha}^{*}(y)\right) \\ &= \sum_{y,y' \in \mathcal{Y}} h(y,y') \left(\pi_{\theta}(y')^{\alpha} \pi^{*}(y) - \pi_{\theta}(y)^{\alpha} \pi^{*}(y')\right) \pi_{\theta}(y') \left(\pi_{\theta}(y) - \pi_{\alpha}^{*}(y)\right) \\ &= \frac{1}{2} \sum_{y,y' \in \mathcal{Y}} h(y,y') \left(\pi_{\theta}(y')^{\alpha} \pi^{*}(y) - \pi_{\theta}(y)^{\alpha} \pi^{*}(y')\right) \pi_{\theta}(y') \left(\pi_{\theta}(y) - \pi_{\alpha}^{*}(y)\right) \\ &+ \frac{1}{2} \sum_{y,y' \in \mathcal{Y}} h(y',y) \left(\pi_{\theta}(y)^{\alpha} \pi^{*}(y) - \pi_{\theta}(y')^{\alpha} \pi^{*}(y)\right) \pi_{\theta}(y) \left(\pi_{\theta}(y') - \pi_{\alpha}^{*}(y')\right) \\ &= \frac{1}{2} \sum_{y,y' \in \mathcal{Y}} h(y,y') \left(\pi_{\theta}(y')^{\alpha} \pi^{*}(y) - \pi_{\theta}(y)^{\alpha} \pi^{*}(y')\right) \left(\pi_{\theta}(y)\pi_{\alpha}^{*}(y') - \pi_{\theta}(y')\pi_{\alpha}^{*}(y)\right) \\ &+ \frac{1}{2} \sum_{y,y' \in \mathcal{Y}} h(y,y') \left(\pi_{\theta}(y')^{\alpha} \pi^{*}(y) - \pi_{\theta}(y)^{\alpha} \pi^{*}(y')\right) \left(\pi_{\theta}(y)\pi_{\alpha}^{*}(y') - \pi_{\theta}(y)\pi_{\theta}(y')\right) \\ &= \frac{1}{2} \sum_{y,y' \in \mathcal{Y}} h(y,y') \left(\pi_{\theta}(y')^{\alpha} \pi^{*}(y) - \pi_{\theta}(y)^{\alpha} \pi^{*}(y')\right) \left(\pi_{\theta}(y)\pi_{\alpha}^{*}(y') - \pi_{\theta}(y')\pi_{\alpha}^{*}(y)\right) \\ &= -\frac{z_{\alpha}}{2} \sum_{y,y' \in \mathcal{Y}} h(y,y') \left(\left(\pi_{\theta}(y')\pi_{\alpha}^{*}(y)\right)^{\alpha} - \left(\pi_{\theta}(y)\pi_{\alpha}^{*}(y')\right)^{\alpha}\right) \left(\pi_{\theta}(y')\pi_{\alpha}^{*}(y) - \pi_{\theta}(y)\pi_{\alpha}^{*}(y')\right) \\ &= -\frac{z_{\alpha}}{2} \sum_{y,y' \in \mathcal{Y}} h(y,y') \left(\pi_{\theta}(y)\pi_{\theta}(y')\right)^{1+\alpha} \left(\left(\frac{\pi_{\alpha}^{*}(y)}{\pi_{\theta}(y)}\right)^{\alpha} - \left(\frac{\pi_{\alpha}^{*}(y')}{\pi_{\theta}(y')}\right)^{\alpha}\right) \left(\frac{\pi_{\alpha}^{*}(y)}{\pi_{\theta}(y)} - \frac{\pi_{\alpha}^{*}(y')}{\pi_{\theta}(y)}\right), \end{aligned}$$

where the second equality follows from (27), the fourth equality is due to the symmetry of h(y, y')with respect to y and y', i.e., h(y, y') = h(y', y), and the sixth equality is from (20). It is easy to see that all terms in the sum in the last line are non-negative, and the sum contains at least one non-zero term if $\pi_{\theta} \neq \pi_{\alpha}^*$. Therefore, $\mathbf{v}^T(\pi_{\theta} - \pi_{\alpha}^*) < 0$ if $\pi_{\theta} \neq \pi_{\alpha}^*$. Consequently, $\|\pi_{\theta} - \pi_{\alpha}^*\|$ is strictly decreasing when moving along v. Since both π_{θ} and π_{α}^* lie on the probability simplex, we have $\prod (\mathbf{v})^T (\pi_\theta - \pi_\alpha^*) \leq \mathbf{v}^T (\pi_\theta - \pi_\alpha^*) < 0$. It follows that for any π_θ in the relative interior of the probability simplex, projection of \mathbf{v} on the probability simplex is a strictly decent direction for $\|\pi_{\theta} - \pi^*_{\alpha}\|.$

As a result, π_{α}^{*} is the globally absorbing unique fixed point of the ODE. Furthermore, when μ is not a function of π_{θ} , then π_{α}^{*} is the unique first order stationary point of the preference loss $\mathcal{L}_{\text{pref}}^{\alpha,\mu}$. In other words, $\mathcal{L}_{\text{pref}}^{\alpha,\mu}$ contains no other local mininum, local maximum, or saddle-point in the probability simplex.

B PROOF OF THEOREM 3

This appendix presents the proof of Theorem 3. The high-level idea, akin to Appendix A, is to show that moving along the ODE direction results in an absolute reduction of the Euclidean distance of π_{θ} from Softmax $(r(\cdot|x)/\alpha)$. The details are however substantially different from Appendix A.

We begin with the following lemma.

Lemma 1. For any $\eta > 0$ and any pair of *n*-dimensional vectors **a** and **b** with positive entries, we have

$$\sum_{i=1}^{n} \left(\frac{a_i}{b_i}\right)^{\eta} \left(\frac{b_i}{\sum_{j=1}^{n} b_j} - \frac{a_i}{\sum_{j=1}^{n} a_j}\right) \le 0,$$
(29)

815 and the equality holds only if a = cb for some scalar c.

Proof of Lemma 1. Fix an arbitrary vector *a* with positive entries, and consider the following function

$$f(\mathbf{x}) \stackrel{\text{def}}{=} \sum_{i=1}^{n} \left(\frac{a_i}{x_i}\right)^{\eta} \left(\frac{x_i}{\sum_{j=1}^{n} x_j} - \frac{a_i}{\sum_{j=1}^{n} a_j}\right), \quad \text{for} \quad \mathbf{x} \in \mathbb{R}^n_+,$$
(30)

defined on the positive quadrant. We will show that $f(\mathbf{x}) \leq 0$, for all $x \in \mathbb{R}^n_+$. Note that if $f(\mathbf{x}) > 0$ for some x, then $f(c\mathbf{x}) = f(\mathbf{x})/c^{\eta} > 0$, for all c > 0. Therefore, without loss of generality, we confine the domain to a compact set, say to the probability simplex $S \stackrel{\text{def}}{=} {\mathbf{x} \in \mathbb{R}^*_+ : \sum_{i=1}^n x_i = 1}$, and show that $f(\mathbf{x}) \leq 0$ for all $\mathbf{x} \in S$. In the same vein, without loss of generality we also assume that

$$\sum_{i=1}^{n} a_i = 1.$$
(31)

Note that $f(\mathbf{x}) = -\infty$ on the boundary of the probability simplex, that is if $x_i = 0$ for some *i*. Therefore, the maximizer \mathbf{x}^* of *f* over *S*, lies in the relative interior of *S*. Consequently, the gradient of the Lagrangian of *f* at \mathbf{x}^* is zero. The Lagrangian *L* of *f* is as follows:

$$L(\mathbf{x},\lambda) \stackrel{\text{def}}{=} f(\mathbf{x}) + \lambda \left(\sum_{i=1}^{n} x_i - 1\right), \quad \text{for } \mathbf{x} \in \mathcal{S}, \, \lambda \in \mathbb{R}.$$
(32)

Then,

$$\frac{d}{dx_k}L(\mathbf{x},\lambda) = \frac{d}{dx_k}f(\mathbf{x}) + \lambda$$

$$= \frac{d}{dx_k}\sum_{i=1}^n \left(\frac{a_i}{x_i}\right)^\eta \left(\frac{x_i}{\sum_{j=1}^n x_j} - \frac{a_i}{\sum_{j=1}^n a_j}\right) + \lambda$$

$$= \frac{d}{dx_k}\sum_{i=1}^n \left(\frac{a_i^\eta x_i^{1-\eta}}{\sum_{j=1}^n x_j} - a_i^{1+\eta} x_i^{-\eta}\right) + \lambda$$

$$= \frac{(1-\eta)a_k^\eta x_k^{-\eta}}{\sum_{j=1}^n x_j} - \frac{\sum_{i=1}^n a_i^\eta x_i^{1-\eta}}{\left(\sum_{j=1}^n x_j\right)^2} + \eta a_k^{1+\eta} x_k^{-\eta-1} + \lambda$$

$$= (1-\eta) \left(\frac{a_k}{x_k}\right)^\eta + \eta \left(\frac{a_k}{x_k}\right)^{1+\eta} + \left[\lambda - \sum_{i=1}^n a_i^\eta x_i^{1-\eta}\right]$$
third equality is due to (21), and the last equality is because $\sum_{i=1}^n x_i = 1$. Consider a condent

where the third equality is due to (31), and the last equality is because $\sum_j x_j = 1$. Consider a scalar function $h : \mathbb{R}_+ \to \mathbb{R}_+$ as follows

$$h(y) \stackrel{\text{def}}{=} (1 - \eta) y^{\eta} + \eta y^{1 + \eta} \quad \text{for} \quad y \ge 0.$$
(34)

Then, (33) simplifies to

$$\frac{d}{dx_k}L(\mathbf{x},\lambda) = h\left(\frac{a_k}{x_k}\right) + C(\lambda, \mathbf{x}, \boldsymbol{a}),\tag{35}$$

where $C(\lambda, \mathbf{x}, \mathbf{a}) = \lambda - \sum_{i=1}^{n} a_i^{\eta} x_i^{1-\eta}$ is independent of k. Therefore, letting $\nabla_{\mathbf{x}} L(\mathbf{x}, \lambda) = 0$ at $\mathbf{x} = \mathbf{x}^*$, it follows that for any $1 \le i < j \le n$,

$$h\left(\frac{a_i}{x_i^*}\right) = h\left(\frac{a_j}{x_j^*}\right). \tag{36}$$

We now consider two cases for η .

864 **Case 1** ($\eta \leq 1$). In this case, h defined in (34) is an strictly increasing function. Therefore, (36) 865 implies that $a_i/x_i^* = a_j/x_i^*$, for all $i, j \le n$. Equivalently, $\mathbf{x}^* = c\mathbf{a}$ for some scalar c > 0. In this 866 case, from (30), $f(\mathbf{x}^*) = 0$. The lemma then follows from the fact that \mathbf{x}^* is the maximizer of f. 867

Case 2 (n > 1). In this case, h is no longer increasing. In this case, h is unimodal. Specifically, h is 868 strictly decreasing over $|0, (\eta - 1)/(\eta + 1)|$ and is strictly increasing over $|(\eta - 1)/(\eta + 1), \infty|$. This unimodality implies that the pre-image of any $y \in \mathbb{R}_+$ (i.e., $h^{-1}(y)$) is a set of at most two 870 points. Consequently, (36) implies that we can partition the indices $1, \ldots, n$ into two groups S_1 and 871 S_2 such that within each group, we have $a_i/x_i^* = a_j/x_j^*$. In other words, $a_i/x_i^* = a_j/x_j^*$ for all 872 $(i, j) \in S_1 \times S_1$ and all $(i, j) \in S_2 \times S_2$. Equivalently, the maximum point, \mathbf{x}^* , belongs to the set 873

 $X^* \stackrel{\text{def}}{=} \{ \mathbf{x} \in \mathbb{R}^n_+ : \ x_i = c_1 a_i \text{ for } i \le k, \text{ and } x_i = c_2 a_i \text{ for } i > k, \text{ for some } c_1, c_2 > 0 \text{ and } k < n \},$

876 where we have assumed without loss of generality that $S_1 = \{1, \ldots, k\}$ and $S_2 = \{k + 1, \ldots, n\}$ 877 for some $k \leq n$. We will show that $f(\mathbf{x}) \leq 0$ for all $\mathbf{x} \in X^*$. 878

Fix some $\mathbf{x} \in X^*$, and corresponding constants c_1, c_2 , and k, as per (37). Let $A = \sum_{i=1}^k a_i$ and 879 $B = \sum_{i=k+1}^{n} a_i$. Then,

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 $f(\mathbf{x}) = \sum_{i=1}^{n} \left(\frac{a_i}{x_i}\right)^{\eta} \left(\frac{x_i}{\sum_{i=1}^{n} x_i} - \frac{a_i}{\sum_{i=1}^{n} a_i}\right)$ $=\sum_{i=1}^{n} \left(\frac{a_i}{x_i}\right)^{\eta} \left(\frac{x_i}{c_1 A + c_2 B} - \frac{a_i}{A + B}\right)$

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890 891 $=\sum_{i=1}^{k} c_{1}^{-\eta} \left(\frac{c_{1}a_{i}}{c_{1}A + c_{2}B} - \frac{a_{i}}{A + B} \right) + \sum_{i=k+1}^{n} c_{2}^{-\eta} \left(\frac{c_{2}a_{i}}{c_{1}A + c_{2}B} - \frac{a_{i}}{A + B} \right)$ $\begin{pmatrix} c^{1-\eta}A & c^{-\eta}A \end{pmatrix} \begin{pmatrix} c^{1-\eta}B & c^{-\eta}B \end{pmatrix}$

 $=\frac{(c_1^{1-\eta}A+c_2^{1-\eta}B)(A+B)-(c_1^{-\eta}A+c_2^{-\eta}B)(c_1A+c_2B)}{(c_1A+c_2B)(A+B)}$

$$= \left(\frac{c_1 A}{c_1 A + c_2 B} - \frac{c_1 A}{A + B}\right) + \left(\frac{c_2 B}{c_1 A + c_2 B} - \frac{c_2 B}{A + B}\right)$$

 $=\frac{c_1^{1-\eta}A+c_2^{1-\eta}B}{c_1A+c_2B}-\frac{c_1^{-\eta}A+c_2^{-\eta}B}{A+B}$

 $=\frac{(c_1-c_2)(c_1^{-\eta}-c_2^{-\eta})AB}{(c_1A+c_2B)(A+B)}$

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and the inequality in the last line holds with equality iff either A or B are zero (note that $c_1, c_2, \eta > 0$), which is the case only if $\mathbf{x} = c_1 \mathbf{a}$ or $\mathbf{x} = c_2 \mathbf{a}$. The lemma then follows from the fact that \mathbf{x}^* is the maximizer of f.

905 This completes the proof of Lemma 1. We proceed with the proof of the theorem. Given the rewards $r(\cdot|\cdot)$ in the *n*-ary BT model (see Section 5), let

$$\pi^*(\cdot|\cdot) \stackrel{\text{def}}{=} \text{Softmax}\left(r(\cdot|\cdot)\right). \tag{38}$$

For any $(x; y_1, \ldots, y_n) \in \mathcal{X} \times \mathcal{Y}^n$, let 911

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$$\bar{\mathcal{D}}(x; y_1, \dots, y_n) \stackrel{\text{def}}{=} \frac{\sum_{i=1}^n \mathcal{D}(x; y_1, \dots, y_n; i)}{\sum_{i=1}^n \pi^*(y_i | x)}.$$
(39)

915 It then follows from the consistency of \mathcal{D} with the *n*-ary BT model that for any $(x; y_1, \ldots, y_n) \in$ 916 $\mathcal{X} \times \mathcal{Y}^n$ and $i = 1, \ldots, n$ 917

> $\mathcal{D}(x; y_1, \dots, y_n; i) = \overline{\mathcal{D}}(x; y_1, \dots, y_n) \, \pi^*(y_i | x).$ (40)

We further define

$$\tilde{\mathcal{D}}(x;[y]) \stackrel{\text{def}}{=} \bar{\mathcal{D}}(x;y_1,\dots,y_n) \,\mu(x;y_1,\dots,y_n). \tag{41}$$

For brevity of notation, we denote y_1, \ldots, y_n by [y] and denote $1, \ldots, n$ by [n]. The loss function $\mathcal{L}^{\alpha,\mu}_{\mathrm{pref-}n}(\pi,\mathcal{D})$ defined in (16) can then be simplified to

$$\begin{aligned} \mathcal{L}_{\text{pref-}n}^{\alpha,\mu}(\pi,\mathcal{D}) &= -\frac{1}{\alpha} \mathbb{E}_{(x;y_1,\dots,y_n;i^*)\sim\mathcal{D}} \left[\mu(y_1,\dots,y_n \mid x) \log \frac{\pi(y_{i^*} \mid x)^{\alpha}}{\sum_{i=1}^n \pi(y_i \mid x)^{\alpha}} \right] \\ &= -\frac{1}{\alpha} \sum_{(x;[y];i^*)\in\mathcal{X}\times\mathcal{Y}^n\times[n]} \mathcal{D}(x;[y];i^*) \, \mu([y]|x) \log \frac{\pi(y_{i^*} \mid x)^{\alpha}}{\sum_{i=1}^n \pi(y_i \mid x)^{\alpha}} \\ &= -\frac{1}{\alpha} \sum_{(x;[y];i^*)\in\mathcal{X}\times\mathcal{Y}^n\times[n]} \tilde{D}(x;[y]) \, \pi^*(y_{i^*}|x) \log \frac{\pi(y_{i^*} \mid x)^{\alpha}}{\sum_{i=1}^n \pi(y_i \mid x)^{\alpha}} \\ &= -\frac{1}{\alpha} \sum_{(x;[y])\in\mathcal{X}\times\mathcal{Y}^n} \tilde{D}(x;[y]) \sum_{i=1}^n \pi^*(y_i|x) \log \frac{\pi(y_i \mid x)^{\alpha}}{\sum_{j=1}^n \pi(y_j \mid x)^{\alpha}}, \end{aligned}$$

where the third equality is due to (40) and (41).

In the rest of the proof, without loss of generality, we consider a single fixed $x \in \mathcal{X}$, and remove x from the notations for the sake of notation brevity. Let

$$\pi_{\alpha}^{*}(\cdot) \stackrel{\text{def}}{=} \operatorname{Softmax} \left(r(\cdot) / \alpha \right).$$
(42)

It follows that for any $y \in \mathcal{Y}$,

$$\pi_{\alpha}^{*}(y) = \frac{\pi^{*}(y)^{1/\alpha}}{\sum_{\tilde{y} \in \mathcal{Y}} \pi^{*}(\tilde{y})^{1/\alpha}}.$$
(43)

Let π and π^*_{α} be the vector representation of $\pi(y)$ and $\pi^*_{\alpha}(y)$ for all $y \in \mathcal{Y}$. Then, for $\mathbf{v} \stackrel{\text{def}}{=} -\nabla_{\pi} \mathcal{L}^{\alpha,\mu}_{\text{pref}-n}(\pi,\mathcal{D})$ we have

Fe iy [y] $= (y_1, \ldots, \mathbf{y}_n) \in \mathcal{Y}^n$, let

$$A([y]) \stackrel{\text{def}}{=} \frac{1}{\alpha} \sum_{k=1}^{n} (\pi(y_k) - \pi_{\alpha}^*(y_k)) \frac{d}{dy_k} \sum_{i=1}^{n} \pi^*(y_i) \log \frac{\pi(y_i \mid x)^{\alpha}}{\sum_{j=1}^{n} \pi(y_j \mid x)^{\alpha}}.$$
 (45)

It then follows from (44) that:

$$\mathbf{v}^{T}\left(\boldsymbol{\pi} - \boldsymbol{\pi}^{*1/\alpha}\right) = \sum_{[y]\in\mathcal{Y}^{n}} \tilde{D}([y]) A([y]).$$
(46)

We proceed to compute A([y]). For k = 1, ..., n,

$$\frac{d}{dy_k} \sum_{i=1}^n \frac{\pi(y_i \mid x)^{\alpha}}{\sum_{j=1}^n \pi(y_j \mid x)^{\alpha}} = \frac{d}{dy_k} \sum_{i=1}^n \pi^*(y_i) \left(\log \pi(y_i)^{\alpha} - \log \sum_{j=1}^n \pi(y_j)^{\alpha} \right)$$
$$= \alpha \frac{\pi^*(y_k)}{\pi(y_k)} - \left(\sum_{i=1}^n \pi^*(y_i) \right) \frac{d}{dy_k} \log \sum_{j=1}^n \pi(y_j)^{\alpha}$$
$$= \alpha \frac{\pi^*(y_k)}{\pi(y_k)} - \alpha \left(\sum_{i=1}^n \pi^*(y_i) \right) \frac{\pi(y_k)^{\alpha-1}}{\sum_{j=1}^n \pi(y_j)^{\alpha}}$$
(47)

Plugging this into the definition of A([y]) in (45), we obtain

$$A([y]) = \sum_{k=1}^{n} (\pi(y_k) - \pi_{\alpha}^*(y_k)) \left(\frac{\pi^*(y_k)}{\pi(y_k)} - \left(\sum_{i=1}^{n} \pi^*(y_i)\right) \frac{\pi(y_k)^{\alpha-1}}{\sum_{j=1}^{n} \pi(y_j)^{\alpha}}\right)$$

$$=\sum_{k=1}^{n} \pi(y_k) \left(\frac{\pi^*(y_k)}{\pi(y_k)} - \left(\sum_{i=1}^{n} \pi^*(y_i)\right) \frac{\pi(y_k)^{\alpha-1}}{\sum_{j=1}^{n} \pi(y_j)^{\alpha}}\right) \\ +\sum_{k=1}^{n} \pi^*_{\alpha}(y_k) \left(\left(\sum_{i=1}^{n} \pi^*(y_i)\right) \frac{\pi(y_k)^{\alpha-1}}{\sum_{j=1}^{n} \pi(y_j)^{\alpha}} - \frac{\pi^*(y_k)}{\pi(y_k)}\right)$$

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$$= \sum_{k=1}^{n} \pi^{*}(y_{k}) - \left(\sum_{i=1}^{n} \pi^{*}(y_{i})\right) \frac{\sum_{k=1}^{n} \pi(y_{k})^{\alpha}}{\sum_{j=1}^{n} \pi(y_{j})^{\alpha}}$$
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 $+\sum_{k=1}^{n} \pi_{\alpha}^{*}(y_{k}) \left(\left(\sum_{i=1}^{n} \pi^{*}(y_{i})\right) \frac{\pi(y_{k})^{\alpha-1}}{\sum_{j=1}^{n} \pi(y_{j})^{\alpha}} - \frac{\pi^{*}(y_{k})}{\pi(y_{k})} \right)$

$$=\sum_{k=1}^{n} \pi_{\alpha}^{*}(y_{k}) \left(\left(\sum_{i=1}^{n} \pi^{*}(y_{i})\right) \frac{\pi(y_{k})^{\alpha-1}}{\sum_{i=1}^{n} \pi(y_{i})^{\alpha}} - \frac{\pi^{*}(y_{k})}{\pi(y_{k})} \right)$$

$$= \frac{\sum_{i=1}^{n} \pi^{*}(y_{i})}{\sum_{i=1}^{n} \pi^{*}(y_{i})^{1/\alpha}} \sum_{k=1}^{n} \left(\frac{\pi^{*}(y_{k})}{\pi(y_{k})^{\alpha}}\right)^{1/\alpha} \left(\frac{\pi(y_{k})^{\alpha}}{\sum_{j=1}^{n} \pi(y_{j})^{\alpha}} - \frac{\pi^{*}(y_{k})}{\sum_{i=1}^{n} \pi^{*}(y_{i})}\right)$$

< 0. ("=" only if $\pi^{*} = c\pi$ for some scalar $c > 0$).

where the last equality is due to (43), and the inequality in the last line follows from Lemma 1 by letting $a_k = \pi^*(y_k)$, $b_k = \pi(y_k)^{\alpha}$, and $\eta = 1/\alpha$. Plugging this into (46), it follows that

$$-\left(\nabla_{\pi}\mathcal{L}_{\text{pref-}n}^{\alpha,\mu}(\pi,\mathcal{D})\right)^{T}(\boldsymbol{\pi}-\boldsymbol{\pi}_{\alpha}^{*})=\mathbf{v}^{T}(\boldsymbol{\pi}-\boldsymbol{\pi}_{\alpha}^{*})<0$$
(49)

1002 if $\pi \neq \pi_{\alpha}^*$. Consequently, $\|\pi - \pi_{\alpha}^*\|$ is strictly decreasing when moving along v. Since both π and 1003 π_{α}^* lie on the probability simplex, we have $\prod (\mathbf{v})^T (\pi - \pi_{\alpha}^*) \leq \mathbf{v}^T (\pi - \pi_{\alpha}^*) < 0$. It follows that for 1004 any π in the relative interior of the probability simplex, projection of v on the probability simplex is 1005 a strictly decent direction for $\|\pi - \pi_{\alpha}^*\|$. As a result, π_{α}^* is the globally absorbing unique fixed point 1006 of the ODE. This completes the proof of Theorem 3.

C PROOF OF THEOREM 4

Here we present the proof of Theorem 4. The high level idea is to show that $\mathcal{L}_{rank}^{\alpha,[\mu]}(\pi, \mathcal{D})$ can be equivalently written as the sum of $\mathcal{L}_{pref-n}^{\alpha,\mu_k}(\pi, \mathcal{D}_k)$ for appropriately defined \mathcal{D}_k , for k = 1, ..., n-1; where each \mathcal{D}_k is consistent with the (n - k + 1)-ary BT model (defined in Section 5). We then use Theorem 3, and in particular (49) in the proof of Theorem 3, to conclude that the softmax distribution is a globally absorbing fixed point of $-\nabla \mathcal{L}_{pref-n}^{\alpha,\mu_k}(\pi,\mathcal{D}_k)$ for k = 1, ..., n-1, and is therefore a globally absorbing fixed point of their sum, $-\nabla \mathcal{L}_{rank}^{\alpha,[\mu]}(\pi,\mathcal{D})$.

As in the previous appendices, without loss of generality we prove the theorem for a single fixed $x \in \mathcal{X}$, and remove x from the equations for notation brevity. To further simplify the notation, without loss of generality, we also remove the permutation τ from the equations, and represent the ranking by mere order of the indices, that is we assume that $y_1 \succ y_2 \succ \cdots \succ y_n$. With these new conventions, the ranking loss (17) simplifies to

$$\mathcal{L}_{\mathrm{rank}}^{\alpha,[\mu]}(\pi,\mathcal{D}) \stackrel{\mathrm{def}}{=} -\frac{1}{\alpha} \mathbb{E}_{(y_1,\dots,y_n)\sim\mathcal{D}} \left[\sum_{k=1}^{n-1} \mu_k(y_k,\dots,y_n) \log \frac{\pi(y_k)^{\alpha}}{\sum_{j=k}^n \pi(y_j)^{\alpha}} \right].$$
(50)

1026 For $k = 1, \ldots, n-1$, we define an (n-k+1)-ary preference distribution \mathcal{D}_k as follows. For any 1027 $(y_1, \ldots, y_{n-k+1}) \in \mathcal{Y}^n$ and $i = 1, \ldots, n-k+1$, 1028

$$\mathcal{D}_{k}(y_{1},\ldots,y_{n-k+1};i) = \frac{1}{(n-k)!} \sum_{\substack{(z_{1},\ldots,z_{k-1})\in\mathcal{Y}^{k-1}\\ \text{Permutation }\tau:(1,\ldots,n-k)\to(1,\ldots,t,n-k+1)}} \mathcal{D}(z_{1},\ldots,z_{k-1},y_{i},y_{\tau(1)},\ldots,y_{\tau(n-k)}).$$
(51)

From (50), we have

$$\mathcal{L}_{rank}^{\alpha,[\mu]}(\pi,\mathcal{D}) = -\frac{1}{\alpha} \mathbb{E}_{(y_1,...,y_n)\sim\mathcal{D}} \left[\sum_{k=1}^{n-1} \mu_k(y_k,...,y_n) \log \frac{\pi(y_k)^{\alpha}}{\sum_{j=k}^n \pi(y_j)^{\alpha}} \right]$$

$$= -\frac{1}{\alpha} \sum_{k=1}^{n-1} \mathbb{E}_{(y_1,...,y_n)\sim\mathcal{D}} \left[\mu_k(y_k,...,y_n) \log \frac{\pi(y_k)^{\alpha}}{\sum_{j=k}^n \pi(y_j)^{\alpha}} \right]$$

$$= -\frac{1}{\alpha} \sum_{k=1}^{n-1} \sum_{(y_1,...,y_n)\in\mathcal{Y}^n} \mathcal{D}(y_1,...,y_n) \left[\mu_k(y_k,...,y_n) \log \frac{\pi(y_k)^{\alpha}}{\sum_{j=k}^n \pi(y_j)^{\alpha}} \right]$$

$$= -\frac{1}{\alpha} \sum_{k=1}^{n-1} \sum_{y_k,...,y_n} \sum_{(y_1,...,y_{k-1})\in\mathcal{Y}^{k-1}} \mathcal{D}(y_1,...,y_n) \log \frac{\pi(y_k)^{\alpha}}{\sum_{j=k}^n \pi(y_j)^{\alpha}} \right]$$

$$= -\frac{1}{\alpha} \sum_{k=1}^{n-1} \sum_{y_k,...,y_n} \frac{\mathcal{D}_k(y_1,...,y_{n-k+1};1)}{((n-k)!)^2} \left[\mu_k(y_k,...,y_n) \log \frac{\pi(y_k)^{\alpha}}{\sum_{j=k}^n \pi(y_j)^{\alpha}} \right]$$

$$= -\frac{1}{\alpha} \sum_{k=1}^{n-1} \frac{\mathcal{D}_k(y_1,...,y_{n-k+1};1)}{(n-k+1)!(n-k)!} \mathbb{E}_{(y_k,...,y_n;i)\sim\mathcal{D}_k} \left[\mu_k(y_k,...,y_n) \log \frac{\pi(y_k)^{\alpha}}{\sum_{j=k}^n \pi(y_j)^{\alpha}} \right]$$

$$= -\frac{1}{\alpha} \sum_{k=1}^{n-1} \frac{\mathcal{L}_{pref,n}^{\alpha,\mu_k}(\pi,\mathcal{D}_k)}{(n-k+1)!(n-k)!} \mathbb{E}_{(y_k,...,y_n;i)\sim\mathcal{D}_k} \left[\mu_k(y_k,...,y_n) \log \frac{\pi(y_k)^{\alpha}}{\sum_{j=k}^n \pi(y_j)^{\alpha}} \right]$$

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Let π and π^*_{α} be the vector representations of π and the softmax distribution π^*_{α} (defined in (43)), and $\mathbf{v} \stackrel{\text{def}}{=} -\nabla_{\pi} \mathcal{L}_{\text{rank}}^{\alpha,[\mu]}(\pi, \mathcal{D})$. Then,

$$(\boldsymbol{\pi} - \boldsymbol{\pi}_{\alpha}^{*})^{T} \mathbf{v} = -(\boldsymbol{\pi} - \boldsymbol{\pi}_{\alpha}^{*})^{T} \nabla \sum_{k=1}^{n-1} \frac{\mathcal{L}_{\text{pref}-n}^{\alpha,\mu_{k}}(\boldsymbol{\pi}, \mathcal{D}_{k})}{(n-k+1)!(n-k)!}$$
$$\overset{n-1}{=} (\boldsymbol{\pi} - \boldsymbol{\pi}^{*})^{T} \nabla \mathcal{L}^{\alpha,\mu_{k}}(\boldsymbol{\pi}, \mathcal{D}_{k})$$

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$$= \sum_{k=1}^{\infty} \frac{-(n-n_{\alpha}) - \sqrt{L_{\text{pref-}n}(n, D_k)}}{(n-k+1)! (n-k)!}$$

$$\leq 0,$$

1064 where the last inequality follows from (49), and it holds with equality only if $\pi \neq \pi_{\alpha}^{*}$. Since both 1065 π and π^*_{α} lie on the probability simplex, we have $\prod(\mathbf{v})^T(\pi - \pi^*_{\alpha}) \leq \mathbf{v}^T(\pi - \pi^*_{\alpha}) < 0$. Then, following a similar argument as in the last paragraph of Appendix B, we conclude that π_{α}^{*} is the globally absorbing unique fixed point of the ODE. This completes the proof of Theorem 4. 1067

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EXPERIMENT DETAILS D

1071 D.1 DETAILS FOR THE ALPACAFARM EXPERIMENT OF SECTION 7.1 1072

We performed the alignment procedure on 4 NVIDIA H100 (94 GiB) GPUs. For each method, we 1074 trained the model for four epochs and reported the maximum win-rate against the SFT model. The 1075 training batch size per GPU device was set to one and the gradient accumulation step was 16. The 1076 range of hyper-parameters considered for each method is given as follows: R-DPO: $\beta \in \{0.01, 0.1\}$, $\alpha \in \{0.001, 0.01, 0.1\}, \text{ CPO: } \beta \in \{0.001, 0.01, 0.1\}, \alpha \in \{0.0001, 0.001, 0.01\}, \text{ SimPO: } \beta \in \{0.001, 0.01, 0.01\}, \beta \in \{0.001, 0.01, 0.01\}, \beta \in \{0.001, 0.01, 0.01\}, \beta \in \{0.001, 0.01, 0.01\}, \beta \in \{0.001,$ 1077 $\{2, 2.5\}, \gamma \in \{1, 1.5\}$ (the suggested range in SimPO), KTO: $\beta \in \{0.01, 0.1\}, \lambda_D = \lambda_U = 1$, 1078 **IPO:** $\tau \in \{0.001, 0.01, 0.1\}$, **DPO:** $\beta \in \{0.001, 0.01, 0.1\}$, and **SPO:** $\alpha \in \{0.001, 0.01\}$, $\beta \in \{0.001, 0.$ 1079 $\{0.001, 0.01\}$. Table 5 shows the sensitivity of SPO to its hyperparameters.

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	$\alpha = 0.01$	$\alpha = 0.001$
$\beta = 0.01$	60.83	59.82
$\beta = 0.001$	57.15	59.99

Table 5: SPO win-rate for different α and β values.

1090 D.2 DETAILS FOR THE EXPERIMENT OF SECTION 7.2 1091

We trained the models on NVIDIA A100 (40 GiB) GPUs. We used a batch size of 32 samples (each containing four responses) for all algorithms. The reference model in all algorithms was identical to the SFT model. All alignment loss functions were optimized using AdamW with 5,000 warm-up iterations.

For SPO, we trained both basic (i.e., $\gamma = 0$) and weighted version. For weighted SPO, we set 1098 $\gamma = 0.01$ without sweeping, and in the ranking experiment we used decayed weight functions 1099 $\eta^k \mu_k$ for $\eta \in 1, 0.5$, see (17). For other SPO parameters, we swept over $\beta \in \{0.01, 0.1\}$, and 1100 $\alpha \in \{0.001\}$. For \mathcal{D}_{KL} computation, we used intermittent batch generation of samples, generating a 1101 batch of 32 samples from π_{θ} once every 8 iterations (i.e., T = 8). For other algorithms, we swept 1102 over the following sets of hyperparameters: DPO: $\beta \in \{0.0001, 0.001, 0.01\}$, S-DPO for ranking: 1103 $\beta \in \{0.0001, 0.001, 0.01\}$, and S-DPO for best-of-*n*: $\beta \in \{0.0001, 0.001, 0.01\}$. For For training 1104 the S-DPO algorithm on the best-of-n dataset, we consider each top-rank response as the positive 1105 response and the corresponding lower-rank responses as the corresponding negative set of responses. For training S-DPO on ranking dataset, each of the 1st, 2nd, and 3rd rank responses serve as positive 1106 responses with the corresponding negative set containing the corresponding lower rank responses. 1107

We computed the win rates of all methods against the best-of-n SFT model using GPT4o-2024-08-06 once every 1000 iterations, and reported the peak win-rate for each method. Each win-rate was averaged over 1,000 story-pair instances, resulting in an estimation error with standard deviation smaller than 0.015.

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E DETAILS OF GENERATION OF RANKING DATASET FOR THE TINYSTORIES EXPERIMENT

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We created a preference dataset to align stories with older age groups. Specifically, for each pair of stories generated by the reference model, we asked GPT4o-2024-08-06 to evaluate them based on clarity and coherence, writing quality, and whether they are interesting and engaging for high school students. The API was asked to evaluate each story independently based on these criteria, and identify its strengths and weaknesses compared to other stories; and then suggest a ranking of stories from best to worst. The prompt used for generating the dataset is provided at the end of this subsection.

We generated a set of 100,000 stories independently from the 110M-parameter pre-trained model (Karpathy, 2023), and grouped them into a set of 25,000 samples each containing four stories. To enhance the quality of the ranking dataset, for each sample we used the prompt to rank the stories twice, reversing the order of the stories in the second evaluation. We retained samples only if both evaluations showed a consistent ranking. After this filtration, 5,000 samples remained for use in the ranking dataset. The dataset is available online at (Anonymous, 2024). 1134 Prompt for Generation of the Ranking Dataset for TinyStories Experiment: 1135 1136 You are tasked with deciding which of the four short stories below, written by high school students, is better suited for publication in the 1137 high school newspaper. 1138 1139 **Story 1:** { } 1140 **Story 2:** { } 1141 **Story 3:** { } 1142 1143 **Story 4:** { } 1144 **Your Task:** 1145 1. **Evaluate Each Story Individually:** 1146 Identify the **strengths** and **weaknesses** of each story, focusing on: - **Engagement:** Is the story interesting and likely to captivate high 1147 school students? 1148 - **Clarity and Coherence:** Is the story well-organized and easy to 1149 follow? 1150 - **Writing Quality:** Assess the grammar, vocabulary, and overall 1151 language use. 1152 2. **Make a Final Decision:** 1153 - Based on your evaluations, decide which story is better suited for 1154 publication. Rank the stories from best to worst. 1155 ****Response Format:**** 1156 * * * 1157 **Evaluation:** **Story 1:** 1158 - **Strengths compared to other stories:** 1159 - [List strengths] 1160 - **Weaknesses compared to other stories:** 1161 - [List weaknesses] 1162 **Story 2:** 1163 - **Strengths compared to other stories:** 1164 - [List strengths] 1165 **Weaknesses compared to other stories:** 1166 - [List weaknesses] 1167 1168 **Story 3:** - **Strengths compared to other stories:** 1169 - [List strengths] 1170 - **Weaknesses compared to other stories:** 1171 - [List weaknesses] 1172 **Story 4:** 1173 - **Strengths compared to other stories:** 1174 - [List strengths] 1175 - **Weaknesses compared to other stories:** 1176 - [List weaknesses] 1177 **Conclusion:** 1178 - **Overall Ranking of the Stories:** 1179 1. **1st Place:** Story [1, 2, 3, or 4] 1180 **2nd Place:** Story [1, 2, 3, or 4] **3rd Place:** Story [1, 2, 3, or 4] 2. 1181 3. 4. **4th Place:** Story [1, 2, 3, or 4] 1182 1183 * * * 1184 **Guidelines:** 1185 - In each evaluation, compare the story to the others, noting unique strengths and weaknesses. 1186 - Evaluation of each story shold not be influenced from prior 1187 evaluations that you provided earlier. - Do not let the presentation order affect your judgment; treat all

stories equally.