Alignment for Foundation Language Models: Mathematical Principle and Algorithmic Designs

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Why We Need RLHF?

- RLHF: A leading technique to adapt LLMs to being preferred by humans.

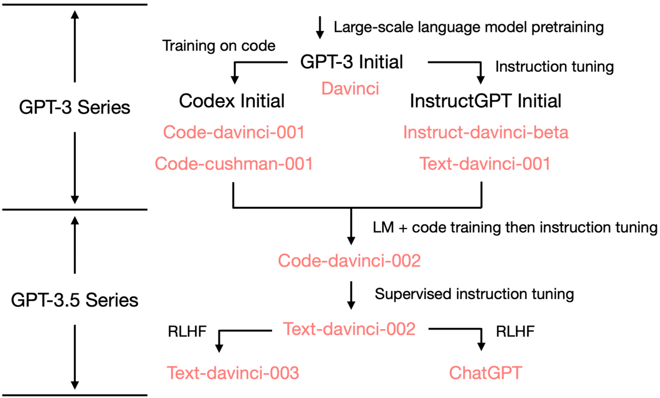


Figure 1: How does GPT Obtain its Ability [FK22]

Training Pipeline

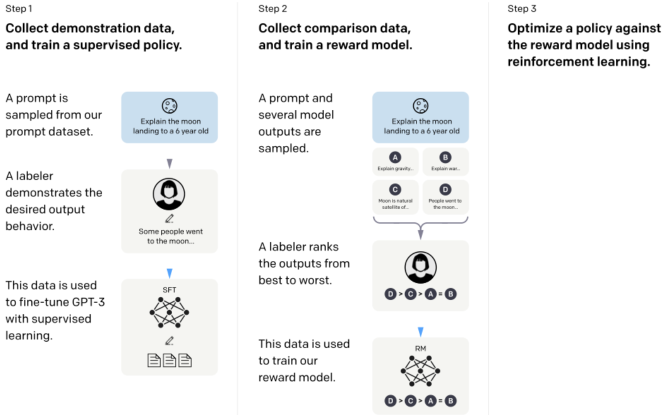


Figure 2: RLHF framework in Instruct-GPT [OWJ+22]

Mathematical Formulation

- Prompt space $\mathcal{X}$: "Human: Can you write a C++ program that prompts the user to enter the name of a country and checks if it borders the Mediterranean Sea? Assistant: ";
- Response space $\mathcal{A}$:
  - A high-quality and correct code ✓
  - A wrong code. ✗
  - "NO, I cannot."
- SFT-policy $\pi_0 : \mathcal{X} \to \Delta(\mathcal{A})$;
- Prompt distribution: $x \sim d_0$.

Mathematical Formulation Continued: Preference Oracle

- Examples: Human, Model from Inverse RL, GPT4 (RLAIF [BKK+22]);
- Goal: making LLM being preferred by $\mathcal{P}$ while stay close to π_0.
  - Fundamental issue: $\mathcal{P}$ is never perfect and can be hacked;
  - Training stability issue;

Definition 1 (General Preference Oracle)

There exists a preference oracle $\mathcal{P} : \mathcal{X} \times \mathcal{A} \times \mathcal{A} \to [0, 1]$, and we can query it to receive the preference signal:

$$y \sim \mathrm{Ber}(\mathcal{P}(a^1 \succ a^2 | x)),$$

where $y = 1$ means a^1 is preferred to a^2, and $y = 0$ means that a^2 is preferred.

RLHF v.s. SFT

SFT	RLHF
Dataset: Prompt+Response positive only	**Dataset:** Prompt+Response Pairs positive & negative
Loss: negative log-likelihood/cross entropy	**Loss:** - Learning reward - Maximize Reward + regularizations
Aim: Approximate the training data distribution	**Aim:** Learning beyond the training datasets, potentially generate better responses than positive data
Components: Generative Model Only	**Components:** Generative Model + Preference Model

Learning in Reward-based RLHF

Mathematical Formulation: Reward-based RLHF

- Implicitly assumes a *total order*: $A \succ B, B \succ C \rightarrow A \succ C$;
- MLE estimation from a preference dataset:

$$\ell_{\mathcal{D}}(\theta) = \sum_{(x,a^1,a^2,y)\in\mathcal{D}} \Big[y \log \Big(\sigma\big(r_\theta(x,a^1) - r_\theta(x,a^2)\big)\Big) + (1-y)\log\Big(\sigma\big(r_\theta(x,a^2) - r_\theta(x,a^1)\big)\Big)\Big]. \tag{1}$$

Definition 2 (Bradley-Terry (BT) model [BT52])

There exists a ground-truth reward function $r^* = r_{\theta^*}$ so that:

$$\mathcal{P}(a^1 \succ a^2 | x) = \frac{\exp(r^*(x,a^1))}{\exp(r^*(x,a^1)) + \exp(r^*(x,a^2))} = \sigma\big(r^*(x,a^1) - r^*(x,a^2)\big).$$

Additionally, we assume that the reward function is parameterized by $r_\theta(x,a) = \langle \theta, \phi(x,a)\rangle$ for feature extractor $\phi : \mathcal{X} \times \mathcal{A} \rightarrow \mathbb{R}^d$.

Reverse-KL Regularized Contextual Bandit [XDY+23]

For iteration t=1,2,...

- A context/prompt $x \sim d_0$;
- An agent selects $a^1, a^2 \in \mathcal{A}$;
- The preference signal y queried from $\mathcal{P}$ is revealed.

Learning objective:

$$\max_{\pi \in \Pi} J(\pi) = \max_{\pi \in \Pi} \mathbb{E}_{x \sim d_0}\Big[\underbrace{\mathbb{E}_{a \sim \pi(\cdot|x)}[r^*(x,a)]}_{\text{Optimize Reward}} - \underbrace{\eta D_{\mathrm{KL}}(\pi(\cdot|x) \| \pi_0(\cdot|x))}_{\text{Stay Close to } \pi_0}\Big].$$

Intractable closed-form Gibbs distribution:

$$\pi^*(a|x) \propto \pi_0(a|x) \exp\Big(\frac{1}{\eta} r^*(x,a)\Big).$$

We assume that we can compute the Gibbs distribution associated with any r by some information-theoretical Oracle $\mathcal{O}(r, \pi_0)$.

Offline Learning: Point-wise Pessimism

Given a pre-collected $\mathcal{D}_{\text{off}} = \{(x, a^1, a^2, y)\}$, we denote r_{MLE} as the MLE estimation on $\mathcal{D}_{\text{off}}$.

Intuition: being conservative at the point with high uncertainty.

- Point-wise confidence interval:

$$\begin{aligned}\underbrace{r_{\mathrm{MLE}}(x,a) - r^*(x,a)}_{\text{Out-of-sample error}} &= \langle \theta_{\mathrm{MLE}} - \theta^*, \phi(x,a)\rangle \\ &\leq \underbrace{\|\theta_{\mathrm{MLE}} - \theta^*\|_{\Sigma_{\mathcal{D}_{\mathrm{off}}}}}_{\text{In-sample error on } \mathcal{D}_{\mathrm{off}} \leq \beta = c\sqrt{d}} \cdot \underbrace{\|\phi(x,a)\|_{\Sigma^{-1}_{\mathcal{D}_{\mathrm{off}}}}}_{\text{Information Ratio}}\end{aligned}$$

- Point-wise pessimism:

$$\hat{\pi} = \mathcal{O}\Big(r_{\mathrm{MLE}}(x,a) - \beta\|\phi(x,a)\|_{\Sigma^{-1}_{\mathcal{D}_{\mathrm{off}}}}, \pi_0\Big).$$

- With high probability, we have

$$J(\pi) - J(\hat{\pi}) \leq 2\beta \cdot \mathbb{E}_{x\sim d_0, a\sim\pi(\cdot|x)}\|\phi(x,a)\|_{\Sigma^{-1}_{\mathcal{D}_{\mathrm{off}}}} - \eta \cdot \mathbb{E}_{x\sim d_0}\big[D_{\mathrm{KL}}(\pi(\cdot|x)\|\hat{\pi}(\cdot|x))\big].$$

Offline Learning: Version-space Pessimism

- Version space $\hat{\Theta}$ consists of θ^* with high probability:

$$\hat{\Theta} := \{\hat{\theta} : \|\theta_{\mathrm{MLE}} - \hat{\theta}\|_{\Sigma_{\mathcal{D}}} \leq \beta = c \cdot \sqrt{d}\}.$$

- Conservative value estimation:

$$\underline{J}(\pi) = \min_{\hat{\theta} \in \hat{\Theta}} \mathbb{E}_{x \sim d_0} \Big[\mathbb{E}_{a \sim \pi(\cdot|x)} [r_{\hat{\theta}}(x, a)] - \eta D_{\mathrm{KL}}(\pi(\cdot|x) \| \pi_0(\cdot|x)) \Big]$$

- Planning: $\hat{\pi} := \mathrm{argmax}_{\pi \in \Pi} \underline{J}(\pi)$, and with high probability,

$$J(\pi) - J(\hat{\pi}) \leq 2\beta \cdot \|\mathbb{E}_{x \sim d_0, a \sim \pi(\cdot|x)}[\phi(x, a)]\|_{\Sigma^{-1}_{\mathcal{D}_{\mathrm{off}}}}.$$

- Compared with point-wise pessimism:
    - Sharper bound due to Jensen's inequality;
    - Lacking general computational guidance.

Offline Learning with Reference Policy

Theorem 3 (Offline Learning with Reference Policy [XDY+23])

If we add a reference in value estimation by:

$$\underline{J}(\pi) = \min_{\hat{\theta}\in\hat{\Theta}} \mathbb{E}_{x\sim d_0}\Big[\mathbb{E}_{a\sim\pi(\cdot|x)}[r_{\hat{\theta}}(x,a)] - \mathbb{E}_{a\sim\pi_{\mathrm{ref}}(\cdot|x)}[r_{\hat{\theta}}(x,a)] - \eta D_{\mathrm{KL}}(\pi(\cdot|x)\|\pi_0(\cdot|x))\Big],$$

it holds that

$$J(\pi) - J(\hat{\pi}) \le c\cdot\sqrt{d}\cdot\|\mathbb{E}_{x\sim d_0}[\phi(x,\pi)] - \mathbb{E}_{x\sim d_0}[\phi(x,\pi_{\mathrm{ref}})]\|_{\Sigma_{\mathrm{off}}^{-1}}.$$

- Robust policy improvement: the resulting $\hat{\pi}$ is never worse than π_{ref} regardless of $\mathcal{D}_{\mathrm{off}}$;
- One common choice of π_{ref} is π_0 [OWJ+22, GSH23].

Online Learning

For iteration $t = 1, 2, \ldots$

- Compute r^t_{MLE} based on $\mathcal{D}^{1:t-1}$;
- The main agent computes $\pi^1_t = \mathcal{O}(r^t_{\mathrm{MLE}}, \pi_0)$;
- The enhancer computes the assistant policy by:

$$\pi^2_t = \mathop{\mathrm{argmax}}_{\pi \in \Pi} \|\phi(x, \pi^1_t) - \phi(x, \pi^2_t)\|_{\Sigma^{-1}_{t,m}}$$

$$\Sigma_{t,m} = \lambda I + \frac{1}{m} \sum_{i=1}^{t-1} \sum_{j=1}^{m} (\phi(x_{i,j}, a^1_{i,j}) - \phi(x_{i,j}, a^2_{i,j}))(\phi(x_{i,j}, a^1_{i,j}) - \phi(x_{i,j}, a^2_{i,j}))^\top.$$

- Collect m comparison pairs by (π^1_t, π^2_t) as $\mathcal{D}^t$.

Intuition: the two policies should be diverse to facilitate exploration.

Online Learning Continued

Theorem 4 (Batch Online Learning Guarantee [XDY+23])

With $m = c_1 \cdot d/\epsilon^2$ and $T = \tilde{\Theta}(d)$, we can find a $\pi^1_{t_0}$ such that

$$J(\pi^*) - J(\pi^1_{t_0}) \lesssim \epsilon - \eta \cdot \mathbb{E}_{x_{t_0} \sim d_0} \Big[D_{\mathrm{KL}}(\pi^*(\cdot|x_{t_0}) \| \pi^1_{t_0}(\cdot|x_{t_0})) \Big] \Big).$$

- Sample complexity scales with the complexity of reward space instance of the generator space;
- Sparse update for $\tilde{\Theta}(d)$ times;
- The techniques extend to regret $\sum_{t=1}^{T} \Big[\frac{2J(\pi^*) - J(\pi^1_t) - J(\pi^2_t)}{2} \Big]$, with enhancer selecting over

$$\Pi_t = \Big\{ \tilde{\pi} \in \Pi : \sqrt{\frac{cd \log(T/\delta)}{m}} \sum_{i=1}^{m} \|\phi(x_{t,i}, \tilde{\pi}) - \phi(x_{t,i}, \pi^1_t)\|_{\Sigma^{-1}_{t,m}} - \eta \sum_{i=1}^{m} D_{\mathrm{KL}}(\tilde{\pi}(\cdot|x_{t,i}) \| \pi^1_t(\cdot|x_{t,i})) \geq 0 \Big\}.$$

Hybrid Learning

For iteration $t = 1, 2, \ldots$

- Compute r_{MLE}^t based on $\mathcal{D}^{1:t-1}$ and $\mathcal{D}_{\mathrm{off}}$;
- The main agent computes $\pi_t^1 = \mathcal{O}(r_{\mathrm{MLE}}^t, \pi_0)$;
- The enhancer takes a fixed π_{ref};
- Collect m comparison pairs by $(\pi_t^1, \pi_{\mathrm{ref}})$ as $\mathcal{D}^t$.

Theorem 5 (Batch Hybrid Learning Guarantee [XDY+23])

With $T = \tilde{\Theta}(d)$, we can find a $\pi_{t_0}^1$ such that

$$J(\pi^*) - J(\pi_{t_0}) \lesssim \underbrace{\sqrt{\frac{d}{\gamma^2 m}}}_{\text{Online exploration}} + \underbrace{\sqrt{d} \cdot \|\mathbb{E}_{x \sim d_0}[\phi(x, \pi^*) - \phi(x, \pi_{\mathrm{ref}})]\|_{\Sigma_{\mathrm{off}}^{-1}}}_{\text{Offline coverage}}$$

$$- \eta \mathbb{E}_{x_{t_0} \sim d_0}\left[D_{\mathrm{KL}}(\pi_{t_0}^1(\cdot|x_{t_0}) \| \pi^*(\cdot|x_{t_0}))\right],$$

Learning Paradigm

Offline	Online	Hybrid
Precondition: $\mathcal{D}_{\mathrm{off}}$	**Precondition:** -	**Precondition:** $\mathcal{D}_{\mathrm{off}}$
Condition: $\\|\mathbb{E}_{x\sim d_0}[\phi(x,\pi^*)-\phi(x,\pi_{\mathrm{ref}})]\\|_{\Sigma_{\mathrm{off}}^{-1}} \le \frac{C_{\mathrm{cov}}}{\sqrt{n_{\mathrm{off}}}}$	**Condition:** Low-rank reward	**Condition:** Both + $n_{\mathrm{off}} \approx mT$
Algorithmic idea: Pessimism	**Algorithmic idea:** π_{r^t} v.s. Optimism	**Algorithmic idea:** π_{r^t} v.s. π_{ref}
#Sample: $O\Big(\frac{dC_{\mathrm{cov}}}{\epsilon^2}\Big)$	**#Sample:** $O\Big(\frac{d^2}{\epsilon^2}\Big)$	**#Sample:** $O\Big(\frac{d^2+dC_{\mathrm{cov}}}{\epsilon^2}\Big)$

We omit the constant factors and some log factors like $\log(T/\delta)$.

Algorithmic Designs in Reward-based RLHF

RLHF v.s. Deep RL

Reward function is never perfect.

- Humans typically possess a set of intricate or even *contradictory* targets: helpful, harmless, honest, verbosity...
- Majority v.s. under-represented groups;
- Human expertise and opinions are diverse.

Essentially, all models are wrong, but some are useful. [Box76]

RL	**RLHF**
Reward:	**Reward:**
Ground truth (Gold reward)	Imperfect reward
	Learned reward / Human / GPT4
Model Selection:	**Model Selection:**
Model with highest reward	Evaluation Benchmarks + Human Raters

Toward a Practical Planning Oracle

Recall the planning oracle:

$$\operatorname*{argmax}_{\pi\in\Pi} \mathbb{E}_{x\sim d_0}\Big[\underbrace{\mathbb{E}_{a\sim\pi(\cdot|x)}[r^*(x,a)]}_{\text{Optimize Reward}} - \underbrace{\eta D_{\mathrm{KL}}(\pi(\cdot|x)\|\pi_0(\cdot|x))}_{\text{Stay Close to } \pi_0}\Big] \propto \pi_0(a|x)\exp\big(\frac{1}{\eta}r(x,a)\big)$$

- PPO [SWD+17] with $\tilde{r}(x,a) = r(x,a) - \eta\log\frac{\pi_\theta(a|x)}{\pi_0(a|x)}$.
  - Complicated hyper-parameter: learning rate, KL coefficient, update epoch, clip range... and code-level optimization;
  - Unstable convergence behavior;
  - Heavy burden on GPU memory: loading 4 models at the same time.
- Direct Preference Optimization (DPO) [RSM+23]:

$$\mathcal{L}(\theta,\pi_0) = -\sum_{(x,\tilde{a}^1,\tilde{a}^2)\in\mathcal{D}_{\mathrm{off}}} \log\sigma\big(\eta\log\frac{\pi_\theta(\tilde{a}^1|x)}{\pi_0(\tilde{a}^1|x)} - \eta\log\frac{\pi_\theta(\tilde{a}^2|x)}{\pi_0(\tilde{a}^2|x)}\big)$$

  - “Direct”: no reward modeling;
  - SFT-based learning: stable with less parameters;
  - DPO enjoys the same solution with PPO.

Iterative Hybrid DPO

- Dataset: Anthropic HH-RLHF, Helpful subset;
  - Human: What is the best way to apologize to someone? Assistant:
- Model: Open-LLaMA-3B V2;

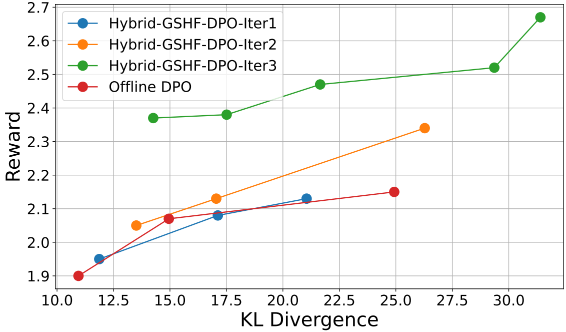


Figure 3: The figure of Reward-KL trade-off. Both the KL and reward are computed on a hand-out test set.

Multi-step Rejection Sampling

[LZJ+23] proposes Rejection Sampling Optimization (RSO):

- DPO: dataset from unknown data distribution, learning target: π^*;
- RSO with a trained reward r:
  - dataset: $a \sim \pi_r$ by ejection sampling with r;
  - label: r;
  - learning target: π_r by running DPO on newly generated dataset.

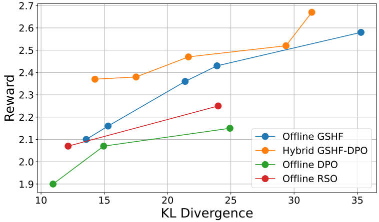
Approximating π_r by π_0 can be inefficient

- Multi-step RS [XDY+23] $\eta_1 > \eta_2 > ... > \eta$:

$$\pi_0 \to \pi_0 \exp(\frac{1}{\eta_1} r) \to \pi_0 \exp(\frac{1}{\eta_2} r) \cdots \to \pi_0 \exp(\frac{1}{\eta} r)$$

More Experimental Results

We remark that the boundary between online and offline is not strict. We can fix $\mathcal{P}$ as some learned preference oracle and use it for the online preference query.



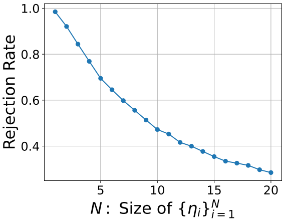


Figure 4: The figure of Reward-KL trade-off. Both the KL and reward are computed on a hand-out test set.

Online Iterative DPO: Uncertainty in LLMs

Essentially, we require

- Exploration: $\|\phi(x, \pi_t^1) - \phi(x, \pi_t^2)\|_{\Sigma_{t,m}^{-1}} \geq \|\phi(x, \pi_t^1) - \phi(x, \pi^*)\|_{\Sigma_{t,m}^{-1}}$;
- Exploitation: π_t^1, π_t^2 are "around" π_{r^t}.

Practical Implementation:

- Rejection sampling:
  - For prompt x, we independently sample (a^1, a^2, a^3, a^4) by π_{r^t};
  - Best-of-4 v.s. Worst-of-4, as ranked by $\mathcal{P}$.
- The concurrent work [HT24] implements rejection-sampling-based online iterative DPO
  - Mistral-7B + pairRM-0.4B;
  - Ranked 2nd in AlpacaEval.

Question: How to quantify the uncertainty in general LLMs?

RLHF Under General Preference

Disadvantage of Reward-based RLHF

- Implicitly assumes a *total order*: $A \succ B, B \succ C \to A \succ C$;
- The total order is not satisfied for the preference *averaged* over a diverse set of human groups;
- The reward function can be easily hacked;
- Win rate is a more robust metric that is close to real-world user experience.

Reverse-KL Regularized Two-player Game

- Relative preference: $R^*(x, a^1, a^2) = \log \mathcal{P}(a^1 \succ a^2|x) - \log \mathcal{P}(a^1 \prec a^2|x)$;
- With BT model, it holds that

$$R^*(x, a^1, a^2) = r^*(x, a^1) - r^*(x, a^2).$$

- Value function

$$\begin{aligned} J(\pi^1, \pi^2) &= \mathbb{E}_{x\sim d_0}\mathbb{E}_{a^1\sim\pi^1, a^2\sim\pi^2}\Big[R^*(x, a^1, a^2) + \eta \log \frac{\pi_0(a^1|x)}{\pi^1(a^1|x)} - \eta \log \frac{\pi_0(a^2|x)}{\pi^2(a^2|x)}\Big] \\ &= \mathbb{E}_{x\sim d_0}\mathbb{E}_{a^1\sim\pi^1, a^2\sim\pi^2}\Big[R^*(x, a^1, a^2) - \eta D_{\mathrm{KL}}(\pi^1(\cdot|x)\|\pi_0(\cdot|x)) + \eta D_{\mathrm{KL}}(\pi^2(\cdot|x)\|\pi_0(\cdot|x))\Big]. \end{aligned} \tag{2}$$

- Nash Equilibrium: $(\pi^1_*, \pi^2_*) = (\pi_*, \pi_*) = \mathrm{argmax}_{\pi^1\in\Pi}\, \mathrm{argmin}_{\pi^2\in\Pi} J(\pi^1, \pi^2)$, which implies $J(\pi_*, \pi_*) = 0$.
- Goal: find a $\hat{\pi}^1$ such that

$$J(\pi_*, \pi_*) - J(\hat{\pi}^1, \dagger) \le \epsilon,$$

where $J(\hat{\pi}^1, \dagger) = \min_{\pi'} J(\hat{\pi}^1, \pi')$.

MLE and Information Ratio

We consider function approximation by $\mathcal{R}$ with $R^* \in \mathcal{R}$.

- Maximum Likelihood Estimation:
$$\ell_{\mathcal{D}_{\mathrm{off}}}(R) = \sum_{(x,a^1,a^2,y)\in\mathcal{D}_{\mathrm{off}}} y \log \sigma(R(x,a^1,a^2)) + (1-y)\log \sigma(-R(x,a^1,a^2)).$$

- Information ratio between prediction error and in-sample error:
$$\Gamma(x,\pi^1,\pi^2) = \sup_{R\in\mathcal{R}} \frac{|R(x,\pi^1,\pi^2) - \hat{R}(x,\pi^1,\pi^2)|}{\sqrt{\lambda + \sum_{i=1}^n (R(x_i,a_i^1,a_i^2) - \hat{R}(x_i,a_i^1,a_i^2))^2}},$$

- Linear reward + BT model:
$$\Gamma(x,\pi^1,\pi^2) \le \|\phi(x,\pi^1) - \phi(x,\pi^2)\|_{\Sigma^{-1}_{\mathcal{D}_{\mathrm{off}}}}.$$

Offline Learning

- Version space consists of R^* with high probability:

$$\widehat{\mathcal{R}} = \Big\{ R \in \mathcal{R} : \sum_{i=1}^{n} (R(x_i, a_i^1, a_i^2) - \hat{R}(x_i, a_i^1, a_i^2))^2 \le O\big(\log(|\mathcal{R}|/\delta)\big) \Big\}.$$

- Conservative value estimations:

$$\underline{J}(\pi^1, \pi^2) = \min_{R \in \widehat{\mathcal{R}}} \mathbb{E}_{x \sim d_0} \mathbb{E}_{a^1 \sim \pi^1, a^2 \sim \pi^2} \Big[R(x, a^1, a^2) + \eta \ln \frac{\pi_0(a^1|x)}{\pi^1(a^1|x)} - \eta \ln \frac{\pi_0(a^2|x)}{\pi^2(a^2|x)} \Big],$$
$$\overline{J}(\pi^1, \pi^2) = \max_{R \in \widehat{\mathcal{R}}} \mathbb{E}_{x \sim d_0} \mathbb{E}_{a^1 \sim \pi^1, a^2 \sim \pi^2} \Big[R(x, a^1, a^2) + \eta \ln \frac{\pi_0(a^1|x)}{\pi^1(a^1|x)} - \eta \ln \frac{\pi_0(a^2|x)}{\pi^2(a^2|x)} \Big].$$

- Compute pessimistic Nash equilibrium

$$\begin{aligned} (\hat{\pi}^1, \tilde{\pi}^2) &= \operatorname*{argmax}_{\pi^1 \in \Pi} \min_{\pi^2 \in \Pi} \underline{J}(\pi^1, \pi^2), \\ (\tilde{\pi}^1, \hat{\pi}^2) &= \operatorname*{argmax}_{\pi^1 \in \Pi} \min_{\pi^2 \in \Pi} \overline{J}(\pi^1, \pi^2). \end{aligned} \tag{3}$$

- Return $(\hat{\pi}^1, \hat{\pi}^2)$.

Theoretical Results of Offline Learning

Theorem 6 (Offline learning guarantee [YXZ+24])

With $\beta^2 = O(\log|\mathcal{R}|/\delta)$, with high probability, we have

$$\mathrm{DuaGP}(\hat{\pi}^1, \hat{\pi}^2) \le 4\beta\sqrt{\frac{\mathcal{C}((\tilde{\pi}^1, \pi_*^2), \pi_D, \mathcal{R})}{n}} + 4\beta\sqrt{\frac{\mathcal{C}((\pi_*^1, \tilde{\pi}^2), \pi_D, \mathcal{R})}{n}}$$

where the coverage coefficient of some policy pair of $\mathcal{D}$ is

$$\mathcal{C}((\pi^1, \pi^2), \pi_D, \mathcal{R}) = \sup_{R \in \widehat{\mathcal{R}}} \frac{(\mathbb{E}_{x \sim d_0}[R(x, \pi^1, \pi^2) - \hat{R}(x, \pi^1, \pi^2)])^2}{\mathbb{E}_{x \sim d_0, a^1 \sim \pi_D^1, a^2 \sim \pi_D^2}(R(x, a^1, a^2) - \hat{R}(x, a^1, a^2))^2}.$$

- Unilateral Coverage [ZXT+22] by $\pi^1 = \tilde{\pi}^1, \pi^2 = \tilde{\pi}^2$:

$$4\beta\sqrt{\tilde{\mathcal{C}}((\tilde{\pi}^1, \pi_*^2), \pi_D, \mathcal{R})/n} + 4\beta\sqrt{\tilde{\mathcal{C}}((\pi_*^1, \tilde{\pi}^2), \pi_D, \mathcal{R})/n} \le \sup_{\pi \in \Pi} \beta\sqrt{\tilde{\mathcal{C}}((\pi, \pi_*), \pi_D, \mathcal{R})/n}.$$

- For reward-based RLHF, the suboptimality is

$$\inf_{\pi \in \Pi} \beta\sqrt{\tilde{\mathcal{C}}((\pi, \pi_*), \pi_D, \mathcal{R})/n}.$$

Refined Coverage Condition

Corollary 7 (Refined Guarantee for Offline Learning)

Under the same condition, we have

$$\mathrm{DuaGP}(\hat{\pi}^1, \hat{\pi}^2) \le \min_{\pi^1, \pi^2} \Big\{ 4\beta \sqrt{\frac{\mathcal{C}((\pi^1, \pi^2_*), \pi_D, \mathcal{R})}{n}} + 4\beta \sqrt{\frac{\mathcal{C}((\pi^1_*, \pi^2), \pi_D, \mathcal{R})}{n}} + \mathrm{subopt}^{\tilde{\pi}^1, \pi^2_*}(\pi^1) + \mathrm{subopt}^{\pi^1_*, \tilde{\pi}^2}(\pi^2) \Big\},$$

where $\mathrm{subopt}^{\tilde{\pi}^1, \pi^2_*}(\pi^1) = \overline{J}(\tilde{\pi}^1, \pi^2_*) - \overline{J}(\pi^1, \pi^2_*)$, $\mathrm{subopt}^{\pi^1_*, \tilde{\pi}^2}(\pi^2) = \underline{J}(\pi^1_*, \pi^2) - \underline{J}(\pi^1_*, \tilde{\pi}^2)$.

- If we take $(\pi^1, \pi^2) = (\tilde{\pi}^1, \tilde{\pi}^2)$, such an upper bound reduces to unilateral coverage case;
- If $\tilde{\mathcal{C}}((\tilde{\pi}^1, \pi^2), \pi_D, \mathcal{R})$ is large, the refined bound adapts to an alternate π^1 in the coverage term;
- Note $\tilde{\pi}^1$ is the best response to $\hat{\pi}^2$ but not necessarily to π^2_* so the subopt can be negative.

Batch Online Learning

For $t = 1, 2, \ldots$

- Compute the MLE $\hat{R}_t$ based on $\mathcal{D}_{1:t-1}$ and construct the bonus:

$$\Gamma_t^m(x, \pi^1, \pi^2) := \sup_{R \in \mathcal{R}} \frac{|R(x, \pi^1, \pi^2) - \hat{R}(x, \pi^1, \pi^2)|}{\sqrt{\lambda + \frac{1}{m}\sum_{s=1}^{t-1}\sum_{j=1}^{m}(R(x_{s,j}, a^1_{s,j}, a^2_{s,j}) - \hat{R}(x_{s,j}, a^1_{s,j}, a^2_{s,j}))^2}},$$

- Compute optimistic Nash policy for the max-player $(\hat{\pi}_t^1, \tilde{\pi}_t^2)$:

$$\operatorname*{argmax}_{\pi^1 \in \Pi} \operatorname*{argmin}_{\pi^2 \in \Pi} \mathbb{E}_{a^1 \sim \pi^1, a^2 \sim \pi^2}\Big[\hat{R}_t(x, a^1, a^2) + \beta \Gamma_t^m(x, \pi^1, \pi^2) + \eta^{-1} \log \frac{\pi_0(a^1|x)}{\pi^1(a^1|x)} - \eta^{-1} \log \frac{\pi_0(a^2|x)}{\pi^2(a^2|x)}\Big],$$

- The min-player aims to approximate the best response for the max-player:

$$\hat{\pi}_t^2 = \operatorname*{argmin}_{\pi^2 \in \Pi} \mathbb{E}_{a^1 \sim \hat{\pi}_t^1, a^2 \sim \pi^2}\Big[\hat{R}_t(x, a^1, a^2) - \beta \Gamma_t^m(x, \hat{\pi}_t^1, \pi^2) - \eta^{-1} \log \frac{\pi_0(a^2|x)}{\pi^2(a^2|x)}\Big].$$

- Collect m comparison pairs by $(\hat{\pi}_t^1, \hat{\pi}_t^2)$ as $\mathcal{D}^t$.

Eluder Coefficient

Definition 8 (Eluder Coefficient [GWZ22, YXGZ23])

We define the information ratio as

$$\tilde{\Gamma}_t(\lambda, \pi_t^1, \pi_t^2) = \sup_{R \in \mathcal{R}} \frac{\mathbb{E}_{x \sim d_0, a^1 \sim \pi_t^1, a^2 \sim \pi_t^2} |R(x, a^1, a^2) - \hat{R}(x, a^1, a^2)|}{\sqrt{\lambda + \sum_{s=1}^{t-1} \mathbb{E}_{x_s \sim d_0, a_s^1 \sim \hat{\pi}_s^1, a_s^2 \sim \hat{\pi}_s^2} (R(x_s, a_s^1, a_s^2) - \hat{R}(x_s, a_s^1, a_s^2))^2}}.$$

Then, the eluder coefficient is given by

$$d(\mathcal{R}, \lambda, T) := \sup_{\pi_{1:T}^1, \pi_{1:T}^2} \sum_{t=1}^{T} \min(1, \tilde{\Gamma}_t^2(\lambda, \pi_t^1, \pi_t^2)).$$

- Information ratio: *Prediction error* (target) v.s. *In-sample error* (guarantee);
- Eluder coefficient: limits the extent to which we can be "surprised" by the new out-of-sample distributions, given the historical data collected so far.

Online Learning Guarantee

Theorem 9 (Online learning guarantee [YXZ+24])

For any $\epsilon > 0$, *with* $T = \min\{n \in \mathbb{N}^+ : n \geq 2d(\mathcal{R}, \lambda, n)\}$, *batch size as* $m = O\big(T \log(T|\mathcal{R}|/\delta)/\epsilon^2\big)$, $\beta = \sqrt{T \log(T|\mathcal{R}|/\delta)/m}$,*then, with high probability, we can find a* $t_0 \in [T]$,

$$J(\pi_1^*, \pi_2^*) - J(\pi_{t_0}^1, \dagger) \leq \epsilon.$$

- $\hat{\pi}^1$ almost beats any competing policy:

$$\min_{\pi^2 \in \Pi} \mathbb{E}_{x \sim d_0} \mathbb{E}_{a^1 \sim \hat{\pi}^1, a^2 \sim \pi^2} \Big[R^*(x, a^1, a^2) - \eta D_{\mathrm{KL}}(\hat{\pi}^1(\cdot|x) \| \pi_0(\cdot|x)) + \eta D_{\mathrm{KL}}(\pi^2(\cdot|x) \| \pi_0(\cdot|x)) \Big] \geq -\epsilon.$$

- $\hat{\pi}^1$ is consistently preferred by $\mathcal{P}$ with small η:

$$\min_{\pi^2 \in \Pi} \mathbb{E}_{x \sim d_0} \mathbb{E}_{a^1 \sim \hat{\pi}^1, a^2 \sim \pi^2} \mathcal{P}(x, a^1, a^2) > \frac{1}{1 + \exp(\epsilon)} \approx 0.5.$$

- $\hat{\pi}^1$ automatically maximizes the regularized reward under BT model:

$$\mathbb{E}_{x \sim d_0} \mathbb{E}_{a^1 \sim \hat{\pi}^1} \Big[r^*(x, a^1) - \eta D_{\mathrm{KL}}(\hat{\pi}^1(\cdot|x) \| \pi_0(\cdot|x)) \Big]$$
$$\geq \max_{\pi^2} \mathbb{E}_{x \sim d_0} \mathbb{E}_{a^2 \sim \pi^2} \Big[r^*(x, a^2) - \eta D_{\mathrm{KL}}(\pi^2(\cdot|x) \| \pi_0(\cdot|x)) \Big] - \epsilon.$$

What we know? & What is next?

What we know:

- Iterative DPO is provably efficient and demonstrates impressive empirical performance;
- Reward hacking: Snorkel-Mistral-PairRM-DPO with output length (2616) beats GPT4 (1365);
- The complexity scales with the complexity of reward space: good if discriminator is simpler than generator (weak to strong?).

What is next?

- More efficient exploration strategy beyond rejection sampling;
- Efficient and effective reward modeling;
- Alignment tax: performance degeneration after RLHF [LLX+24];
- Practical implementation of NLHF.

Thanks for listening!

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