Token-weighted Direct Preference Optimization with Attention

Abstract

Direct Preference Optimization (DPO) aligns Large Language Models with human preferences without the need for a separate reward model. However, DPO treats all tokens in responses equally, neglecting the differing importance of individual tokens. Existing token-level PO methods compute the token weights using either token-position-based heuristic functions or probability estimates given by a separately trained model, which lacks robustness and incurs extra training cost. In contrast, we propose Token-weighted DPO (TwDPO)—a novel training objective grounded on token-weighted RL—and AttentionPO—an instantiation of TwDPO that uses attention from the LLM itself to estimate token weights. AttentionPO prompts the LLM to serve as a pairwise judge and check where the model attends when comparing the responses. This design makes AttentionPO *content-aware*, adjusting weights based on response content, and *efficient*, incurring only two extra forward passes per example. Experiment results show that AttentionPO significantly improves performance on AlpacaEval, MT-Bench, and ArenaHard, surpassing existing Preference Optimization methods.

1 Introduction

The alignment of Large Language Models (LLMs) with human preferences and values is critical for ensuring the quality and safety of generated outputs. Early efforts in this domain utilized policy-gradient reinforcement learning (RL) algorithms like Proximal Policy Optimization (PPO) (Schulman et al., 2017; Ouyang et al., 2022). However, these traditional RL methods require training a separate reward model on annotated preference pairs to provide feedback during training (Ouyang et al., 2022). To address this complexity, Preference Optimization (PO) methods such as Direct Preference Optimization (DPO) (Rafailov et al., 2023) have emerged. DPO's training objective is derived from

Figure 1: AttentionPO weighs each token by attention, surpassing DPO and various other baselines.

the policy gradient, but it learns the reward landscape directly from preference pairs, avoiding the need for an external reward model.

Despite the advancements introduced by DPO and its variants—including IPO (Azar et al., 2024), KTO (Ethayarajh et al., 2024), and SimPO (Meng et al., 2024)—these methods generally treat every token within a response as equally important (Meng et al., 2024). This uniform weighting neglects the fact that different tokens contribute variably to the overall quality of a response (Meng et al., 2024). Consequently, traditional PO methods fail to provide the fine-grained credit assignment necessary to account for the specific importance of individual tokens to human preference.

Recent research has attempted to enable token-level credit assignment through various estimation techniques. Grounded in token-level policy gradient methods, TDPO adds sequence KL terms to the DPO objective (Zeng et al., 2024). Other approaches, such as TIS-DPO (Liu et al., 2025), SePO (Yang et al., 2025), and cDPO (Lin et al., 2024), estimate token importance by contrasting probabilities between different policies or models. Alternatively, TI-DPO utilizes gradient norms and Gaussian priors (Yang et al., 2026), while D^2PO

employs heuristic temporal decay functions that prioritize earlier tokens (Shao et al., 2025). However, many of these methods either require the training of additional models to estimate weights (Yang et al., 2025; Liu et al., 2025; Lin et al., 2024) or rely on heuristic functions based on token positions rather than the specific semantic content of the tokens (Yang et al., 2026; Shao et al., 2025).

In this work, we propose Token-weighted DPO (TwDPO), a training objective that is theoretically-grounded on token-weighted RL, and **AttentionPO**, an instantiation of TwDPO that utilizes the attentions from the LLM itself to estimate token weights. By obtaining attention weights for response tokens from a pairwise judge prompt, AttentionPO provides a content-aware importance metric. These weights are then normalized and applied during the credit assignment process to better align the model with human preferences.

Experimental results demonstrate the effectiveness of our proposed approach. AttentionPO achieves significant performance improvements across several models and standard benchmarks. On LLaMA-3-8B-Base-SFT (Grattafiori et al., 2024; Meng et al., 2024), AttentionPO improves performance by 12% (win rate against GPT-4-1106-preview (Hurst et al., 2023)) on AlpacaEval (Li et al., 2023; Dubois et al., 2024), 1.05 (LLM-judged score) on MT-Bench (Zheng et al., 2023), and 40% (win rate against GPT-4-0314) on Are-naHard (Li et al., 2024, 2025). On LLaMA-3-8B-Insturct, AttentionPO improves performance by 27% on AlpacaEval, 1.41 on MT-Bench, and 14% on ArenaHard. AttentionPO also surpasses strong baselines such as SimPO (up to 4% on AlpacaEval; 0.20 on MT-Bench). AttentionPO highlights the value of using intrinsic model attentions for precise, token-level preference optimization.

2 Methodology

We first introduce the notations (§ 2.1) and preliminaries (§ 2.2), then present our TwDPO objective (§ 2.3) and its math derivations (§ 2.4). Finally, we discuss an instantiation of the TwDPO, AttentionPO, which uses attentions as weights. AttentionPO takes three steps: (1) First, we prompt the initial LLM to act as a pairwise judge to extract the attention weights (§ 2.5); (2) We post-process the attention weights to obtain a weight distribution (§ 2.6); (3) We apply TwDPO using the attention weight distribution. See Figure 2 for visualization.

2.1 Notations

We initialize our main policy π_θ with a reference model π_{ref}. We train π_θ on a preference dataset $\mathcal{D} = \{x^{(i)}, y_w^{(i)}, y_l^{(i)}\}_{i=1}^N$, where each example contains a prompt $x^{(i)}$, a preferred response $y_w^{(i)}$ and a dispreferred response $y_l^{(i)}$. Each response y consists of tokens $\{y^1, \cdots, y^{|y|}\}$.

2.2 Preliminaries

Direct Preference Optimization is an offline variant of traditional policy gradient methods to align LLMs with human preferences. It avoids the need for a separate reward model. Instead, it trains LLMs as reward models themselves, on the annotated preference pairs. In particular, DPO maximizes the model's predicted probability of y_w being preferred over y_l. Formally, given the preference dataset $\mathcal{D}$, DPO trains π_θ using the following objective:

$$\mathcal{L} = -\mathbb{E}_{(x,y_w,y_l)\sim\mathcal{D}}\left[log\left(p_\theta(y_w \succ y_l|x)\right)\right]. \quad (1)$$

where $p_\theta(y_w \succ y_l|x)$ is the model's predicted preference probability. Following the Bradley-Terry model (Bradley and Terry, 1952),

$$p_\theta(y_w \succ y_l|x) = \frac{\exp(r(x,y_w))}{\exp(r(x,y_w)) + \exp(r(x,y_l))} \quad (2)$$
$$= \sigma(r_\theta(x,y_w) - r_\theta(x,y_l)).$$

where $r_\theta(x,y_w)$ is model's predicted reward and σ is the sigmoid function. Further, DPO derives the model's predicted reward to be $r_\theta(x,y) = \beta log\frac{\pi_\theta(y|x)}{\pi_{ref}(y|x)} + \beta log(Z(x))$, where $Z(x)$ is a partition function depending only on x. Thus, the final DPO objective is to minimize

$$\mathcal{L} = -\mathbb{E}_{(x,y_w,y_l)\sim\mathcal{D}}\left[log\sigma\left(\beta log\frac{\pi_\theta(y_w|x)}{\pi_{ref}(y_w|x)} - \beta log\frac{\pi_\theta(y_l|x)}{\pi_{ref}(y_l|x)}\right)\right]. \quad (3)$$

Equation 3 can be rewritten into the token-level form:

$$\mathcal{L} = -\mathbb{E}_{(x,y_w,y_l)\sim\mathcal{D}}\left[log\sigma\left(\beta \sum_{t=1}^{|y_w|} \log \frac{\pi_\theta(y_w^t|x,y_w^{<t})}{\pi_{ref}(y_w^t|x,y_w^{<t})} - \beta \sum_{t=1}^{|y_l|} log \frac{\pi_\theta(y_l^t|x,y_l^{<t})}{\pi_{ref}(y_l^t|x,y_l^{<t})}\right)\right]. \quad (4)$$

Note that DPO assigns an equal weight of 1 to all the $\frac{\pi_\theta(y^t|x,y^{<t})}{\pi_{ref}(y^t|x,y^{<t})}$ terms. This does not consider the varying degrees of importance of different tokens to the final response quality.

Figure 2: Workflow of AttentionPO. First, we prompt π_{ref} to act as a pairwise judge and indicate which response is better in a single output token $y_{verdict}$. We extract π_{ref}'s attentions at layer $\mathcal{L}$ that attend from $y_{verdict}$ to the response tokens of both y_w and y_l. Prompting and weight extraction are repeated two times with the position of y_w and y_l swapped, and the final attention weights A_w and A_l are averaged over the two rounds. Second, we post-process the weights by applying normalization and fixing the attention sink. Finally, we apply TwDPO with the post-processed attention weights.

2.3 Token-weighted DPO

Instead, our objective multiplies each probability ratio term in Equation 4 with a token weight a^t:

$$\mathcal{L} = -\mathbb{E}_{\mathcal{D}}\Bigg[log\sigma\Bigg(\beta|y_w|\sum_{t=1}^{|y_w|} a_w^t \log \frac{\pi_\theta(y_w^t|x,y_w^{<t})}{\pi_{ref}(y_w^t|x,y_w^{<t})} \\ -\beta|y_l|\sum_{t=1}^{|y_l|} a_l^t log\frac{\pi_\theta(y_l^t|x,y_l^{<t})}{\pi_{ref}(y_l^t|x,y_l^{<t})}\Bigg)\Bigg]. \tag{5}$$

2.4 Mathematical Derivation

We closely follow the proof of Rafailov et al. (2023) to derive the token-weighted DPO objective from a token-weighted RL objective. First, we find the closed-form expression of the near-optimal policy π^* and reward function r^* attained by the token-weighted RL objective (§ 2.4.1). Next, we derive the token-weighted DPO objective (§ 2.4.2).

2.4.1 Deriving the Near Optimum of the Token-weighted Objective

DPO (Rafailov et al., 2023) derives the equivalence between their optimal policy and the one attained by a sequence-level RL objective, which maximizes response reward with KL constraints:

$$\max_\pi \mathbb{E}_{x\sim\mathcal{D},y\sim\pi(\cdot|x)}\left[r(x,y)\right] - \beta\mathbb{D}_{\mathbb{KL}}(\pi_\theta(y|x)||\pi_{ref}(y|x))$$

$$= \max_\pi \mathbb{E}_{x\sim\mathcal{D},y\sim\pi(\cdot|x)}\left[r(x,y) - \beta\sum_{t=1}^{|y|}\frac{\pi_\theta(y^t|x,y^{<t})}{\pi_{ref}(y^t|x,y^{<t})}\right]. \tag{6}$$

Instead, we show that our objective 5 gives a model equivalent to the near-optimal policy produced by a token-weighted RL objective. We start by reformulating objective 6. For a given prompt x, a policy π, and a reference model π_{ref}, our objective is to find an optimal policy that maximizes the reward under a token-weighted KL penalty. As we will show in § 2.4.3, this objective naturally induces a token-weighted reward function r. Our KL penalty weighs the log-probability ratios at each token step t by the weight a^t:

$$\max_\pi \mathbb{E}_{x\sim\mathcal{D},y\sim\pi(\cdot|x)}\bigg[r(x,y) - \\ \beta|y|\sum_{t=1}^{|y|} a^t \log\frac{\pi(y^t|x,y^{<t})}{\pi_{ref}(y^t|x,y^{<t})}\bigg]. \tag{7}$$

Note that a^t is a proper distribution and sums up to 1. In light of this, we scale the KL term by the sequence length $|y|$ so that the total weight of the logprob ratio terms $|y|\sum_{t=1}^{|y|} a^t$ equals $|y|$, which is consistent with the DPO objective 6.

To solve this mathematically, we define a sequence-level "weighted" log-probability for both the policy and the reference model:

$$\log\tilde{\pi}(y|x) = |y|\sum_{t=1}^{|y|} a^t \log\pi(y^t|x,y^{<t}),$$

$$\log\tilde{\pi}_{ref}(y|x) = |y|\sum_{t=1}^{|y|} a^t \log\pi_{ref}(y^t|x,y^{<t}). \tag{8}$$

Substituting these into our objective, we can follow the standard derivation steps:

$$\max_{\pi} \mathbb{E}_{x\sim\mathcal{D}} \mathbb{E}_{y\sim\pi(\cdot|x)} \left[r(x,y) - \beta \log \frac{\tilde{\pi}(y|x)}{\tilde{\pi}_{ref}(y|x)} \right]$$

$$= \min_{\pi} \mathbb{E}_{x\sim\mathcal{D}} \mathbb{E}_{y\sim\pi(\cdot|x)} \left[\log \frac{\tilde{\pi}(y|x)}{\tilde{\pi}_{ref}(y|x)} - \frac{1}{\beta} r(x,y) \right]$$

$$= \min_{\pi} \mathbb{E}_{x\sim\mathcal{D}} \mathbb{E}_{y\sim\pi(\cdot|x)} \left[\log \frac{\tilde{\pi}(y|x)}{\frac{1}{Z(x)}\tilde{\pi}_{ref}(y|x)\exp(\frac{1}{\beta}r(x,y))} \right.$$
$$\left. - \log Z(x) \right],$$

where $Z(x) = \sum_y \tilde{\pi}_{ref}(y|x)\exp(\frac{1}{\beta}r(x,y))$ is the partition function.

The near optimal weighted policy $\tilde{\pi}^*$ (we analyze the error bounds between $\tilde{\pi}^*$ and the intractable true optimal policy in Appendix B) that minimizes this expression satisfies:

$$\tilde{\pi}^*(y|x) = \frac{1}{Z(x)}\tilde{\pi}_{ref}(y|x)\exp\left(\frac{1}{\beta}r(x,y)\right). \tag{9}$$

By taking the logarithm of both sides and rearranging the terms, we can express the true reward $r^*(x,y)$ entirely in terms of the optimal policy:

$$r^*(x,y) = \beta \log \frac{\tilde{\pi}^*(y|x)}{\tilde{\pi}_{ref}(y|x)} + \beta \log Z(x). \tag{10}$$

Substituting the expanded definition of our weighted log-probabilities back into this reward expression yields:

$$r^*(x,y) = \beta|y|\sum_{t=1}^{|y|} a^t \log \frac{\pi^*(y^t|x,y^{<t})}{\pi_{ref}(y^t|x,y^{<t})} + \beta \log Z(x). \tag{11}$$

2.4.2 Deriving the Objective Under the Bradley-Terry Model

We substitute our token-weighted reparameterization of $r^*(x,y)$ into the Bradley-Terry preference model (Equation 2):

$$p^*(y_w \succ y_l|x) = \sigma(r^*(x,y_w) - r^*\theta(x,y_l))$$

$$= \sigma\left(\left(\beta|y_w|\sum_{t=1}^{|y_w|} a_w^t \log \frac{\pi^*(y_w^t|x,y_w^{<t})}{\pi_{ref}(y_w^t|x,y_w^{<t})} + \beta \log Z(x) \right) \right.$$
$$\left. - \left(\beta|y_l|\sum_{t=1}^{|y_l|} a_l^t \log \frac{\pi^*(y_l^t|x,y_l^{<t})}{\pi_{ref}(y_l^t|x,y_l^{<t})} + \beta \log Z(x) \right) \right).$$

Crucially, the partition function terms $\beta \log Z(x)$ cancel out, leaving:

$$p^*(y_w \succ y_l|x) = \sigma\left(\beta|y_w|\sum_{t=1}^{|y_w|} a_w^t \log \frac{\pi^*(y_w^t|x,y_w^{<t})}{\pi_{ref}(y_w^t|x,y_w^{<t})} \right.$$
$$\left. - \beta|y_l|\sum_{t=1}^{|y_l|} a_l^t \log \frac{\pi^*(y_l^t|x,y_l^{<t})}{\pi_{ref}(y_l^t|x,y_l^{<t})} \right). \tag{12}$$

To frame this as a maximum likelihood objective for training a parameterized policy π_θ, we take the negative log-likelihood over the preference dataset $\mathcal{D}$. This leads to our final objective in Equation 5.

2.4.3 Properties

Reward function is token-weighted. Equation 10 shows that r weighs tokens by a^t. For tokens with higher a^t, their logprob ratio between $\pi^*(y^t|x,y^{<t})$ and $\pi_{ref}(y^t|x,y^{<t})$ significantly affect r, while tokens with lower a^t affect r less.

Token-weighted KL penalty enables locally-adaptive trust region. Our KL penalty in objective 7 scales the KL divergence at the token level via a^t. Consequently, the model is granted greater freedom to deviate from the reference policy on low-importance tokens, while being strictly constrained on high-importance ones. While restricting the most critical tokens may seem counterintuitive, this adaptive weighting is essential because important tokens dominate the implicitly derived reward function, and thus are highly susceptible to reward hacking and over-optimization. The token-weighted KL term acts as a locally adaptive regulator: for high-weight tokens, the massive incentives to deviate are safely balanced by proportionally stricter penalties, ensuring the model only updates when the expected reward justifies the risk.

The above suggests that objective 7 is indeed a token-weighted RL objective in terms of both the reward function and KL penalty. Consequently, both its derived policy and the near-optimal policy derived from objective 5 learn more signals from important tokens, which is what we desire. We further provide an analysis on the gradient in Appendix C. While we use attention as the weights, there are no assumptions about how the weights are derived, and AttentionPO is only one possible instantiation.

2.5 Token Weights Extraction Through Attention Scores

We hypothesize that if we ask the LLM to judge the response quality, the tokens that get more attention are more important. As such, we prompt π_{ref} with a general pairwise judge prompt (See Appendix 6) that asks it to predict which of y_w and y_l has better quality. We explicitly require π_{ref} to output the identifier ("A" or "B") of the better response, and we denote this single token as $y_{verdict}$. To avoid bias, we hide the preference labels in the prompt

and call π_{ref} two rounds, each round with the positions of y_w and y_l swapped. For each round, we do a single forward pass and obtain the attention weights at a fixed layer L. We extract the attention weights from $y_{verdict}$ to all the tokens in y_w and denote them as $A_w^{round\_r} = [a_w^1, \cdots, a_w^{|y_w|}]$. Similarly, we extract the attention weights from $y_{verdict}$ to all the tokens in y_l as $A_l^{round\_r} = [a_l^1, \cdots, a_l^{|y_l|}]$. For simplicity, we compute the final attention weight of each token as the mean attention weight for that token across attention heads.

For rounds $r \in \{1, 2\}$, This produces $A_w^{round\_1}$, $A_w^{round\_2}$, $A_l^{round\_1}$, $A_l^{round\_2}$. The final attention is the average of the two rounds:

$$
\begin{aligned}
a_w^t &= \frac{1}{2} a_w^{t,round\_1} + \frac{1}{2} a_w^{t,round\_2}, \\
a_l^t &= \frac{1}{2} a_l^{t,round\_1} + \frac{1}{2} a_l^{t,round\_2}.
\end{aligned}
\tag{13}
$$

2.6 Post-Processing

Normalization. π_{ref} also attends to other tokens in the pairwise judge prompt and so neither A_w nor A_l form a proper distribution (i.e., it does not sum up to 1.0). Therefore, we normalize the attention weights A_w and A_l: $a_w^t \leftarrow a_w^t/(\sum_{q=1}^{|y_w|} a_w^q)$, $a_l^t \leftarrow a_l^t/(\sum_{q=1}^{|y_l|} a_l^q)$.

Fixing Attention Sink. Attention sink is a phenomenon where the LLMs predominantly attend to the initial tokens (Xiao et al., 2024). Manual inspection on our dataset $\mathcal{D}$ suggests that these initial tokens are usually of low importance, consisting of starting phrases. As such, for any response with at least K' tokens, we reset the attention weights of the first K tokens of each response y to the average weight $1/|y|$ and renormalize the remaining tokens:

$$
\begin{aligned}
\forall t \in \{K+1, \cdots, |y_w|\}, a_w^t \leftarrow a_w^t \frac{1 - \frac{K}{|y_w|}}{\sum_{q=K+1}^{|y_w|} a_w^q} \\
\forall t \in \{K+1, \cdots, |y_l|\}, a_l^q \leftarrow a_l^q \frac{1 - \frac{K}{|y_l|}}{\sum_{q=K+1}^{|y_l|} a_l^q}
\end{aligned}
\tag{14}
$$

3 Experiment Setup

Models and Datasets. We follow the settings from Meng et al. (2024). For the initial model π_{ref}, we experiment with **Llama-3-8B-Base-SFT** from Meng et al. (2024) (princeton-nlp/Llama-3-Base-8B-SFT), which is supervised-finetuned from the pretrained model LLaMA-3-8B (Grattafiori et al., 2024) on UltraChat-200K (Ding et al., 2023); and

LLaMA-3-8B-Instruct (Grattafiori et al., 2024) (meta-llama/Meta-Llama-3-8B-Instruct).

For the SFT model (Llama-3-8B-Base-SFT), we apply AttentionPO on the UltraFeedback binarized dataset (Cui et al., 2024) (HuggingFaceH4/ultrafeedback_binarized). This dataset contains 61,135/2,000 training/validation examples covering diverse instruction-following tasks such as creative writing, document-assisted writing, and open-ended QA. Each query is accompanied by four responses generated by diverse LLMs and graded by GPT-4 in terms of instruction-following, helpfulness, honesty, and truthfulness. y_w is set to the response with the highest overall score, and y_l is chosen randomly from the remaining three.

For the Instruction-Tuned model (LLaMA-3-8B-Instruct), we use the dataset produced by Meng et al. (2024) (princeton-nlp/llama3-ultrafeedback). It contains 59,876/1,961 training/validation examples. The questions are subsampled from the binarized datasets, but for each question, five responses are sampled from π_{ref} and then scored by a reward model PairRM (Jiang et al., 2023b). y_w is set to the response with the highest score and y_l is set to the one with the lowest score.

Attention Weights. We set L to the index of the last layer for every model (i.e., we take the attention weights from the last layer). To fix the attention sink issue, we use $K = 1$ and $K' = 5$. That is, for response y that has at least 5 tokens, we set the attention weight of its first token to $1/|y|$. The rationale is that for our models, the attention sink primarily concentrates on the first token. For LLaMA3-8B-Base-SFT, significant attention weights are on the first token (12.55%), whereas the weights on the second (3.35%) and third (2.55%) tokens are much smaller. For LLaMA-3-8B-Instruct, the proportion is 8.25%/2.11%/1.55% for the first, second, and third tokens, respectively.

We show detailed statistics of the attention weights in Table 1. The standard deviation of the weights from both SFT and Instruct models is above 0.01, suggesting that the weights vary across tokens. We also show the ten most weighted tokens in Table 2. For the SFT model, 7/10 tokens are related to binary judgment words (e.g., "Yes", "True") for both y_w and y_l. The highly weighted tokens of the Instruct model not only include these but also negation words (e.g., "doesn").

Training Details. We set learning rate to $1e-6$ with a cosine scheduler and a warmup ratio of 0.1.

	π_{ref}=LLaMA-3-8B-Base-SFT			π_{ref}=LLaMA-3-8B-Instruct		
	Std	Max	Len	Std	Max	Len
y_w	0.0177	0.1242	269.0895	0.0126	0.0915	356.9848
y_l	0.0175	0.1202	235.3978	0.0137	0.0959	365.8176

Table 1: Statistics of the attention weights after post-processing in § 2.6. Std: Standard deviation of token weights within a response. Max: Maximum weights; Len: Response length; Metrics are averaged across the training set.

π_{ref}=LLaMA-3-8B-Base-SFT				π_{ref}=LLaMA-3-8B-Instruct			
y_w		y_l		y_w		y_l	
Token	Weight	Token	Weight	Token	Weight	Token	Weight
True	0.1237	Ye	0.8212	(Note	0.1269	(Note	0.1276
idence	0.1227	Neutral	0.1213	YES	0.0918	Yes	0.0853
Neutral	0.1184	ye	0.1065	"What	0.0844	"What	0.0673
POS	0.1148	Completion	0.0987	doesn	0.0643	doesn	0.0618
False	0.1016	idence	0.0886	wouldn	0.0606	No	0.0598
Completion	0.0997	No	0.0845	False	0.0572	!ĊĊ	0.0529
No	0.0990	True	0.0796	Yes	0.0563	didn	0.0528
Negative	0.0788	Ent	0.0721	No	0.0556	wouldn	0.0510
Positive	0.0668	Negative	0.0692	Explanation	0.0505	don	0.0497
Yes	0.0591	False	0.0686	don	0.0492	"The	0.0447

Table 2: Most weighted tokens after post-processing in § 2.6. Weight: Weights averaged across all occurrences of the token in the training set. We only keep tokens that occur at least 100 times.

We use the AdamW optimizer (Loshchilov and Hutter, 2019). The KL regularizer β is set to 0.005. See more details in Appendix E.

Baselines. We compare AttentionPO against the initial model π_{ref} and models trained with common PO methods, including **RRHF** (Yuan et al., 2023), **SLiC-HF** (Zhao et al., 2023), **DPO** (Rafailov et al., 2023), **TDPO** (Zeng et al., 2024), **TI-DPO** (Yang et al., 2026), **IPO** (Azar et al., 2024), **CPO** (Xu et al., 2024), **KTO** (Ethayarajh et al., 2024), **ORPO** (Hong et al., 2024), **R-DPO** (Park et al., 2024), and **SimPO** (Meng et al., 2024). Except TDPO and TI-DPO, we adopt the training hyperparameters from Meng et al. (2024), which have been separately searched to be optimal.

Evaluation. Following prior work (Meng et al., 2024; Yang et al., 2025; Huang and Goyal, 2025), we evaluate the models on AlpacaEval (Li et al., 2023), MT-Bench (Zheng et al., 2023), and Arena-Hard (Li et al., 2024). For AlpacaEval, we report the raw and length-controlled win rate of our model against GPT-4-1106-preview. For MT-Bench, we report the LLM-judged quality score of our model's generated response on a scale of 1 to 10. For Arena-Hard, we report the win rate of our model against GPT4-0314. We use GPT-4o-mini (Achiam et al., 2024) as the judge model for these benchmarks. See more evaluation details in Appendix E.

4 Results

We first present the main results (§ 4.1), followed by comparing our method with other choices of token weights (§ 4.2), and finally conducting an ablation study (§ 4.3).

4.1 Main Results

As shown in Table 3, **AttentionPO significantly improves the performance over the base model** π_{ref} **in all settings**. On LLaMA-3-8B-Base-SFT, performance increases by 12% on AlpacaEval, 1.05 on MT-Bench, 40% on ArenaHard. On LLaMA-3-8B-Instruct, performance increases by 27% on AlpacaEval, 0.41 on MT-Bench, and 14% on ArenaHard. Furthermore, **AttentionPO outperforms the baselines in most settings**. For the SFT model, AttentionPO ranks first on ArenaHard, second on MT-Bench, and third on AlpacaEval. For the Instruct model, AttentionPO outperforms all baselines on AlpacaEval and MT-Bench. Across the benchmarks, AttentionPO achieves the best overall rank for both models.

4.2 Impact of Token Weight Sources

There are alternative ways to obtain token-level weights. Prior work (Lin et al., 2024; Yang et al., 2025; Liu et al., 2025; Shao et al., 2025; Yang et al., 2026) either requires training a separate model to

	π_{ref}=LLaMA-3-8B-Base-SFT					π_{ref}=LLaMA-3-8B-Instruct				
	AlpacaEval		MT	ArenaHard	**Avg Rank ↓**	AlpacaEval		MT	ArenaHard	**Avg Rank ↓**
	LR ↑	WR ↑	Score ↑	WR ↑		LR ↑	WR ↑	Score ↑	WR ↑	
Base	9.20	4.63	5.47	9.92	12.75	33.60	32.60	6.78	37.57	11.25
+RRHF	11.29	6.63	6.18	26.00	8.25	43.75	37.65	6.63	41.91	9.00
+SLiC-HF	16.73	12.08	5.95	13.08	9.00	38.38	37.03	6.76	42.76	9.12
+DPO	22.88	17.70	**6.54**	38.54	2.75	49.02	44.72	6.73	53.98	5.50
+TDPO	11.96	6.18	5.68	12.09	10.75	37.74	37.34	6.64	41.00	10.50
+TI-DPO	9.94	4.77	5.29	10.14	12.25	35.41	34.57	6.80	38.73	9.75
+IPO	20.69	19.73	6.23	34.56	4.25	48.94	47.47	6.99	50.50	4.00
+CPO	18.94	**24.56**	6.13	36.04	4.62	41.26	45.13	6.67	52.07	6.75
+KTO	18.24	15.05	5.93	18.28	8.00	43.10	39.73	6.79	48.98	6.38
+ORPO	19.36	13.47	5.72	17.32	8.25	40.92	36.95	6.76	44.64	8.88
+R-DPO	20.94	15.57	6.33	28.72	4.75	52.11	46.98	6.79	**54.98**	3.12
+SimPO	**32.26**	19.11	6.13	47.01	3.38	56.79	47.73	6.51	54.94	4.75
+AttentionPO	21.55	20.23	6.52	**49.72**	**2.00**	**60.77**	**58.29**	**7.19**	52.06	**2.00**

Table 3: Main results. Base: π_{ref}; MT: MT-Bench; AlpacaEval: LR is the length-controlled win rate and WR is the raw win rate against GPT-4-1106-Preview; MT-Bench: LLM-judged quality score of the model's responses, on a scale of 1 to 10; ArenaHard: Win rate against GPT-4-0314. Avg Rank: arithmetic mean of the method's ranks across all individual metrics. AttentionPO achieves the best overall ranking across both Base-SFT and Instruct settings.

Figure 3: Results for different layers. x-axis: index of the layer from which attention weights are extracted; y-axis: benchmark performance.

estimate weights or relies on strong heuristics. Instead, we stick to our setting where the weights are attained through self-judging, but we experiment with various changes to the current design. This includes (1) Extracting the attention weights from a different hidden layer L of π_{ref}; (2) Using attention rollout (Abnar and Zuidema, 2020) to aggregate the weights across different hidden layers; (3) Prompting π_{ref} to verbally assign a weight for each token. For these experiments, we use LLaMA-3-8B-Instruct as an example.

Changing layers. LLaMA-3-8B-Instruct consists of 32 hidden layers. We use $L = 32$ for our main experiments. Here, we experiment with $L \in \{1, 8, 16, 24, 32\}$ and present the results in Figure 3. We find that **the first and last layers perform better than the middle ones, with the last layer achieving the best results**. We leave more investigation on this to future work.

Attention rollout (w/ attn rollout). Attention rollout aggregates the attentions across all the layers to estimate the total attentions from tokens in the final output layer to tokens in the initial input layer. Table 4 shows that using their aggregated weights underperforms our method. This is potentially associated with our previous observation that middle-layer attentions are not suitable for AttentionPO, since attention rollout incorporates attentions from these layers into the final weights.

Verbalized self-judged weights (w/ verbal w). Instead of using attention, we ask π_{ref} to verbally assign an importance score on a scale of 1 to 5 to each token in the response. We observe that it is difficult for the model to precisely give a score for every token (e.g., malformed scoring report; not being able to recall every token in the response). Therefore, we adapt a coarser granularity and ask the model to first partition the response into parts and then assign a score for each part (See prompts in Appendix I). Even with a coarser granularity, π_{ref} still cannot perfectly recall the response tokens. We filter out examples where fewer than 90% of the tokens are matched with a verbalized weight for either y_w or y_l. After filtering, we get 10,111/343 train/validation examples. To compensate for a smaller dataset, we increase the number of training epochs from 1 to 5 and validate at each epoch. Table 4 shows that this method outperforms ours on ArenaHard but underperforms on AlpacaEval and MT-Bench. A potential reason is the use of a coarser granularity. We leave more investigation on the viability of this approach to future work.

4.3 Ablation Study

Restoring the attention sink (w/ attn sink). We restore the attention sink, in which case the first

| | π_{ref}=LLaMA-3-8B-Instruct | | | |
| | AlpacaEval | | MT | ArenaHard |
	LR ↑	WR ↑	Score ↑	WR ↑
Base	33.60	32.60	6.78	37.57
+DPO	49.02	44.72	6.73	53.98
+AttentionPO	**60.77**	**58.29**	**7.19**	52.06
w/ attn rollout	54.84	54.87	6.71	48.23
w/ verbal w	57.95	57.76	6.89	**61.41**

Table 4: Results with different weight sources.

| | π_{ref}=LLaMA-3-8B-Instruct | | | |
| | AlpacaEval | | MT | ArenaHard |
	LR ↑	WR ↑	Score ↑	WR ↑
Base	33.60	32.60	6.78	37.57
+DPO	49.02	44.72	6.73	**53.98**
+AttentionPO	60.77	**58.29**	**7.19**	52.06
w/ attn sink	61.14	57.27	6.93	51.64
w/ len norm	**62.00**	55.69	6.79	44.59

Table 5: Ablation Results.

token occupies roughly 8.25% of the total weights. Table 5 shows that this variant underperforms our method on all benchmarks, indicating the benefits of averaging out the attention sink.

Adding length normalization (w/ len norm). Prior work (Yang et al., 2025; Meng et al., 2024) argues that DPO is biased toward lengthy responses (i.e., lengthy responses receive more gradient updates than concise ones). They add a length normalizer to the objective. Similarly, we remove the $|y|$ multiplier in front of the logprob ratio term for y_w and y_l, giving a weighted, length-normalized variant:

$$\mathcal{L}' = -\mathbb{E}_{\mathcal{D}}\left[log\sigma\left(\beta \sum_{t=1}^{|y_w|} a_w^t \log \frac{\pi_\theta(y_w^t|x, y_w^{<t})}{\pi_{ref}(y_w^t|x, y_w^{<t})} \right. \right.$$
$$\left. \left. -\beta \sum_{t=1}^{|y_l|} a_l^t log \frac{\pi_\theta(y_l^t|x, y_l^{<t})}{\pi_{ref}(y_l^t|x, y_l^{<t})} \right) \right] \quad (15)$$

Adding the length normalization effectively reduces the KL regularization constant β. Therefore, we increase β to 2.0 for this baseline. For these experiments, we use LLaMA-3-8B-Instruct as an example. Table 5 shows that applying length normalization significantly hurts performance on MT-Bench and AreaHard. One speculated reason for this is the misalignment with the original RL objective. Instead of maximizing the total rewards of the entire rollout y, the dual-RL objective of objective 15 (which is the same as objective 7 but with $|y|$ removed in both the reward function and the KL penalty) maximizes the average per-token reward of y, undermining the total rewards.

5   Related Work

Preference Optimization. Aligning LLMs with human preferences originally relied on RLHF via PPO (Ouyang et al., 2022; Schulman et al., 2017), which requires a separate reward model. Modern Preference Optimization (PO) methods bypass this by training the policy directly on preference pairs (y_w, y_l) using contrastive objectives. For instance, RRHF (Yuan et al., 2023) and SLiC-HF (Zhao et al., 2023) apply ranking losses, while DPO (Rafailov et al., 2023) derives a reference-normalized objective from policy gradients. Subsequent variants introduce bounded objectives (IPO (Azar et al., 2024)), pointwise formulations (KTO (Ethayarajh et al., 2024)), auxiliary SFT objectives (CPO (Xu et al., 2024), ORPO (Hong et al., 2024)), length penalties (R-DPO (Park et al., 2024)), or reference-free length normalization with reward margins (SimPO (Meng et al., 2024)). However, these methods weight all response tokens equally, failing to capture token-level importance.

Token-level PO. To enable fine-grained credit assignment, recent work explores token-level weighting. TDPO (Zeng et al., 2024) incorporates token-level sequential KL terms. TIS-DPO (Liu et al., 2025), SePO (Yang et al., 2025), and cDPO (Lin et al., 2024) estimate token importance by contrasting probabilities between reference/negative models and oracle/positive models. TI-DPO (Yang et al., 2026) combines Gaussian priors with logit gradient norms. Alternatively, heuristic approaches like D^{2}PO (Shao et al., 2025) decay weights based on token position. Nonetheless, these methods either demand expensive auxiliary models or rely on rigid, position-based heuristics rather than semantic content.

6   Conclusion

We propose TwDPO—a token-weighted DPO objective, theoretically grounded on token-weighted RL—and AttentionPO—an instantiation of TwDPO that prompts the model to judge the response qualities and extract attentions from the model itself to weigh the response tokens. Experiment results show that AttentionPO significantly improves the performance of the base model across AlpacaEval, MT-Bench, and ArenaHard, outperforming various prior PO methods. We hope AttentionPO paves the way for highly-performant and efficient preference alignment with humans.

Limitations

Due to computational constraints, we do not experiment with our method on larger models. In addition, our training and evaluation focus on the instruction-following task. Analysing the performance and generalizability of AttentionPO on other models and tasks is an important future direction.

Moreover, the search space for the optimal choice of attention weights for TwDPO is large. For example, while we simply take the mean across attention heads, future work could investigate selecting a specific head or group of heads for weight extraction. However, we argue that such a choice of attention heads is likely model-dependent and may not transfer across settings.

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A Extended Related Work

Preference Optimization. The alignment with human preferences and values is critical for LLM-generated output. Early work (Ouyang et al., 2022) trains LLM using policy-gradient RL-algorithm such as PPO (Schulman et al., 2017). However, these methods require training a separate reward model on annotated preference pairs to provide RL rewards. Preference Optimization (PO) methods avoid the need for an extra reward model and train the main policy directly on the preference pairs to learn the reward landscape. On a high level, PO methods use a contrastive learning objective between a preferred response y_w and a dispreferred response y_l. For example, RRHF (Yuan et al., 2023) and SLiC-HF (Zhao et al., 2023) use ranking losses. DPO (Rafailov et al., 2023) drives its training objective from policy gradient, which normalizes the model's probability with the reference model's probability. IPO (Azar et al., 2024) uses a bounded objective in contrast to DPO. KTO (Ethayarajh et al., 2024) avoids the pairwise assumption and uses a pointwise formulation. CPO (Xu et al., 2024) and ORPO (Hong et al., 2024) add an SFT term in addition to the contrastive term. R-DPO (Park et al., 2024) adds an extra term to the original DPO objective to avoid the length exploitation. SimPO (Meng et al., 2024) modifies DPO by removing dependencies on the reference model, incorporating length normalization, and adding a reward margin term. However, all the methods above assign equal weights to every response token, which cannot account for the fine-grained importance of each token to the overall response quality.

Token-level PO. Various attempts are made to enable fine-grained, token-level credit assignment during PO training. TDPO (Zeng et al., 2024) is grounded on token-level policy gradient methods. It adds two sequence KL terms to the original DPO objective. TIS-DPO (Liu et al., 2025) and cDPO (Lin et al., 2024) estimate the token importance via contrasting the probability to produce the token from a positive policy with the one from a negative policy, given the same prefix. The positive and negative policies are induced either from prompts or training. SePO (Yang et al., 2025) takes a similar approach, but it trains an oracle model with DPO on a subset of the original training set and contrasts the probability from the oracle against the one from the reference model. TI-DPO (Yang et al., 2026) estimates the token weights by combining

a pre-defined Gaussian prior distribution with the gradient norm of the last token's maximum logit with respect to each token. Certain methods use heuristics to assign weights. For example, D^2PO (Shao et al., 2025) gives earlier tokens more weight than later ones. However, many of these methods require training extra models to estimate weights. The rest compute weights using heuristic functions, which are purely based on token positions rather than the tokens themselves.

Attention Weights. Early studies on transformers (Vaswani et al., 2017) indicate that specific attention heads capture linguistic properties like coreference resolution, framing attention weights as transparent windows into model reasoning (Clark et al., 2019). However, subsequent research challenges this notion by demonstrating that attention distributions can be manipulated without altering model predictions, implying that attention correlates with but does not cause model outputs (Jain and Wallace, 2019; Serrano and Smith, 2019). Counter-counter-arguments suggest attention remains a useful, albeit incomplete, diagnostic signal when contextualized (Wiedemann et al., 2019). While individual attention heads specialize (Vig, 2019), they operate redundantly. Furthermore, attention patterns are frequently associated with superficial heuristics rather than deep semantic understanding (McCoy et al., 2019). When aggregated across multiple layers with residual connections, the aggregated attentions show a higher correlation with gold token importance scores, compared with raw attentions (Abnar and Zuidema, 2020). These findings suggest that attention could potentially provide a complementary view of information flow. In summary, whether attention is interpretable is still under debate. As such, in this work, we do not explicitly assume the interpretability of attentions.

B Theoretical Analysis and Error Bounds

Because the sequence-level expectation $\mathbb{E}_{y \sim \pi}$ in the TwDPO objective is coupled with token-weighted log-probabilities, deriving an exact analytical closed-form solution for the optimal policy is intractable without invoking complex token-level dynamic programming. In this section, we establish a formal theoretical guarantee for TwDPO by framing it as a bounded perturbation around the standard Direct Preference Optimization (DPO) objective (Rafailov et al., 2023). We first bound the divergence between the true, intractable TwDPO

optimal policy π_{opt} and the standard DPO optimal policy π_{DPO}. We then bound the distance between our empirical autoregressive heuristic policy $\tilde{\pi}^*$ and π_{DPO}, concluding with a unified Total Variation (TV) distance bound between the empirical heuristic and the true optimum.

B.1 Objective Formulation and Perturbation Setup

Let $\mathcal{D}$ denote the dataset of prompts x, and let $y = (y^1, y^2, \ldots, y^{|y|})$ represent a generated sequence of length $|y|$. For a given prompt x, policy π, and reference policy π_{ref}, the TwDPO objective $J_{\text{TwDPO}}(\pi)$ modifies the standard sequence-level KL penalty by weighting individual token steps using attention weights a^t:

$$J_{\text{TwDPO}}(\pi) = \mathbb{E}_{x \sim \mathcal{D}} \mathbb{E}_{y \sim \pi(\cdot | x)}$$
$$\left[r(x, y) - \beta |y| \sum_{t=1}^{|y|} a^t \log \frac{\pi(y^t \mid x, y^{<t})}{\pi_{\text{ref}}(y^t \mid x, y^{<t})} \right], \tag{16}$$

where $\beta > 0$ is the global scaling parameter. By definition, the token attention weights are normalized such that $\sum_{t=1}^{|y|} a^t = 1$. Let us define the effective token weights as $w^t = |y| a^t$, satisfying $\frac{1}{|y|} \sum_{t=1}^{|y|} w^t = 1$.

We parameterize the deviation of these attention weights from a uniform distribution as a perturbation vector ϵ^t:

$$w^t = 1 + \epsilon^t, \quad \text{where} \quad \sum_{t=1}^{|y|} \epsilon^t = 0. \tag{17}$$

Assumption 1 (Bounded Attention Deviation). *There exists a constant $\delta \geq 0$ such that the maximum token-level attention perturbation is strictly bounded for all sequences:*

$$\max_t |\epsilon^t| \leq \delta. \tag{18}$$

Assumption 2 (Bounded Trust Region Log-Ratios). *The log-probability ratio between any valid policy π under consideration and the reference policy π_{ref} is bounded at the token level by a finite constant $C > 0$:*

$$\max_t \left| \log \frac{\pi(y^t \mid x, y^{<t})}{\pi_{ref}(y^t \mid x, y^{<t})} \right| \leq C. \tag{19}$$

Using this formulation, we decompose the TwDPO objective into the standard DPO objective $J_{\text{DPO}}(\pi)$ and a descriptive perturbation term:

$$J_{\text{TwDPO}}(\pi) = \mathbb{E}_{x \sim \mathcal{D}} \mathbb{E}_{y \sim \pi(\cdot | x)}$$
$$\left[r(x, y) - \beta \sum_{t=1}^{|y|} (1 + \epsilon^t) \log \frac{\pi(y^t \mid x, y^{<t})}{\pi_{\text{ref}}(y^t \mid x, y^{<t})} \right]$$
$$= J_{\text{DPO}}(\pi) - \beta \mathbb{E}_{x \sim \mathcal{D}} \mathbb{E}_{y \sim \pi(\cdot | x)} \left[R_\epsilon(\pi; x, y) \right],$$

where the point-wise sequence perturbation $R_\epsilon(\pi; x, y)$ is defined as:

$$R_\epsilon(\pi; x, y) = \sum_{t=1}^{|y|} \epsilon^t \log \frac{\pi(y^t \mid x, y^{<t})}{\pi_{\text{ref}}(y^t \mid x, y^{<t})}. \tag{20}$$

B.2 Bounding the Objective Discrepancy

We now bound the magnitude of the expected perturbation term. Under Assumptions 1 and 2, the sequence-level perturbation can be upper-bounded via the triangle inequality:

$$|R_\epsilon(\pi; x, y)| \leq \sum_{t=1}^{|y|} |\epsilon^t| \cdot \left| \log \frac{\pi(y^t \mid x, y^{<t})}{\pi_{\text{ref}}(y^t \mid x, y^{<t})} \right|$$
$$\leq \sum_{t=1}^{|y|} \delta C = |y| \delta C. \tag{21}$$

Taking the expectation over the prompt and sequence distributions, the discrepancy between the two objectives is strictly bounded by:

$$|J_{\text{TwDPO}}(\pi) - J_{\text{DPO}}(\pi)| \leq \beta \delta C \mathbb{E}_{x \sim \mathcal{D}} \mathbb{E}_{y \sim \pi(\cdot | x)}[|y|]. \tag{22}$$

For ease of notation, let $B(\pi) = \beta \delta C \mathbb{E}_\pi[|y|]$ denote the policy-dependent bound constraint.

B.3 Distance Bound for True Optima

Let $\pi_{\text{opt}} = \arg \max_\pi J_{\text{TwDPO}}(\pi)$ be the true, intractable optimal policy under the token-weighted framework, and let $\pi_{\text{DPO}} = \arg \max_\pi J_{\text{DPO}}(\pi)$ be the analytical optimal policy for the standard DPO objective.

From the exact mathematical properties of KL-constrained reinforcement learning objectives, the suboptimality gap of any arbitrary policy π evaluated under J_{DPO} is exactly equal to its generalized KL divergence from the optimal DPO policy:

$$J_{\text{DPO}}(\pi_{\text{DPO}}) - J_{\text{DPO}}(\pi)$$
$$= \beta \mathbb{E}_{x \sim \mathcal{D}} \left[D_{\text{KL}}(\pi(\cdot \mid x) \parallel \pi_{\text{DPO}}(\cdot \mid x)) \right]. \tag{23}$$

Evaluating the true optimal policy π_{opt} using the identity in Equation 23 yields:

$$J_{\text{DPO}}(\pi_{\text{DPO}}) - J_{\text{DPO}}(\pi_{\text{opt}})$$
$$= \beta \mathbb{E}_{x \sim \mathcal{D}} \left[D_{\text{KL}}(\pi_{\text{opt}}(\cdot \mid x) \parallel \pi_{\text{DPO}}(\cdot \mid x)) \right]. \tag{24}$$

By the definition of functional optimality, π_{opt} maximizes J_{TwDPO}, meaning $J_{\text{TwDPO}}(\pi_{\text{opt}}) \geq J_{\text{TwDPO}}(\pi_{\text{DPO}})$. We construct a double inequality chain by introducing the objective boundaries $B(\pi_{\text{opt}})$ and $B(\pi_{\text{DPO}})$:

$$
\begin{aligned}
J_{\text{DPO}}(\pi_{\text{opt}}) + B(\pi_{\text{opt}}) &\geq J_{\text{TwDPO}}(\pi_{\text{opt}}) \\
&\geq J_{\text{TwDPO}}(\pi_{\text{DPO}}) \\
&\geq J_{\text{DPO}}(\pi_{\text{DPO}}) - B(\pi_{\text{DPO}}).
\end{aligned}
\tag{25}
$$

Rearranging the outermost components of this inequality gives an upper bound on the DPO objective gap:

$$
J_{\text{DPO}}(\pi_{\text{DPO}}) - J_{\text{DPO}}(\pi_{\text{opt}}) \leq B(\pi_{\text{DPO}}) + B(\pi_{\text{opt}}). \tag{26}
$$

Substituting this directly back into the identity in Equation 24, we obtain:

$$
\begin{aligned}
\beta \mathbb{E}_{x \sim \mathcal{D}} &\left[D_{\text{KL}}(\pi_{\text{opt}}(\cdot \mid x) \parallel \pi_{\text{DPO}}(\cdot \mid x)) \right] \\
&\leq \beta \delta C \left(\mathbb{E}_{\pi_{\text{DPO}}}[|y|] + \mathbb{E}_{\pi_{\text{opt}}}[|y|] \right).
\end{aligned}
\tag{27}
$$

Dividing both sides by the regularization parameter β establishes our first localized distance guarantee.

Lemma 1 (Optima Distance Bound). *The expected KL divergence between the true optimal token-weighted policy π_{opt} and the standard DPO policy π_{DPO} is linearly bounded by the maximum attention perturbation δ:*

$$
\begin{aligned}
\mathbb{E}_{x \sim \mathcal{D}} &\left[D_{KL}(\pi_{opt}(\cdot \mid x) \parallel \pi_{DPO}(\cdot \mid x)) \right] \\
&\leq \delta C \left(\mathbb{E}_{\pi_{DPO}}[|y|] + \mathbb{E}_{\pi_{opt}}[|y|] \right).
\end{aligned}
\tag{28}
$$

B.4 Bounding the Autoregressive Heuristic Policy

We now address our empirical heuristic policy, denoted as $\tilde{\pi}^*$. While $\tilde{\pi}^*$ is derived via a localized parameterization mapping, it is generated sequentially in an autoregressive fashion, ensuring that $\tilde{\pi}^*(y \mid x) = \prod_{t=1}^{|y|} \tilde{\pi}^*(y^t \mid x, y^{<t})$ constitutes a mathematically proper, normalized probability distribution over sequence space ($\sum_y \tilde{\pi}^*(y \mid x) = 1$).

By definition, our empirical token-weighted optimal parameterization satisfies the equality:

$$
\sum_{t=1}^{|y|} w^t \log \frac{\tilde{\pi}^*(y^t \mid x, y^{<t})}{\pi_{\text{ref}}(y^t \mid x, y^{<t})} = \frac{1}{\beta} r(x, y) - \log Z(x). \tag{29}
$$

Expanding $w^t = 1 + \epsilon^t$ yields:

$$
\log \frac{\tilde{\pi}^*(y \mid x)}{\pi_{\text{ref}}(y \mid x)} + R_\epsilon(\tilde{\pi}^*; x, y) = \frac{1}{\beta} r(x, y) - \log Z(x). \tag{30}
$$

Recall that the standard sequence-level DPO optimal policy satisfies:

$$
\log \frac{\pi_{\text{DPO}}(y \mid x)}{\pi_{\text{ref}}(y \mid x)} = \frac{1}{\beta} r(x, y) - \log Z_{\text{DPO}}(x). \tag{31}
$$

Subtracting Equation 31 from Equation 30 isolates the log-ratio between our heuristic policy and the standard DPO policy:

$$
\log \frac{\tilde{\pi}^*(y \mid x)}{\pi_{\text{DPO}}(y \mid x)} = \log Z_{\text{DPO}}(x) - \log Z(x) - R_\epsilon(\tilde{\pi}^*; x, y). \tag{32}
$$

Let $\Delta Z(x) = \log Z_{\text{DPO}}(x) - \log Z(x)$. Taking the expectation of Equation 32 under $\tilde{\pi}^*$ yields the forward KL divergence:

$$
D_{\text{KL}}(\tilde{\pi}^* \parallel \pi_{\text{DPO}}) = \Delta Z(x) - \mathbb{E}_{y \sim \tilde{\pi}^*} \left[R_\epsilon(\tilde{\pi}^*; x, y) \right]. \tag{33}
$$

Similarly, taking the expectation of Equation 32 under the standard DPO policy yields the reverse KL divergence:

$$
-D_{\text{KL}}(\pi_{\text{DPO}} \parallel \tilde{\pi}^*) = \Delta Z(x) - \mathbb{E}_{y \sim \pi_{\text{DPO}}} \left[R_\epsilon(\tilde{\pi}^*; x, y) \right]. \tag{34}
$$

Subtracting Equation 34 from Equation 33 cancels the intractable partition scaling term $\Delta Z(x)$:

$$
\begin{aligned}
D_{\text{KL}}(\tilde{\pi}^* &\parallel \pi_{\text{DPO}}) + D_{\text{KL}}(\pi_{\text{DPO}} \parallel \tilde{\pi}^*) \\
&= \mathbb{E}_{y \sim \pi_{\text{DPO}}} \left[R_\epsilon(\tilde{\pi}^*; x, y) \right] - \mathbb{E}_{y \sim \tilde{\pi}^*} \left[R_\epsilon(\tilde{\pi}^*; x, y) \right].
\end{aligned}
\tag{35}
$$

Since the reverse KL divergence is strictly non-negative ($D_{\text{KL}}(\pi_{\text{DPO}} \parallel \tilde{\pi}^*) \geq 0$), we drop it to establish an upper bound, and apply the triangle inequality across expectations:

$$
\begin{aligned}
D_{\text{KL}}(\tilde{\pi}^* \parallel \pi_{\text{DPO}}) &\leq |\mathbb{E}_{y \sim \pi_{\text{DPO}}} \left[R_\epsilon(\tilde{\pi}^*; x, y) \right]| + \\
&\quad |\mathbb{E}_{y \sim \tilde{\pi}^*} \left[R_\epsilon(\tilde{\pi}^*; x, y) \right]| \\
&\leq \delta C \mathbb{E}_{y \sim \pi_{\text{DPO}}}[|y|] + \delta C \mathbb{E}_{y \sim \tilde{\pi}^*}[|y|].
\end{aligned}
$$

Taking the expectation across the entire prompt distribution $\mathcal{D}$ establishes our second localization lemma.

Lemma 2 (Heuristic Distance Bound). *The expected KL divergence between the empirical autoregressive heuristic policy $\tilde{\pi}^*$ and the closed-form standard DPO policy π_{DPO} is strictly bounded by:*

$$
\begin{aligned}
\mathbb{E}_{x \sim \mathcal{D}} &\left[D_{KL}(\tilde{\pi}^*(\cdot \mid x) \parallel \pi_{DPO}(\cdot \mid x)) \right] \\
&\leq \delta C \left(\mathbb{E}_{\pi_{DPO}}[|y|] + \mathbb{E}_{\tilde{\pi}^*}[|y|] \right).
\end{aligned}
\tag{36}
$$

B.5 Unified Suboptimality Guarantee via Total Variation Distance

We now unify Lemma 1 and Lemma 2 to bound the final distance between our empirical heuristic policy $\tilde{\pi}^*$ and the true intractable optimal policy π_{opt}. We map our KL bounds to Total Variation (TV)

distance using Pinsker's inequality, which states that for any distributions P and Q, $D_{\text{TV}}(P, Q) \leq \sqrt{\frac{1}{2} D_{\text{KL}}(P \parallel Q)}$.

Applying Pinsker's inequality to Lemma 1 and Lemma 2 gives:

$$
\begin{aligned}
&\mathbb{E}_{x \sim \mathcal{D}}[D_{\text{TV}}(\pi_{\text{opt}}, \pi_{\text{DPO}})] \\
&\leq \mathbb{E}_{x \sim \mathcal{D}}\left[\sqrt{\frac{1}{2} D_{\text{KL}}\left(\pi_{\text{opt}}(\cdot \mid x) \parallel \pi_{\text{DPO}}(\cdot \mid x)\right)}\right] \\
&\leq \mathbb{E}_{x \sim \mathcal{D}}\left[\sqrt{\frac{\delta C}{2}\left(\mathbb{E}_{y \sim \pi_{\text{DPO}}}[|y|] + \mathbb{E}_{y \sim \pi_{\text{opt}}}[|y|]\right)}\right] \\
&\leq \sqrt{\frac{\delta C}{2}\left(\mathbb{E}_{\pi_{\text{DPO}}}[|y|] + \mathbb{E}_{\pi_{\text{opt}}}[|y|]\right)},
\end{aligned}
\tag{37}
$$

where the first inequality comes from Pinsker's inequality, the second comes from equation 28 with $\mathcal{D}$ containing only a single query x, the third comes from Jensen's inequality.

Similarly, applying Pinsker's inequality, equation 36 with $\mathcal{D}$ containing only a single query x, and Jensen's inequality, we get

$$
\mathbb{E}_{x \sim \mathcal{D}}[D_{\text{TV}}(\tilde{\pi}^*, \pi_{\text{DPO}})] \leq \sqrt{\frac{\delta C}{2}\left(\mathbb{E}_{\pi_{\text{DPO}}}[|y|] + \mathbb{E}_{\tilde{\pi}^*}[|y|]\right)}.
\tag{38}
$$

Finally, by utilizing the triangle inequality property of Total Variation distances, we bound the direct distance between the empirical heuristic and the true functional optimum:

$$
D_{\text{TV}}(\pi_{\text{opt}}, \tilde{\pi}^*) \leq D_{\text{TV}}(\pi_{\text{opt}}, \pi_{\text{DPO}}) + D_{\text{TV}}(\tilde{\pi}^*, \pi_{\text{DPO}}).
\tag{39}
$$

Taking expectations over $\mathcal{D}$ and substituting Equations 37 and 38 leads directly to our main result.

Theorem 1 (TwDPO Suboptimality Consistancy). *Under Assumptions 1 and 2, the expected Total Variation distance between the empirical autoregressive heuristic policy $\tilde{\pi}^*$ and the true, intractable token-weighted optimal policy π_{opt} is strictly bounded by $\mathcal{O}(\sqrt{\delta})$:*

$$
\mathbb{E}_{x \sim \mathcal{D}}[D_{TV}(\pi_{opt}(\cdot \mid x), \tilde{\pi}^*(\cdot \mid x))] \leq \sqrt{\frac{\delta C}{2}}
$$
$$
\left(\sqrt{\mathbb{E}_{\pi_{DPO}}[|y|] + \mathbb{E}_{\pi_{opt}}[|y|]} + \sqrt{\mathbb{E}_{\pi_{DPO}}[|y|] + \mathbb{E}_{\tilde{\pi}^*}[|y|]}\right).
\tag{40}
$$

This theorem provides a rigorous theoretical safety net for TwDPO. It demonstrates that while a clean closed-form sequence-level derivation is structurally impossible due to token-weight expectation coupling, the empirical objective remains mathematically consistent. As long as the attention variance deviation from uniform is controlled

($\delta \to 0$), the empirical policy behaves predictably and stays bounded within a localized neighborhood of the true mathematical optimum.

C   Gradient Analysis

The gradient of objective 5 is:

$$
\begin{aligned}
\nabla_\theta \mathcal{L} = -\beta \mathbb{E}_{(x, y_w, y_l) \sim \mathcal{D}}\bigg[&\sigma\left(r'_\theta(x, y_l) - r'_\theta(x, y_w)\right) \\
&\left(|y_w| \sum_{t=1}^{|y_w|} a_w^t \nabla_\theta log \pi_\theta(y_w^t | x, y_w^{<t}) - \right. \\
&\left. |y_l| \sum_{t=1}^{|y_l|} a_l^t \nabla_\theta log \pi_\theta(y_l^t | x, y_l^{<t})\right)\bigg],
\end{aligned}
\tag{41}
$$

where $r'_\theta(x, y) = \beta |y| \sum_{t=1}^{|y|} a^t \log \frac{\pi_\theta(y^t | x, y^{<t})}{\pi_{ref}(y^t | x, y^{<t})}$.

Similar to DPO, the $\sigma(r'_\theta(x, y_l) - r'_\theta(x, y_w))$ term scales up our combined gradient when the reward margin between y_w and y_l is smaller or negative. The main difference from DPO is that we weigh the gradient of each token at position t by a^t, so that higher-weighted tokens get more gradient updates and the model learns more on these tokens.

D   Token Matching

We note that certain attention scores may not be matched to any tokens, and certain tokens may not be assigned an attention weight. This is because when we extract the attention weights in § 2.5, the response y is tokenized with the pairwise judge prompt as the surrounding context. During training, y is tokenized with a different surrounding context, and consequently, the first and last several tokens do not match the original tokens extracted from the pairwise judge prompt. In case no perfect match is found, we use the "edit_distance" Python library to match the attention weight to the response tokens during training. For tokens without a match, we assign a weight of 0. We observe that in most cases, more than 95% of the tokens are matched to attention weights.

E   Hyperparameters

Training. We tune our training β in the range {2e-2, 1e-2, 5e-3, 1e-3} and show the final training hyperparameters for AttentionPOfor both LLaMA-3-8B-Base-SFT and LLaMA-3-8B-Instruct in Figure 6. We train for around 2K steps and validate every 500 steps to pick the best checkpoint for evaluation. For the baselines except TDPO and

Parameter	Value
Max Context Length	2048
Max Prompt Length	1800
Learning Rate	1e-6
β	5e-3
Batch Size	32
# Epochs	1
# Train Examples	∼60K
# Validation Examples	∼2K
Scheduler	Cosine
Warmup Ratio	0.1
Optimizer	AdamW

Table 6: Training Hyperparameters

Parameter	Value
Max New Tokens	1024
Temperature	varies
Judge Max New Tokens	2048
Judge Temperature	0

Table 8: Hyperparameters for MT-Bench. We use the default temperature, which varies between different task subsets.

Parameter	Value
Max New Tokens	2048
Temperature	0
Judge Max New Tokens	16000
Judge Temperature	0
Baseline Model	GPT-4-0314

Table 9: Hyperparameters for ArenaHard

TI-DPO, we take the existing checkpoints from Meng et al. (2024) and use their hyperparameters. For TDPO and TI-DPO, since the original method is applied on different task and training datasets, we retrain new checkpoints on our datasets. For TDPO, we use the TDPO$_2$ variant due to its superior performance over TPO$_1$, as reported in the original paper. We tune β in the range {1e-2, 1e-1} and adopt the default for other hyperparameters. The final hyperparameters are $\beta = $ 1e-2, $\alpha = $ 0.5, Learning Rate = 5e-6. For TI-DPO, we tune β in the range {1e-2, 1e-1} and Learning Rate in the range {5e-6, 1e-6, 1e-5}. We adopt the default for the other hyperparameters. The final hyperparameters are $\beta = $ 1e-2, $\alpha = $ 0.5, $\alpha_{\text{triplet}} = $ 1e-3, $\gamma = 0.1$, $\lambda = 0.7$, Learning Rate = 5e-6.

Parameter	Value
Max New Tokens	4096
Temperature	0.7
Top K	50
Top P	0.9
Presence Penalty	0.1
Frequency Penalty	0.1
Judge Max New Tokens	1
Judge Temperature	1.0
Baseline Model	GPT4-1106-preview

Table 7: Hyperparameters for AlpacaEval

Evaluation. The default hyperparameters are used whenever they are available. See the details in Figure 7, 8, and 9.

F Additional Results

F.1 Results on other models

We additionally experiment with zephyr-7b-sft-full (Tunstall et al., 2023), which is a model supervised-finetuned from Mistral-7B-v0.1 (Jiang et al., 2023a) on UltraChat-200K (Ding et al., 2023). We denote this model as **Mistral-7B-Base-SFT**. We use the same UltraFeedback binarized dataset (Cui et al., 2024) (HuggingFaceH4/ultrafeedback_binarized) and the same hyperparameters to train it. The results are shown in Table 10.

Compared with π_{ref}, AttentionPO significantly enhances performances across different benchmarks. We observe a 14% increase on AlpacaEval, a 0.82 increase on MT-Bench, and a 12% increase on ArenaHard. In addition, AttentionPO outperforms DPO in terms of AlpacaEval and ArenaHard, but DPO has a higher MT-Bench score.

F.2 Using attentions from other models

We investigate whether attention weights from one model can be used to train another model. In par-

	π_{ref}=Mistral-7B-Base-SFT			
	AlpacaEval		MT	ArenaHard
	LR ↑	WR ↑	Score ↑	WR ↑
Base	8.77	4.20	4.54	2.26
+DPO	18.56	14.62	**5.85**	12.45
+AttentionPO	**22.39**	**19.47**	5.36	**13.88**

Table 10: Results on Mistral-7B-Base-SFT.

| | π_{ref}=LLaMA-3-8B-Base-SFT | | | | π_{ref}=LLaMA-3-8B-Instruct | | | |
| | AlpacaEval | | MT | ArenaHard | AlpacaEval | | MT | ArenaHard |
	LR ↑	WR ↑	Score ↑	WR ↑	LR ↑	WR ↑	Score ↑	WR ↑
Base	9.20	4.63	5.47	9.92	33.60	32.60	6.78	37.57
+DPO	22.88	17.70	**6.54**	38.54	49.02	44.72	6.73	**53.98**
+AttentionPO	21.55	20.23	6.52	49.72	**60.77**	**58.29**	**7.19**	52.06
w/ attn from sft	-	-	-	-	48.54	44.67	6.99	45.71
w/ attn from inst	**26.97**	**27.74**	6.44	**58.21**	-	-	-	-

Table 11: Results of using attentions from other models.

ticular, we use the attentions from LLaMA-3-8B-Base-SFT to train LLaMA-3-8B-Instruct (w/ attn from sft) and vice versa (w/ attn from inst). The results are shown in Table 11.

Training the SFT model with attentions from the stronger Instruct model (w/ attn from inst) leads to a further increase in performance on AlpacaEval and ArenaHard on top of the original AttentionPO results. In contrast, training the instruction model with attentions from the SFT model (w/ attn from sft) gives worse performance than the original AttentionPO, but the results are nonetheless better than π_{ref} by a significant margin across benchmarks. This suggests that attentions from a stronger model gives stronger performance. AttentionPO can still deliver performance gains even with attentions from a model weaker than π_{ref}, but to a lesser extent.

F.3 Analysis of Response Length

| | π_{ref}=SFT | | π_{ref}=Instruct | |
	WR ↑	#Tokens	WR ↑	#Tokens
Base	9.92	1254	37.57	580
+RRHF	26.00	1506	41.91	506
+SLiC-HF	13.08	556	42.76	575
+DPO	38.54	921	53.98	533
+TDPO	12.09	1233	41.00	565
+TI-DPO	10.14	1238	38.73	585
+IPO	34.56	675	50.50	546
+CPO	36.04	**1588**	52.07	**631**
+KTO	18.28	516	48.98	535
+ORPO	17.32	594	44.64	540
+R-DPO	28.72	731	**54.98**	524
+SimPO	47.01	796	54.94	505
+AttentionPO	**49.72**	1157	52.06	553

Table 12: ArenaHard Results. WR: Win Rate against GPT-4-0314. #Tokens: Number of response tokens.

We report the length of generated responses on ArenaHard in Table 12. For both the SFT and Instruct model, responses produced by AttentionPO are not longer than those from either the base model or other baseline methods. This shows that the perfor-

mance boost does not come from verbosity.

G Examples

We show an example of attention weights for LLaMA-3-8B-Base-SFT in Figure 4 and LLaMA-3-8B-Instruct in Figure 5.

H Compute

We run all experiments on a single node with 40 CPU cores, 256 GB of memory, and 2 Nvidia A100 80 GB GPUs.

I Prompt

Figure 4: An example for LLaMA-3-8B-Base-SFT.

Figure 5: An example for LLaMA-3-8B-Instruct.

Pairwise Judge Prompt

Please act as an impartial judge and evaluate the quality of the two responses to the user prompt displayed below. You will be given answer A and answer B. Your job is to evaluate which answer is better.

Consider if the answers are helpful, relevant, and concise. Helpful means the answer correctly responds to the prompt or follows the instructions. Relevant means all parts of the response closely connect or are appropriate to what is being asked. Concise means the response is clear and not verbose or excessive.

Then consider the creativity and novelty of the answers when needed. Finally, identify any missing important information in the answers that would be beneficial to include when responding to the user prompt.

After providing your explanation, you must output exactly one of the following choices as your final verdict:

1. Answer A is better: A
2. Answer B is better: B

<|The Start of User Prompt|>
{question}
<|The End of User Prompt|>

<|The Start of Answer A|>
{answer_a}
<|The End of Answer A|>

<|The Start of Answer B|>
{answer_b}
<|The End of Answer B|>

Now, output one of the following identifiers and nothing else (no quotes, no spaces, no new lines, no thinking or reasoning, ...): A or B.

Your choice:

Figure 6: Pairwise Judge Prompt

Verbalized Self Judge System Prompt

You are an expert in linguistics. Given a question and a response, split the response into parts and rate the importance of each part relative to the user's question on a scale of 1 (filler) to 5 (critical content).

Guidelines

* Split the response into parts that are as fine-grained as possible. The split needs to be on phrase-level or word-level. Try not to simply split by sentences or paragraphs, as this is too coarse.
* The parts need to be a disjoint partition of the original response. When concatenated, they should cover all the tokens in the original response. Each part needs to be non-empty. Different parts cannot overlap with each other.
* Part M needs to contain text that immediately follow part M-1.
* For example, given a response consisting of 5 tokens (i.e., resposne = "t1 t2 ... t5"), (part_1="t1 t2" part_2="t3 t4 t5") is a legal split, (part_1="t1 t2" part_2="t4 t5") is an illegal split.

Format

* Output ONLY a JSON list of tuples in the format: [["part_1_text", score_1], ["part_2_text", score_2] ..., ["part_M_text", score_(M)]]
* The accompanied score for each part needs to be an integer from 1 to 5.

Figure 7: Verbalized Self-judge System Prompt

Verbalized Self Judge User Prompt

Question: {prompt}

Response: {tokens}

Figure 8: Verbalized Self-judge User Prompt