

Towards Efficient Exact Optimization of Language Model Alignment

*Haozhe Ji¹, Cheng Lu², Yilin Niu³, Pei Ke¹,
Hongning Wang¹, Jun Zhu², Jie Tang⁴, Minlie Huang¹*

¹CoAI Group, ²TSAIL Group, ³Zhipu AI, ⁴KEG



清华大学
Tsinghua University



Introduction



- ◉ *Aligning language models (LMs) to generate human preferred responses is crucial to the development of **reliable** AI systems.*
- ◉ *It is essential to develop **principled** and **scalable** alignment method.*
- ◉ **Principle:** *Theoretically grounded in principle.*
- ◉ **Scalable:** *Accommodate to growing scale.*

Introduction



◉ The Recipe of LM alignment [Ouyang et al., 2022]:

◆ SFT stage: Supervised Fine-Tuning

$$\begin{array}{c} \mathbf{x} \longrightarrow \text{[Human Icon]} \longrightarrow \mathbf{y} \\ \text{prompt} \qquad \qquad \qquad \text{response} \end{array} \quad \longrightarrow \quad \mathcal{L}_{\text{sft}}(\pi_{\theta}) = \mathbb{E}_{(\mathbf{x}, \mathbf{y}) \sim \mathcal{D}^{\text{sft}}} \left[-\log \pi_{\theta}(\mathbf{y}|\mathbf{x}) \right]$$

◆ RM stage: Reward Modeling

$$\begin{array}{c} \mathbf{x} \quad \mathbf{y}_1, \dots, \mathbf{y}_n \longrightarrow \text{[Human Icon]} \longrightarrow \mathbf{y}_w > \mathbf{y}_l \\ \text{prompt} \quad \text{responses} \qquad \qquad \qquad \text{preference} \end{array} \quad \longrightarrow \quad \mathcal{L}_r(r_{\phi}) = \mathbb{E}_{(\mathbf{x}, \mathbf{y}_w, \mathbf{y}_l) \sim \mathcal{D}^{\text{pref}}} \left[-\log \frac{e^{r_{\phi}(\mathbf{x}, \mathbf{y}_w)}}{e^{r_{\phi}(\mathbf{x}, \mathbf{y}_w)} + e^{r_{\phi}(\mathbf{x}, \mathbf{y}_l)}} \right]$$

◆ Alignment stage: Learning with (proxy) Human Feedback

$$\mathcal{J}_{\text{hf}}^{\beta}(\pi_{\theta}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\underbrace{\mathbb{E}_{\pi_{\theta}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})]}_{\text{Reward model (from RM stage)}} - \beta \mathbb{D}_{\text{KL}}[\pi_{\theta}(\mathbf{y}|\mathbf{x}) \parallel \underbrace{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})}_{\text{SFT policy (from SFT stage)}}] \right)$$

Introduction



- ◉ Reinforcement Learning from Human Feedback (RLHF) [Ouyang et al., 2022]:
 - ◆ PPO: Framing as **KL-regularized reward maximization** and solved by RL.

$$\mathcal{J}_{\text{hf}}^{\beta}(\pi_{\theta}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\mathbb{E}_{\pi_{\theta}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})] - \beta \mathbb{D}_{\text{KL}}[\pi_{\theta}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})] \right)$$

Introduction



- ◉ Reinforcement Learning from Human Feedback (RLHF) [Ouyang et al., 2022]:
 - ◆ PPO: Framing as **KL-regularized reward maximization** and solved by RL.

$$\mathcal{J}_{\text{hf}}^{\beta}(\pi_{\theta}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\underbrace{\mathbb{E}_{\pi_{\theta}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})] - \beta \mathbb{D}_{\text{KL}}[\pi_{\theta}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})]}_{R(\mathbf{x}, \mathbf{y}) = r_{\phi}(\mathbf{x}, \mathbf{y}) - \beta \log \frac{\pi_{\theta}(\mathbf{y}|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})}} \right)$$

Introduction



⊙ Reinforcement Learning from Human Feedback (RLHF) [Ouyang et al., 2022]:

◆ PPO: Framing as **KL-regularized reward maximization** and solved by RL.

$$\mathcal{J}_{\text{lhf}}^{\beta}(\pi_{\theta}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\underbrace{\mathbb{E}_{\pi_{\theta}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})] - \beta \mathbb{D}_{\text{KL}}[\pi_{\theta}(\mathbf{y}|\mathbf{x}) \| \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})]}_{R(\mathbf{x}, \mathbf{y}) = r_{\phi}(\mathbf{x}, \mathbf{y}) - \beta \log \frac{\pi_{\theta}(\mathbf{y}|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})}} \right)$$

$$\nabla_{\theta} \mathcal{J}_{\text{lhf}}^{\beta}(\pi_{\theta}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}, \mathbf{y} \sim \pi_{\theta}(\mathbf{y}|\mathbf{x})} [R(\mathbf{x}, \mathbf{y}) \nabla_{\theta} \log \pi_{\theta}(\mathbf{y}|\mathbf{x})]$$

Policy gradient method, e.g., PPO [Schulman et al., 2017]

Introduction



◉ Reinforcement Learning from Human Feedback (RLHF) [Ouyang et al., 2022]:

◆ PPO: Framing as **KL-regularized reward maximization** and solved by RL.

$$\mathcal{J}_{\text{lhf}}^{\beta}(\pi_{\theta}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\underbrace{\mathbb{E}_{\pi_{\theta}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})] - \beta \mathbb{D}_{\text{KL}}[\pi_{\theta}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})]}_{R(\mathbf{x}, \mathbf{y}) = r_{\phi}(\mathbf{x}, \mathbf{y}) - \beta \log \frac{\pi_{\theta}(\mathbf{y}|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})}} \right)$$

$$\nabla_{\theta} \mathcal{J}_{\text{lhf}}^{\beta}(\pi_{\theta}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}, \mathbf{y} \sim \pi_{\theta}(\mathbf{y}|\mathbf{x})} [R(\mathbf{x}, \mathbf{y}) \nabla_{\theta} \log \pi_{\theta}(\mathbf{y}|\mathbf{x})]$$

Policy gradient method, e.g., PPO [Schulman et al., 2017]

RL has **high variance** in policy gradient estimation
RL needs to **sample in training loop** } **Inefficiency of convergence**

Introduction



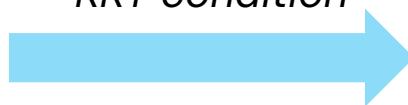
◉ Direct Preference Optimization (DPO) [Rafailov et al., 2023]:

◆ **Key intuition:** Policy optimization as reward modeling.

$$\mathcal{J}_{\text{hf}}^{\beta}(\pi_{\theta})$$

Alignment objective

KKT condition



$$\pi_{\beta}^{*}(\mathbf{y}|\mathbf{x}) = \pi_{\text{sft}}(\mathbf{y}|\mathbf{x}) \frac{e^{\frac{1}{\beta} r_{\phi}(\mathbf{x}, \mathbf{y})}}{Z_{\beta}(\mathbf{x})}$$

Analytic solution of maximizing $\mathcal{J}_{\text{hf}}^{\beta}(\pi_{\theta})$



Simple algebra

$$r_{\phi}(\mathbf{x}, \mathbf{y}) = \beta \log \frac{\pi_{\beta}^{*}(\mathbf{y}|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} + \beta \log Z_{\beta}(\mathbf{x})$$

Reward model as a function of π_{β}^{*}

BT model



$$\mathcal{L}_{\text{dpo}}(\pi_{\theta}) = \mathbb{E}_{(\mathbf{x}, \mathbf{y}_w, \mathbf{y}_l) \sim \mathcal{D}^{\text{pref}}} \left[-\log \sigma \left(\beta \log \frac{\pi_{\theta}(\mathbf{y}_w|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}_w|\mathbf{x})} - \beta \log \frac{\pi_{\theta}(\mathbf{y}_l|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}_l|\mathbf{x})} \right) \right]$$

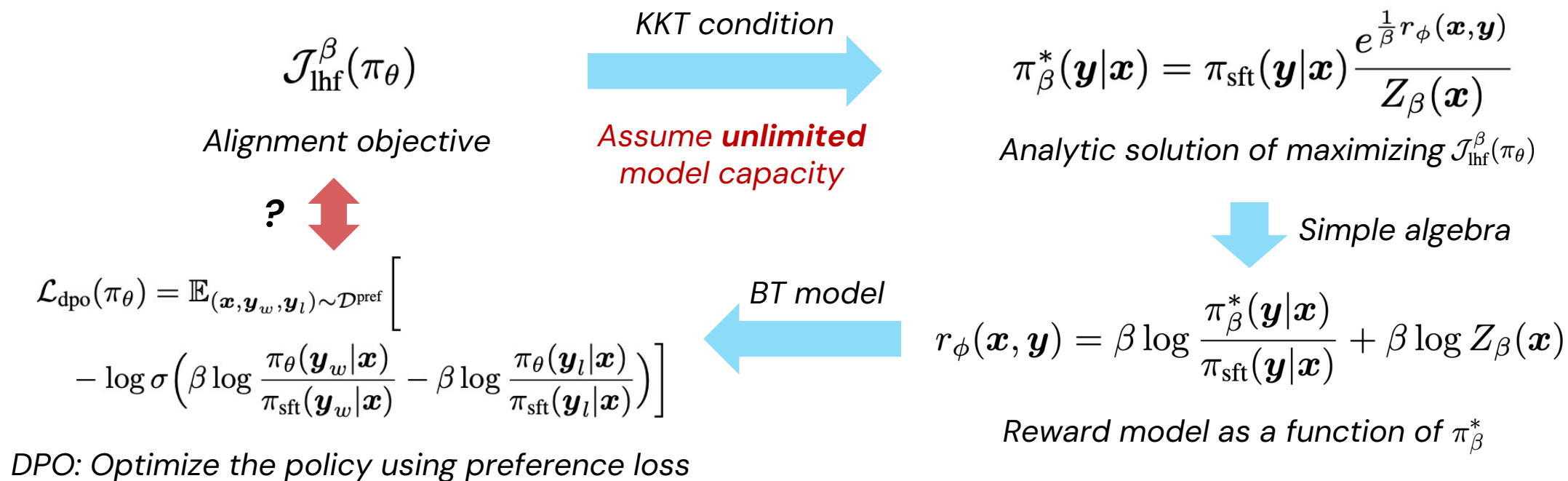
DPO: Optimize the policy using preference loss

Introduction



◉ *Direct Preference Optimization (DPO)* [Rafailov et al., 2023]:

◆ **Key intuition:** Policy optimization as reward modeling.



◆ DPO is **not exactly** optimizing the alignment objective.

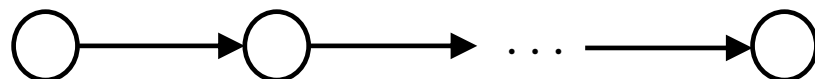
Introduction



- ⊙ *Practical constraint: The expressivity gap between π_θ and π_β^**

Local-normalization

$$\pi_\theta(\mathbf{y}|\mathbf{x}) = \pi_\theta(y_1|\mathbf{x}) \pi_\theta(y_2|\mathbf{x}, y_1) \cdots \pi_\theta(y_n|\mathbf{x}, y_1, \dots, y_{n-1})$$



Auto-Regressive Model (ARM)

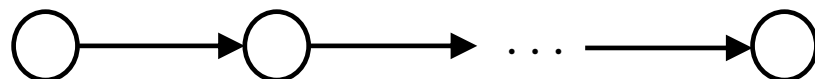
Introduction



- Practical constraint: The expressivity gap between π_θ and π_β^*

Local-normalization

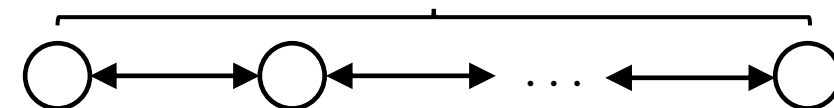
$$\pi_\theta(\mathbf{y}|\mathbf{x}) = \pi_\theta(y_1|\mathbf{x}) \pi_\theta(y_2|\mathbf{x}, y_1) \cdots \pi_\theta(y_n|\mathbf{x}, y_1, \dots, y_{n-1})$$



Auto-Regressive Model (ARM)

Global-normalization

$$\pi_\beta^*(\mathbf{y}|\mathbf{x}) \propto \exp \left[\beta^{-1} r_\phi(\mathbf{x}, y_1, y_2, \dots, y_n) \right]$$



Energy-Based Model (EBM)

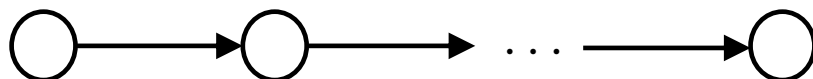
Introduction



- Practical constraint: The expressivity gap between π_θ and π_β^*

Local-normalization

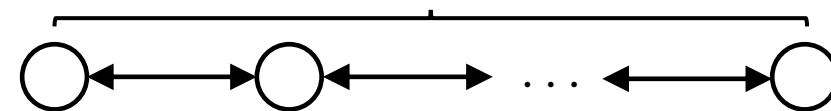
$$\pi_\theta(\mathbf{y}|\mathbf{x}) = \pi_\theta(y_1|\mathbf{x}) \pi_\theta(y_2|\mathbf{x}, y_1) \cdots \pi_\theta(y_n|\mathbf{x}, y_1, \dots, y_{n-1})$$



Auto-Regressive Model (ARM)

Global-normalization

$$\pi_\beta^*(\mathbf{y}|\mathbf{x}) \propto \exp \left[\beta^{-1} r_\phi(\mathbf{x}, y_1, y_2, \dots, y_n) \right]$$



Energy-Based Model (EBM)

Pros: Efficient sampling in $O(\text{Poly}(n))$ time

Cons: Assume AR factorization of $\text{Prob}(\text{sequence})$

Pros: No assumption on modeling $\text{Prob}(\text{sequence})$

Cons: Inefficient sampling in $O(\text{Superpoly}(n))$

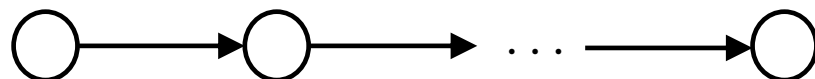
Introduction



- Practical constraint: The expressivity gap between π_θ and π_β^*

Local-normalization

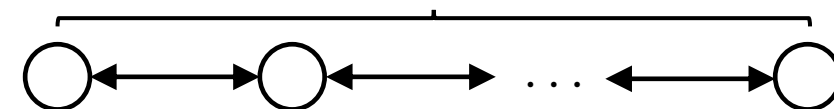
$$\pi_\theta(\mathbf{y}|\mathbf{x}) = \pi_\theta(y_1|\mathbf{x}) \pi_\theta(y_2|\mathbf{x}, y_1) \cdots \pi_\theta(y_n|\mathbf{x}, y_1, \dots, y_{n-1})$$



Auto-Regressive Model (ARM)

Global-normalization

$$\pi_\beta^*(\mathbf{y}|\mathbf{x}) \propto \exp \left[\beta^{-1} r_\phi(\mathbf{x}, y_1, y_2, \dots, y_n) \right]$$



Energy-Based Model (EBM)

Pros: Efficient sampling in $O(\text{Poly}(n))$ time

Cons: Assume AR factorization of $\text{Prob}(\text{sequence})$

Pros: No assumption on modeling $\text{Prob}(\text{sequence})$

Cons: Inefficient sampling in $O(\text{Superpoly}(n))$

- Theoretical justification [Lin et al., 2021]:

- There are some “hard” sequences whose unnormalized scores are easy to compute, yet the conditional local probabilities are **intractable**.
- ARMs **cannot perfectly** capture all EBM distributions with $O(\text{Poly}(n))$ -sized parameters.

Introduction



⊙ What does the solution of RLHF look like under this practical constraint?

◆ KL-regularized RL as probability matching [Korbak et al., 2021].

$$\mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\mathbb{E}_{\pi_{\theta}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})] - \beta \mathbb{D}_{\text{KL}}[\pi_{\theta}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})] \right) \overset{\text{equivalent}}{\longleftrightarrow} \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left[\mathbb{D}_{\text{KL}}(\pi_{\theta}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\beta_r}^*(\mathbf{y}|\mathbf{x})) \right]$$

Maximize reward with KL penalty *Minimize reverse KL divergence*

Introduction



What does the solution of RLHF look like under this practical constraint?

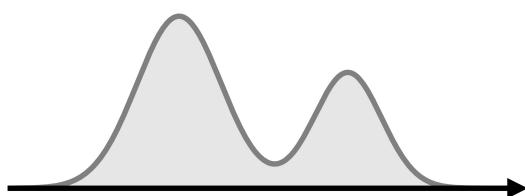
◆ KL-regularized RL as probability matching [Korbak et al., 2021].

$$\mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\mathbb{E}_{\pi_{\theta}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})] - \beta \mathbb{D}_{\text{KL}}[\pi_{\theta}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})] \right) \overset{\text{equivalent}}{\longleftrightarrow} \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left[\mathbb{D}_{\text{KL}}(\pi_{\theta}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\beta_r}^*(\mathbf{y}|\mathbf{x})) \right]$$

Maximize reward with KL penalty
Minimize reverse KL divergence

◆ The asymmetry of KL divergence:

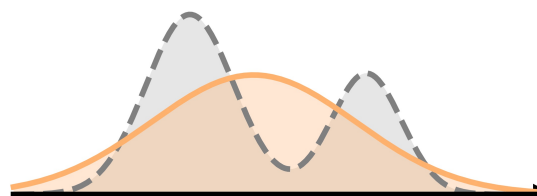
- Estimate the density of p



Target distribution $p(x)$

Forward KL

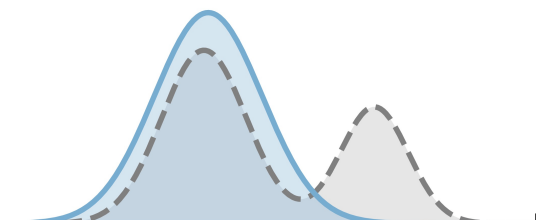
$$\mathbb{D}_{\text{KL}}(p \parallel \hat{p}) = \mathbb{E}_{x \sim p} \left[\log \frac{p(x)}{\hat{p}(x)} \right]$$



Mean-seeking solution

Reverse KL

$$\mathbb{D}_{\text{KL}}(\hat{p} \parallel p) = \mathbb{E}_{x \sim \hat{p}} \left[\log \frac{\hat{p}(x)}{p(x)} \right]$$



Mode-seeking solution

Method



- ◉ **Key motivation:** Policy optimization as probability matching.
- ◉ Without loss of generality, consider the generalized alignment objective:

$$\mathcal{J}_{\text{hf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\mathbb{E}_{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})] - \beta_r \mathbb{D}_{\text{KL}}[\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})] \right)$$

Method



- ◉ **Key motivation:** Policy optimization as probability matching.
- ◉ Without loss of generality, consider the generalized alignment objective:

$$\mathcal{J}_{\text{hf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\mathbb{E}_{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})] - \beta_r \mathbb{D}_{\text{KL}}[\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})] \right)$$

- ◆ $\pi_{\theta}^{\beta_{\pi}}$ is the geometric mean of π_{θ} and π_{sft}

$$\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x}) \propto \pi_{\theta}(\mathbf{y}|\mathbf{x})^{\beta_{\pi}} \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})^{1-\beta_{\pi}}$$

- ◉ **Key motivation:** Policy optimization as probability matching.
- ◉ Without loss of generality, consider the generalized alignment objective:

$$\mathcal{J}_{\text{hf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \left(\mathbb{E}_{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})} [r_{\phi}(\mathbf{x}, \mathbf{y})] - \beta_r \mathbb{D}_{\text{KL}}[\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})] \right)$$

- ◆ $\pi_{\theta}^{\beta_{\pi}}$ is the geometric mean of π_{θ} and π_{sft}

$$\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x}) \propto \pi_{\theta}(\mathbf{y}|\mathbf{x})^{\beta_{\pi}} \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})^{1-\beta_{\pi}}$$

- ◆ Decompose the KL regularization

$$\beta = \beta_r \cdot \beta_{\pi}$$

regularize reward regularize policy

- ◆ Analytic solution is also π_{β}^* .

- ◆ Unify the regularization setting of PPO ($\beta_{\pi} = 1, \beta_r = \beta$) and DPO ($\beta_{\pi} = \beta, \beta_r = 1$)

- Deriving the probability matching objective of $\mathcal{J}_{\text{hf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})} \left[\log \frac{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})}{\pi_{\beta_r}^*(\mathbf{y}|\mathbf{x})} \right]$$

- Calculating reverse KL requires sampling from $\pi_{\theta}^{\beta_{\pi}}$, which prohibits straightforward back propagation.

- Deriving the probability matching objective of $\mathcal{J}_{\text{lhf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})} \left[\log \frac{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})}{\pi_{\beta_r}^*(\mathbf{y}|\mathbf{x})} \right]$$



Importance Sampling (IS)
 π_{sft} as the proposal distribution

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[\frac{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \log \frac{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})}{\pi_{\beta_r}^*(\mathbf{y}|\mathbf{x})} \right]$$

- Deriving the probability matching objective of $\mathcal{J}_{\text{lhf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})} \left[\log \frac{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})}{\pi_{\beta_r}^*(\mathbf{y}|\mathbf{x})} \right]$$



Importance Sampling (IS)
 π_{sft} as the proposal distribution

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[\frac{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \log \frac{\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x})}{\pi_{\beta_r}^*(\mathbf{y}|\mathbf{x})} \right]$$



Define $f_{\theta}(\mathbf{x}, \mathbf{y}) = \log \pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x}) - \log \pi_{\text{sft}}(\mathbf{y}|\mathbf{x})$
as the log policy ratio

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[e^{f_{\theta}(\mathbf{x}, \mathbf{y})} \log \frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y})}}{\frac{1}{Z_{\beta_r}(\mathbf{x})} e^{\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r}}} \right]$$

Method



- Deriving the probability matching objective of $\mathcal{J}_{\text{hf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[e^{f_{\theta}(\mathbf{x}, \mathbf{y})} \log \frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y})}}{\frac{1}{Z_{\beta_r}(\mathbf{x})} e^{\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r}}} \right]$$

- The partition function $Z_{\beta_r}(\mathbf{x})$ is intractable.

- Deriving the probability matching objective of $\mathcal{J}_{\text{lhf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[e^{f_{\theta}(\mathbf{x}, \mathbf{y})} \log \frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y})}}{\frac{1}{Z_{\beta_r}(\mathbf{x})} e^{\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r}}} \right]$$

- The partition function $Z_{\beta_r}(\mathbf{x})$ is intractable.
- Inspiration from Self-Normalized Importance Sampling (SNIS)
 - Estimate $\mathbb{E}_{x \sim p}[f(x)]$ where we can only compute the **unnormalized** $P(x)$

- Deriving the probability matching objective of $\mathcal{J}_{\text{lhf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[e^{f_{\theta}(\mathbf{x}, \mathbf{y})} \log \frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y})}}{\frac{1}{Z_{\beta_r}(\mathbf{x})} e^{\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r}}} \right]$$

- The partition function $Z_{\beta_r}(\mathbf{x})$ is intractable.
- Inspiration from Self-Normalized Importance Sampling (SNIS)
 - Estimate $\mathbb{E}_{x \sim p}[f(x)]$ where we can only compute the **unnormalized** $P(x)$

$$\mathbb{E}_{x \sim p}[f(x)] = \sum_x p(x) f(x)$$

$$p(x) = \frac{P(x)}{\sum_x P(x)} \quad \downarrow \quad \rightarrow \quad \frac{\sum_x P(x) f(x)}{\sum_x P(x)} = \frac{\mathbb{E}_q \left[\frac{P(x)}{q(x)} f(x) \right]}{\mathbb{E}_q \left[\frac{P(x)}{q(x)} \right]} \quad \rightarrow \quad \mathbb{E}_{x \sim p}[f(x)] = \lim_{N \rightarrow \infty} \frac{\sum_{i=1}^N \frac{P(x_i)}{q(x_i)} f(x_i)}{\sum_{i=1}^N \frac{P(x_i)}{q(x_i)}}$$

$$\mathbb{E}_{x \sim p}[f(x)] = \frac{\sum_x P(x) f(x)}{\sum_x P(x)}$$

where $x_1, \dots, x_N \sim q$ are i.i.d. samples

- Deriving the probability matching objective of $\mathcal{J}_{\text{hf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[e^{f_{\theta}(\mathbf{x}, \mathbf{y})} \log \frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y})}}{\frac{1}{Z_{\beta_r}(\mathbf{x})} e^{\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r}}} \right]$$
$$Z_{\beta_r}(\mathbf{x}) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[\exp\left(\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r}\right) \right]$$

- Deriving the probability matching objective of $\mathcal{J}_{\text{lhf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[e^{f_{\theta}(\mathbf{x}, \mathbf{y})} \log \frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y})}}{\frac{1}{Z_{\beta_r}(\mathbf{x})} e^{\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r}}} \right]$$

$$Z_{\beta_r}(\mathbf{x}) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} [\exp(\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r})]$$

- Sample K i.i.d. continuations $\mathbf{y}_{1:K} = \{\mathbf{y}_1, \dots, \mathbf{y}_K\}$ from $\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \lim_{K \rightarrow \infty} \sum_{k=1}^K \frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y}_k)}}{\sum_{j=1}^K e^{f_{\theta}(\mathbf{x}, \mathbf{y}_j)}} \log \frac{\frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y}_k)}}{\sum_{j=1}^K e^{f_{\theta}(\mathbf{x}, \mathbf{y}_j)}}}{\frac{e^{\frac{1}{\beta_r} r_{\phi}(\mathbf{x}, \mathbf{y}_k)}}{\sum_{j=1}^K \frac{1}{\beta_r} e^{r_{\phi}(\mathbf{x}, \mathbf{y}_j)}}}$$

Distribution of log policy ratio

Distribution of reward model

- Deriving the probability matching objective of $\mathcal{J}_{\text{lhf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} \left[e^{f_{\theta}(\mathbf{x}, \mathbf{y})} \log \frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y})}}{\frac{1}{Z_{\beta_r}(\mathbf{x})} e^{\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r}}} \right]$$
$$Z_{\beta_r}(\mathbf{x}) = \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})} [\exp(\frac{r_{\phi}(\mathbf{x}, \mathbf{y})}{\beta_r})]$$

- Sample K i.i.d. continuations $\mathbf{y}_{1:K} = \{\mathbf{y}_1, \dots, \mathbf{y}_K\}$ from $\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})$

$$\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}} \parallel \pi_{\beta_r}^*) = \lim_{K \rightarrow \infty} \sum_{k=1}^K \frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y}_k)}}{\sum_{j=1}^K e^{f_{\theta}(\mathbf{x}, \mathbf{y}_j)}} \log \frac{\frac{e^{f_{\theta}(\mathbf{x}, \mathbf{y}_k)}}{\sum_{j=1}^K e^{f_{\theta}(\mathbf{x}, \mathbf{y}_j)}}}{\frac{e^{\frac{1}{\beta_r} r_{\phi}(\mathbf{x}, \mathbf{y}_k)}}{\sum_{j=1}^K \frac{1}{\beta_r} e^{r_{\phi}(\mathbf{x}, \mathbf{y}_j)}}}$$

Reverse KL $\mathbb{D}_{\text{KL}}(p_{f_{\theta}} \parallel p_{r_{\phi}})$ of $p_{f_{\theta}}$ and $p_{r_{\phi}}$

- ◉ Introduce the Efficient Exact Optimization (**EXO**) objective of alignment

- ◆ **Learning from the reward model**

$$\mathcal{L}_{\text{exo}}(\pi_{\theta}) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}_{1:K} | \mathbf{x})} \left[\mathbb{D}_{\text{KL}}(p_{f_{\theta}}(\cdot | \mathbf{y}_{1:K}, \mathbf{x}) \| p_{r_{\phi}}(\cdot | \mathbf{y}_{1:K}, \mathbf{x})) \right]$$

- Where we define: *regularize policy*

$$p_{f_{\theta}}(i | \mathbf{y}_{1:K}, \mathbf{x}) = \frac{e^{\beta_{\pi} \log \frac{\pi_{\theta}(\mathbf{y}_i | \mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}_i | \mathbf{x})}}}{\sum_{j=1}^K e^{\beta_{\pi} \log \frac{\pi_{\theta}(\mathbf{y}_j | \mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}_j | \mathbf{x})}}}$$

regularize reward

$$p_{r_{\phi}}(i | \mathbf{y}_{1:K}, \mathbf{x}) = \frac{e^{\frac{1}{\beta_r} r_{\phi}(\mathbf{x}, \mathbf{y}_i)}}{\sum_{j=1}^K e^{\frac{1}{\beta_r} r_{\phi}(\mathbf{x}, \mathbf{y}_j)}}$$

- ◆ **Learning from the preference data ($K=2$)**

$$\mathcal{L}_{\text{exo-pref}}(\pi_{\theta}) = \mathbb{E}_{(\mathbf{x}, \mathbf{y}_w, \mathbf{y}_l) \sim \mathcal{D}^{\text{pref}}} \left[\mathbb{D}_{\text{KL}}(p_{f_{\theta}}(\cdot | \mathbf{y}_w, \mathbf{y}_l, \mathbf{x}) \| p_{r_h}(\cdot | \mathbf{y}_w, \mathbf{y}_l, \mathbf{x})) \right]$$

- Where the preference probability $p_{r_h}(\cdot | \mathbf{y}_w, \mathbf{y}_l, \mathbf{x})$ is a label-smoothed one-hot distribution.

◉ Justification of exactness

- ◆ The gradient of EXO aligns with the gradient of the generalized alignment objective and the reverse KL asymptotically for policy with **arbitrary** θ when $K \rightarrow \infty$.

$$\begin{aligned}\nabla_{\theta} \mathcal{L}_{\text{exo}}(\pi_{\theta}) &= \nabla_{\theta} \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} [\mathbb{D}_{\text{KL}}(\pi_{\theta}^{\beta_{\pi}}(\mathbf{y}|\mathbf{x}) \parallel \pi_{\beta_r}^*(\mathbf{y}|\mathbf{x}))] \\ &= -\frac{1}{\beta_r} \nabla_{\theta} \mathcal{J}_{\text{lhf}}^{\beta_r}(\pi_{\theta}^{\beta_{\pi}}).\end{aligned}$$

- ◆ EXO reaches the same **mode-seeking** solution as RLHF.
- ◆ In practice, EXO converges effectively and efficiently with finite K (will be shown later empirically).

Comparison with DPO



Generalizing DPO:

- ◆ Sample K completions $\mathbf{y}_{1:K} = \{\mathbf{y}_1, \dots, \mathbf{y}_K\}$ from $\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})$
- ◆ Substitute hard human preference with soft distribution defined by reward model

$$\mathcal{L}_{\text{dpo-rw}}(\pi_\theta) = \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} \mathbb{E}_{\pi_{\text{sft}}(\mathbf{y}_{1:K}|\mathbf{x})} \left[- \sum_{i=1}^K \frac{e^{\frac{1}{\beta_r} r_\phi(\mathbf{x}, \mathbf{y}_i)}}{\sum_{j=1}^K e^{\frac{1}{\beta_r} r_\phi(\mathbf{x}, \mathbf{y}_j)}} \log \frac{e^{\beta_\pi \log \frac{\pi_\theta(\mathbf{y}_i|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}_i|\mathbf{x})}}}{\sum_{j=1}^K e^{\beta_\pi \log \frac{\pi_\theta(\mathbf{y}_j|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}_j|\mathbf{x})}} \right]$$

Forward KL $\mathbb{D}_{\text{KL}}(p_{f_\theta} || p_{r_\phi})$ of p_{f_θ} and p_{r_ϕ} (up to a constant)

- ◆ The gradient of DPO-rw aligns with the gradient of the forward KL asymptotically for policy with **arbitrary** θ when $K \rightarrow \infty$.

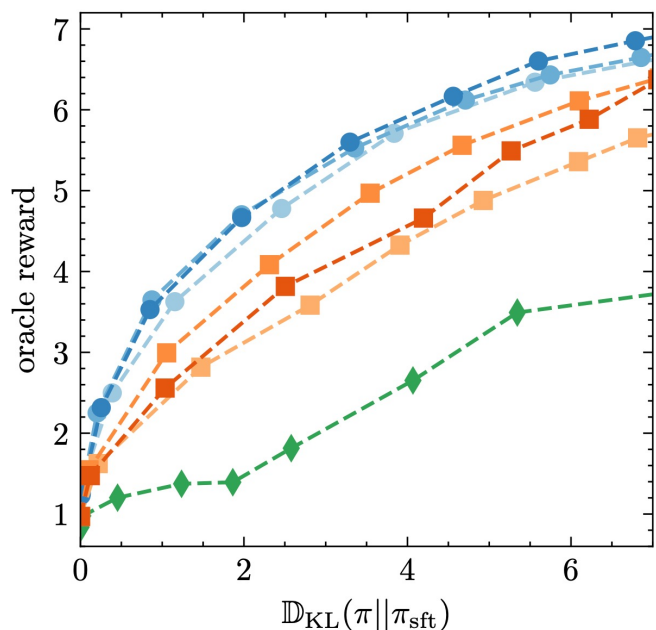
$$\nabla_\theta \mathcal{L}_{\text{dpo-rw}}(\pi_\theta) = \nabla_\theta \mathbb{E}_{\mathbf{x} \sim \mathcal{D}^{\text{pref}}} [\mathbb{D}_{\text{KL}}(\pi_{\beta_r}^*(\mathbf{y}|\mathbf{x}) || \pi_\theta^{\beta_\pi}(\mathbf{y}|\mathbf{x}))]$$

- **Inexactness:** DPO minimizes the forward KL, while RLHF, e.g., PPO minimizes the reverse KL.

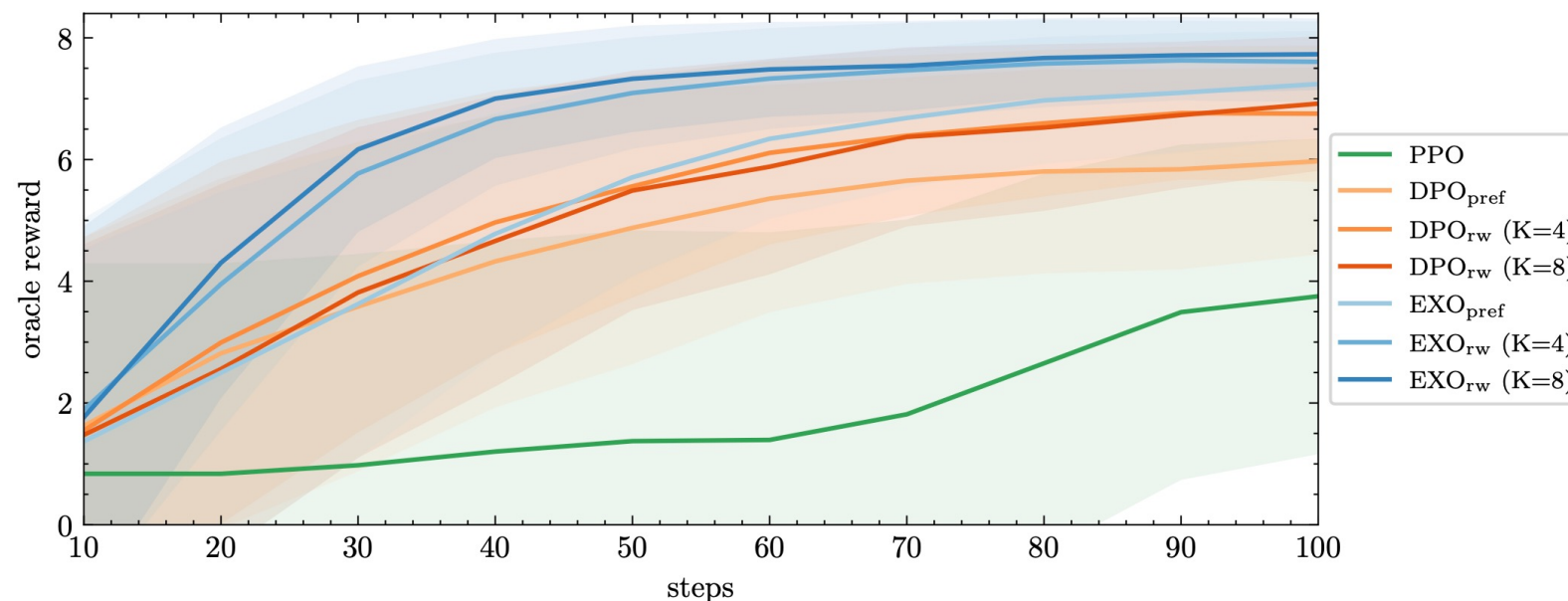
Experiments



- Synthetic experiment: Generate IMDB review with positive sentiment
 - ◆ Oracle reward (Human labeler): Classifier trained on IMDB review classification dataset



Oracle reward vs KL



Oracle reward vs Training steps

Experiments

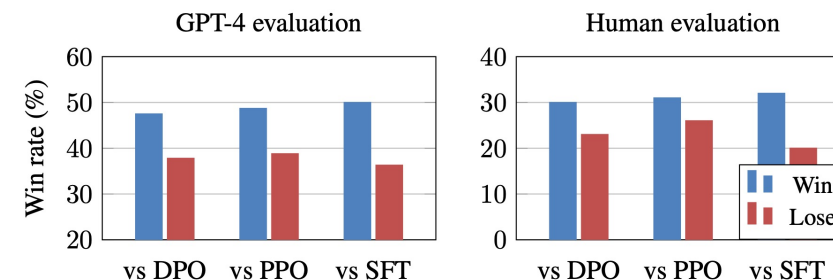


Alignment on real human preferences:

- ◆ Text summarization: TL;DR preference dataset
- ◆ Dialogue generation: Anthropic-HH dataset (helpfulness subset)
- ◆ Instruction following: Filtered real user query from an online API

Method	Reward Model (%)		GPT-4 (%)	
	vs SFT	vs Chosen	vs SFT	vs Chosen
w/ Preferences				
DPO _{pref}	68.3	23.7	57.0	30.5
EXO_{pref}	92.5	60.1	83.0	55.0
w/ Reward Model				
Best-of- <i>N</i>	99.3	75.8	83.5	60.0
PPO	93.2	58.3	77.0	52.0
DPO _{rw}	82.7	39.8	70.0	41.0
EXO_{rw}	97.3	76.4	88.5	64.0

Method	Reward Model (%)		GPT-4 (%)	
	vs SFT	vs Chosen	vs SFT	vs Chosen
w/ Preferences				
DPO _{pref}	66.3	65.1	58.0	37.0
EXO_{pref}	76.4	76.7	73.0	51.0
w/ Reward Model				
Best-of- <i>N</i>	94.6	98.2	86.0	63.0
PPO	75.0	74.0	66.5	52.0
DPO _{rw}	79.9	81.3	75.5	49.0
EXO_{rw}	85.6	87.2	83.5	60.0



- ◆ Outperforms DPO and PPO in both settings of learning from preferences & reward model.
- ◆ On par with Best-of-*N* (*N*=128) but much more computationally efficient in inference.
- ◆ Scaling to realistic instruction-following dataset with consistent improvement.

Experiments



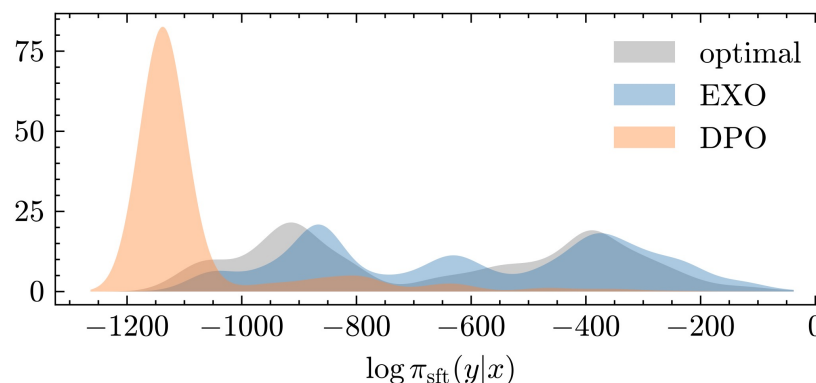
○ Visualization: Compare the density of DPO and EXO with the optimal policy

◆ Given a test prompt **“This Fox spectacle was a big hit when released in ”**

◆ Estimate the empirical policy distribution of π_θ and π_β^* by SNIS:

$$\hat{\pi}_\theta(\mathbf{y}_i|\mathbf{x}) = \frac{M\pi_\theta(\mathbf{y}_i|\mathbf{x})}{\sum_{j=1}^M \pi_\theta(\mathbf{y}_j|\mathbf{x})/\pi_{\text{sft}}(\mathbf{y}_j|\mathbf{x})} \quad \hat{\pi}_\beta^*(\mathbf{y}_i|\mathbf{x}) = \frac{M\pi_{\text{sft}}(\mathbf{y}_i|\mathbf{x}) \exp(r(\mathbf{x}, \mathbf{y}_i)/\beta)}{\sum_{j=1}^M \exp(r(\mathbf{x}, \mathbf{y}_j)/\beta)}$$

◆ Use Kernel Density Estimation to estimate the density and plot the ratio $\rho_{\hat{\pi}}(\mathbf{y}|\mathbf{x}) = \frac{\hat{\pi}(\mathbf{y}|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})}$



Experiments

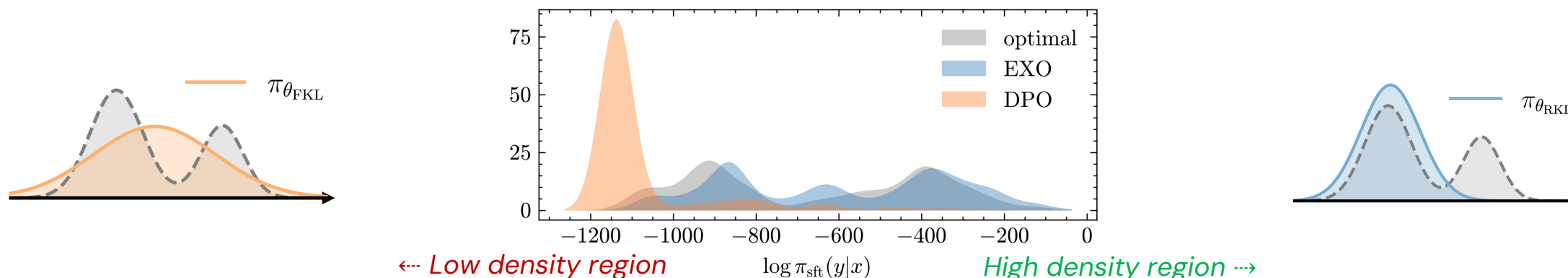


Visualization: Compare the density of DPO and EXO with the optimal policy

- Given a test prompt **"This Fox spectacle was a big hit when released in "**
- Estimate the empirical policy distribution of π_θ and π_β^* by SNIS:

$$\hat{\pi}_\theta(\mathbf{y}_i|\mathbf{x}) = \frac{M\pi_\theta(\mathbf{y}_i|\mathbf{x})}{\sum_{j=1}^M \pi_\theta(\mathbf{y}_j|\mathbf{x})/\pi_{\text{sft}}(\mathbf{y}_j|\mathbf{x})} \quad \hat{\pi}_\beta^*(\mathbf{y}_i|\mathbf{x}) = \frac{M\pi_{\text{sft}}(\mathbf{y}_i|\mathbf{x}) \exp(r(\mathbf{x}, \mathbf{y}_i)/\beta)}{\sum_{j=1}^M \exp(r(\mathbf{x}, \mathbf{y}_j)/\beta)}$$

- Use Kernel Density Estimation to estimate the density and plot the ratio $\rho_{\hat{\pi}}(\mathbf{y}|\mathbf{x}) = \frac{\hat{\pi}(\mathbf{y}|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})}$



Experiments

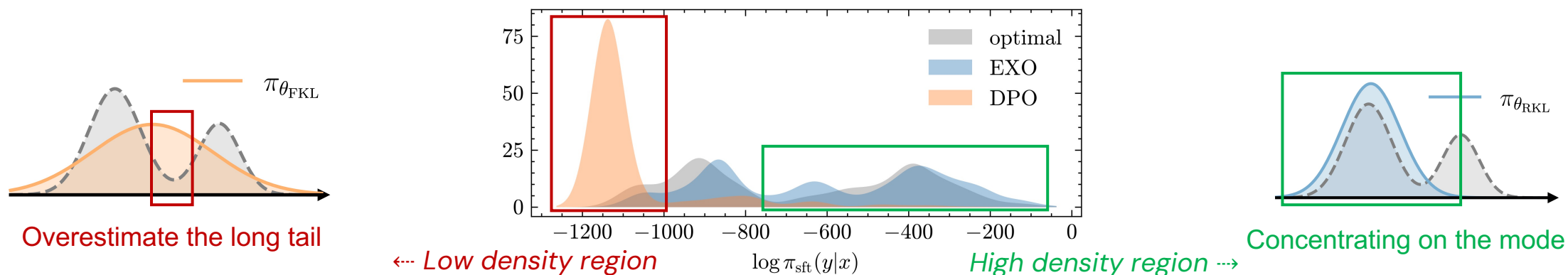


Visualization: Compare the density of DPO and EXO with the optimal policy

- Given a test prompt **"This Fox spectacle was a big hit when released in "**
- Estimate the empirical policy distribution of π_θ and π_β^* by SNIS:

$$\hat{\pi}_\theta(\mathbf{y}_i|\mathbf{x}) = \frac{M\pi_\theta(\mathbf{y}_i|\mathbf{x})}{\sum_{j=1}^M \pi_\theta(\mathbf{y}_j|\mathbf{x})/\pi_{\text{sft}}(\mathbf{y}_j|\mathbf{x})} \quad \hat{\pi}_\beta^*(\mathbf{y}_i|\mathbf{x}) = \frac{M\pi_{\text{sft}}(\mathbf{y}_i|\mathbf{x}) \exp(r(\mathbf{x}, \mathbf{y}_i)/\beta)}{\sum_{j=1}^M \exp(r(\mathbf{x}, \mathbf{y}_j)/\beta)}$$

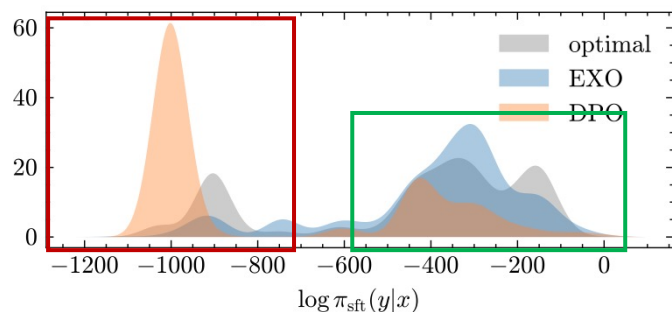
- Use Kernel Density Estimation to estimate the density and plot the ratio $\rho_{\hat{\pi}}(\mathbf{y}|\mathbf{x}) = \frac{\hat{\pi}(\mathbf{y}|\mathbf{x})}{\pi_{\text{sft}}(\mathbf{y}|\mathbf{x})}$



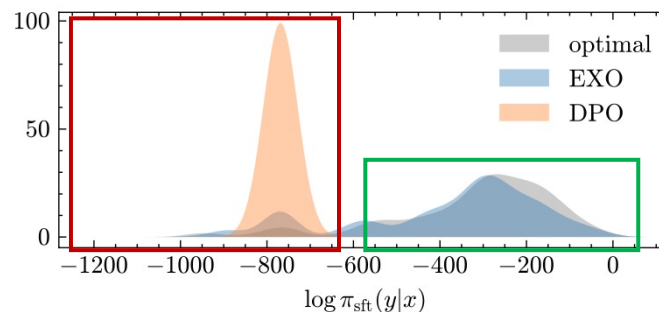
Experiments



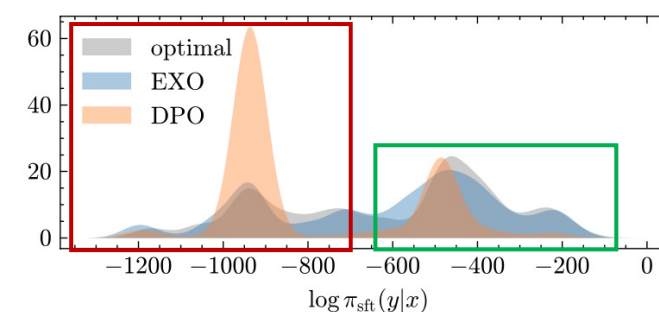
More visualization cases: (prevailing phenomenon, no cherry-picking)



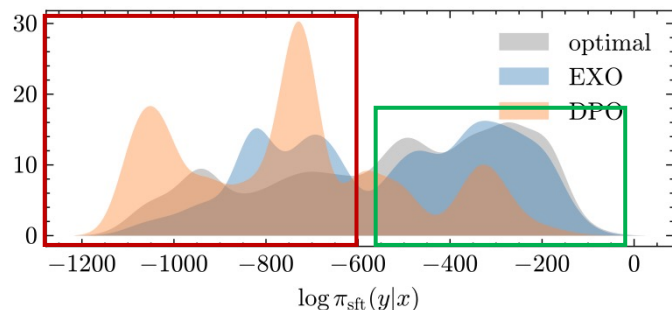
Estimated density ratio of the EXO, DPO and optimal policy given the prompt "Is this supposed to be serious? I hope not".



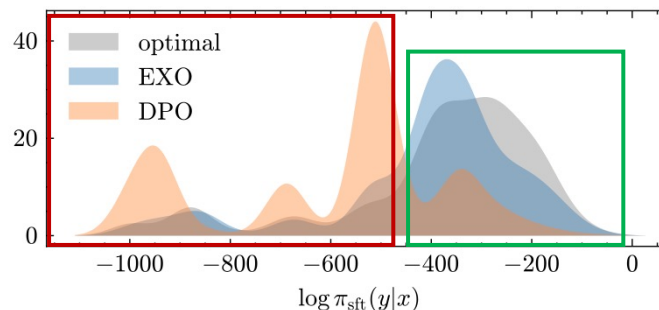
Estimated density ratio of the EXO, DPO and optimal policy given the prompt "Great book, great movie, great soundtrack. Frank".



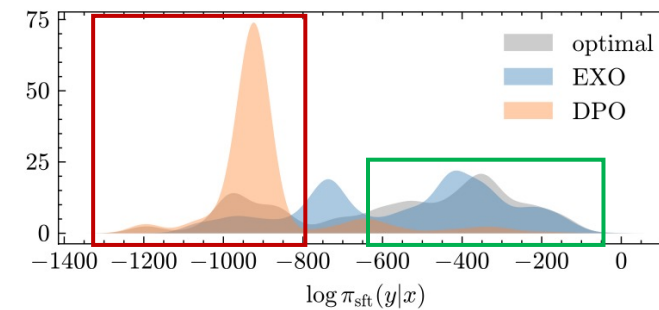
Estimated density ratio of the EXO, DPO and optimal policy given the prompt "What we have here the standard Disney direct to DVD".



Estimated density ratio of the EXO, DPO and optimal policy given the prompt "This is indeed the film that popularized kung".



Estimated density ratio of the EXO, DPO and optimal policy given the prompt "This movie is about a group of people who are".



Estimated density ratio of the EXO, DPO and optimal policy given the prompt "Once the slow beginning gets underway, the film kicks".

Conclusion



- ◉ We unify PPO and DPO under the framework of density estimation, and examine that PPO is actually minimizing the **reverse KL** to the optimal policy; while DPO is minimizing the **forward KL** to the optimal policy.
- ◉ We propose efficient exact optimization (EXO) for language model alignment problem. Specifically, EXO **exactly** optimizes the alignment objective in RLHF, while being **efficient** in optimization by formulating as probability matching.

Q & A

Homepage: <https://haozheji.github.io>

GitHub repo: <https://github.com/haozheji/exact-optimization>

Conversational AI Group of Tsinghua University: <http://coai.cs.tsinghua.edu.cn/>



清华大学
Tsinghua University

