Reinforcement Learning from Human Feedback: From Theory to Algorithm

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RL Research for Large Language Models



Foundation Generative Models

General ChatBot









Coding Assistant

Music, Video, Image Generation



Copilot







Foundation Model Pipeline



- **1.** LLM is trained on a large amount of *unlabelled* data, to predict next token: P(next token | prior tokens);
- 2. Goal: acquire general knowledge.

Yao Fu, How does GPT Obtain its Ability? Tracing Emergent Abilities of Language Models to their Sources

Instruction-following training

Foundation Model Pipeline



Instruction-following training

Ability to follow humans' instructions.



Tell me something about the sushi

> ... Sushi is a traditional Japanese dish that consists of vinegared rice combined with various ingredients



- 1. RLHF is the leading technique to adapt the generation distribution to be preferred by the humans: helpful, harmless, and honest;
- 2. RLHF learns from *relative feedback*





Which response do you prefer?

Your choice will help make ChatGPT better



Response 2 S)

I'm just a program, so I don't have feelings, but thanks for asking! How about you? How are you doing today?

Formulation of LLM and RLHF

Language Model as RL/Bandit Agent

- 1. **Prompt** $x \in \mathscr{C}$: state from some distribution d_0
 - 1. Explain the moon landing to a 6 year old child.
- 2. **Response** $a \in \mathscr{A}$: action
 - 1. Explain gravity ...
 - 2. Explain war...
 - 3. Moon is natural satellite of ...
- 3. LLM: policy $\pi : \mathscr{X} \to \Delta(\mathscr{A})$
 - 1. Initial policy π_0 .

Bradley-Terry (BT) Model



- The Bradley-Terry model is a *proxy* of the Human preference
- Linear parameterization: $r^{\star}(x, a)$

$$\mathbb{R} \longrightarrow \mathscr{P}_{\theta}(a^{1} \succ a^{2} x) = \frac{e^{r_{1}}}{e^{r_{1}} + e^{r_{2}}}$$
$$\mathbb{R}$$

$$a) = \left\langle \phi(x, a), \theta^{\star} \right\rangle$$

RLHF as Reverse-KL Regularized Contextual Bandit

In practice, the following regularized learning objective is adopted: $\max_{\pi \in \Pi} J(\pi) = \max_{\pi \in \Pi} \mathbb{E}_{x \sim d_0} \left[\mathbb{E}_{a \sim \pi(\cdot x)} \left[\prod_{\pi \in \Pi} \mathbb{E}_{x \sim d_0} \left[\mathbb{E}_{x \sim \pi(\cdot x)} \right] \right] \right]$ Stay Close to π_0 **Optimize Reward**

$$[r^{\star}(x,a)] \quad -\eta \mathrm{KL}(\pi(\cdot x) \| \pi_0(\cdot x)) \|.$$

RLHF as Reverse-KL Regularized Contextual Bandit

In practice, the following regularized learning objective is adopted: $\max_{\pi \in \Pi} J(\pi) = \max_{\pi \in \Pi} \mathbb{E}_{x \sim d_0} \left[\mathbb{E}_{a \sim \pi(\cdot x)} \right]$

- The BT model is not perfect: the major difference from traditional DRL
- The KL-constraint framework admits a stochastic optimal policy;
- The KL constraint optimization problem admits a closed-form solution:

$$\arg \max_{\pi} \left[\mathbb{E}_{a \sim \pi(\cdot x)} [r(x, a)] - \eta \operatorname{KL}(\pi(\cdot x) \| \pi_0(\cdot x)) \right] = \frac{1}{Z(x)} \cdot \pi_0(a \ x) \exp(\frac{1}{\eta} r(x, a))$$

where $Z(x) = \sum_{a' \in \mathscr{A}} \pi_0(a' \ x) \exp(\frac{1}{\eta} r(x, a'))$.

• Assume the computational oracle: $\mathcal{O}(r, \eta, \pi_0)$

$$[r^{\star}(x,a)] \quad -\eta \mathrm{KL}(\pi(\cdot x) \| \pi_0(\cdot x)) \Big] \,.$$

Stay Close to π_0 **Optimize Reward**



Instruct-GPT Framework to Make Chat-GPT

- Preference Data Collection:

 - Preference signal: $y \sim \mathscr{P}_{RT}^{\star}(\cdot x, a^1, a^2)$
- Learning Reward model as MLE:

•
$$\mathscr{C}_{\mathscr{D}}(\theta) = \sum_{(x,a^w,a^l)\in\mathscr{D}} \log\Big(\sigma\big(r_{\theta}(x_{\theta})\big)\Big)$$

Optimize the learned reward using PPO.

Ouyang, Long et al., Training language models to follow instructions with human feedback

• Contextual bandit: $x \sim d_0$, $a^1, a^2 \sim \pi_b(\cdot x)$ (typically π_0)

 $(x, a^w) - r_\theta(x, a^l))$

Fundamental Issue: Reward Hacking

- Heavily optimize the proxy reward leads to reward hacking:
 - Higher reward
 - But worse performance
- The learned *proxy reward* are of issues:

 - - of-distribution.

Collin Burns et al., Weak-to-Strong Generalization: Eliciting Strong Capabilities With Weak Supervision

SOTA RMs achieve accuracy ~75% (due to noise and human disagreement)

• Sensitivity to sampling distribution (determined by the behavior policy)

Fine-tuning improves in-distribution generalization, but often performs poorly out-



Fundamental Issue: Reward Hacking



Distribution shift: KL between π_0 and tuned policy

Simplified Figure from Leo Gao et al., Scaling Laws for Reward Model Overoptimization

Offline Learning from a Fixed Preference Dataset

Insufficient Dataset Coverage

- Unbalanced Preference Coverage
 - Prompt A: Can you write a code for ...
 - A good code v.s. another good code;
 - A good code v.s. a bad code;
 - A bad code v.s. another bad code.

• Prompt B: What is the best fitness app?

• a^1 : what is fitness app? v.s. a^2 : I am sorry, but I am an AI model...



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Ying Jin, Zhuoran Yang, and Zhaoran Wang, Is Pessimism Provably Efficient for Offline RL?





RLHF with Pessimism

- Construct the Pessimistic Reward

 - Where $x,a^1,a^2 \in \mathcal{D}_{off}$
- **Planning with the Pessimistic Reward:**

•
$$\hat{\pi}(\cdot x) = \mathcal{O}(r,\eta,\pi_0)$$
.

Xiong, Wei, et al., Iterative Preference Learning from Human Feedback: Bridging Theory and Practice for RLHF under KL-Constraint

Lower confidence bound (LCB) • Compute $\hat{r}(x, a) = r_{\text{MLE}}(x, a) - c \cdot \sqrt{d} \| \phi(x, a) - \phi(x, \pi_0) \|_{\Sigma_{\text{off}}^{-1}}$ reference $\Sigma_{\text{off}} = \lambda I + \sum_{(\phi(x, a^1) - \phi(x, a^2))(\phi(x, a^1) - \phi(x, a^2))^{\top}.$

RLHF with Pessimism

Theorem: Guarantee for the Pessimistic RLHF

If the offline dataset covers the target

 $\mathbb{E}_{x \sim d_0, a^1 \sim \pi^*(\cdot x), a^2 \sim \pi_0(\cdot x)} \| \phi(x, a^1) - \phi(x$

least $1 - \delta$, we have

 $J(\pi^{\star}) - J(\hat{\pi}) + \eta \mathbf{K}$

Partial coverage:

Xiong, Wei, et al., Iterative Preference Learning from Human Feedback: Bridging Theory and Practice for RLHF under KL-Constraint

$$(\pi^{\star}, \pi_0)$$
 well:
 $(x, a^2) \|_{\Sigma_{\text{off}}^{-1}} \leq \frac{C^{\star}}{\sqrt{n_{\text{off}}}}$, then with probability

$$\mathrm{KL}(\pi^{\star} \| \hat{\pi}) \lesssim \frac{\sqrt{d} \cdot C^{\star}}{\sqrt{n_{\mathrm{off}}}}$$

• C^{\star} : distribution shift between behavior policy and target policy (π^{\star}, π_0)



Is a Good Coverage Assumption Practical?

- C^{\star} : distribution shift between behavior policy and coverage target
- Significant shift in open-source dataset due to the long sequence nature

Average
$$\frac{\pi_{\text{Mistral}-7B-v0.1}(a \ x)}{\pi_{\text{Gemma}-2B-it}(a \ x)} \approx ex$$

Bai, et al. Training a Helpful and Harmless Assistant with Reinforcement Learning from Human Feedback





RLHF with **Pessimism**

- **Pessimism by Ensemble**
 - A popular heuristic implementation of pessimism is based on ensemble $\hat{r}(x, a) = \min_{k=1,...5} r_k(x, a)$ where r_k are independently trained



Batch Hybrid Learning with Online Exploration

RLHF with Only Exploration

- **Batch Hybrid Leanring**
 - Hybrid: we start with an offline set but can also query the human during training \bullet
 - Batch: we use a large batch size for a sparse update
 - **Remark:** PPO with a fixed learned reward: offline learning \bullet
- Intuition: Online Exploration Improves RLHF Policy
 - π_0 can only sample low-reward responses (in-distribution for learned reward);
 - During PPO training, the reward gets higher and higher (out-of-distribution);
 - Querying human feedback for these high-reward responses mitigates the OOD issue.

Initialized with $\mathcal{D} = \mathcal{D}_{off}$ and define the covariance matrix:

- For t = 1, 2, 3, ... $\Sigma_{t.m} = \lambda I$
 - Exploitation with the main agent: π
 - Choose the enhancer policy:

• (1)
$$\pi_t^2 = \arg \max_{\pi' \in \Gamma_t} \|\phi(x, \pi') - \phi(x, \pi_t^1)\|_{\Sigma_{t,m}^{-1}}$$

• (2)
$$\pi_t^2 = \pi_0;$$

• Collect the m new samples $x_{t,j}, a_{t,j}^{1}, a_{t,j}^{1}$

$$+\frac{1}{m}\sum_{i=1}^{t-1}\sum_{j=1}^{m}(\phi(x_{i,j},a_{i,j}^{1})-\phi(x_{i,j},a_{i,j}^{2})(\phi(x_{i,j},a_{i,j}^{1})-\phi(x_{i,j},a_{i,j}^{2})^{\mathsf{T}}$$

$$\pi_t^1 = \mathcal{O}(\hat{r}_t, \eta, \pi_0)$$
, with \hat{r}_t as the MLE on \mathcal{D} ;

Confidence set: $\Pi_t = \left\{ \pi' : \beta \| \phi(x, \pi') - \phi(x, \pi_t^1) \|_{\Sigma_{t,m}^{-1}} \ge \eta \operatorname{KL}(\pi'(\cdot x) \| \pi_t^1(\cdot x)) \right\}$

$$u_{t,j}^2, y_{t,j} \sim (d_0, \pi_t^1, \pi_t^2, \mathscr{P}_{BT}^{\star}) \text{ into } \mathscr{D}.$$



Theorem 2 Part 1: Guarantee for the Online Iterative RLHF with optimism

 $T = \tilde{\Omega}(d)$ times, w.p. at least $1 - \delta$, we can find a $t_0 \in [T]$ such that

Xiong, Wei, et al., Iterative Preference Learning from Human Feedback: Bridging Theory and Practice for RLHF under KL-Constraint

With Option I, if we run the online iterative RLHF with batch size $m = c \cdot \frac{d}{c^2}$ for $J(\pi^{\star}) - J(\pi_{t_0}^1) + \eta \operatorname{KL}(\pi^{\star} \| \pi_{t_0}^1) \leq \epsilon$

Theorem 2 Part 2: Guarantee for the Online Iterative RLHF with offline dataset

 $T = \tilde{\Omega}(d)$ times, w.p. at least $1 - \delta$, we can find a $t_0 \in [T]$ such that $J(\pi^{\star}) - J(\pi_{t_0}^1) + \eta \text{KL}(\pi^{\star} \| \pi_{t_0}^1) \leq$

- collected by (π_t, π_0) may cover (π^*, π_0) better;
- **Online v.s. Hybrid:** optimism v.s. additional offline dataset coverage.

Xiong, Wei, et al., Iterative Preference Learning from Human Feedback: Bridging Theory and Practice for RLHF under KL-Constraint

With Option II, if we run the hybrid iterative RLHF with batch size $m = c \cdot \frac{d}{c^2}$ for

$$\leq \epsilon + \sqrt{d} \|\mathbb{E}[\phi(x, \pi^*) - \phi(x, \pi_0)]\|_{\Sigma_{\mathrm{off}+1:t_0}^{-1}}$$

• Offline v.s. Hybrid : under the offline coverage condition, $\pi_t \to \pi^*$, online data



Practical Algorithm: Approximate the Computational Oracle

- **PPO** with regularized reward $\hat{r}(x, a) =$
 - Loading 4 models at the same time: tuned model, critic, reward, and π_0 .
- DPO, SLiC, IPO, InfoNCA, GPO: different choices of the binary classification loss
 - Direct Preference Optimization skips the reward modeling and optimize

$$L(\theta,\eta,\pi_0) = -\sum_{(x,a^w,a^l)\in\mathscr{D}} \log \sigma \left(\eta \log \frac{\pi_{\theta}(a^w \ x)}{\pi_0(a^w \ x)} - \eta \log \frac{\pi_{\theta}(a^l \ x)}{\pi_0(a^l \ x)}\right).$$

Computation oracle: $\mathcal{O}(r,\eta,\pi_0) := \arg \max \mathbb{E}_{a \sim \pi(\cdot x)} [r(x,a) - \eta \text{KL}(\pi(\cdot x) \| \pi_0(\cdot x))]$

$$r(x,a) - \eta \log \frac{\pi(a x)}{\pi_0(a x)}$$



Online Iterative RLHF: Experimental Result 1



Setup

- \bullet Ultra-LLaMA-13B RM to *approximate* human
- sample more in-distribution data from π_0

Scaling Laws for Reward Model Overoptimization

Main message: sampling new data from online exploration is far more efficient than

Online Iterative RLHF: Experimental Result 2

- 1. The same setup but with
 - 1. Model: Zephyr trained from Mistral-7B-v0.1
 - 2. Prompt set: Ultra feedback 60K
- 2. Online Exploration
 - 1. Exploitation: close to π_t^1 (MLE);
 - 2. Exploration: maximize policy difference;
 - 3. *Rejection sampling*: we sample 4 responses and use the best sample.

Dong H, Xiong W, et al. Raft: Reward ranked finetuning for generative foundation model alignment



Beyond the Reward-based Framework: RLHF with General Preference

Bradley-Terry (BT) Model



- The Bradley-Terry model is a *proxy* of the preference oracle with **issues**:
 - Its transitivity may not hold in practice

$$P(a^1 \prec a^2) > 0.5 \& P(a^2)$$

 $\mathscr{P}_{BT}^{\star}(a^{1} \succ a^{2} \ x, a^{1}, a^{2}) = \frac{e^{r_{1}}}{e^{r_{1}} + e^{r_{2}}}$

 $\langle a^3 \rangle > 0.5 \Rightarrow P(a^1 < a^3) > 0.5$



Preference Model



- Anti-symmetric Relative preference

$$R^{\star}(x, a^{1}, a^{2}) = \log \frac{\mathscr{P}^{\star}(a^{1} \succ a^{2} \ x, a^{1}, a^{2})}{\mathscr{P}^{\star}(a^{1} \prec a^{2} \ x, a^{1}, a^{2})} = \underbrace{r^{\star}(x, a^{1}) - r^{\star}(x, a^{2})}_{\text{If BT is true.}}$$

 $\begin{array}{l} \begin{array}{l} \text{Preference} \\ \text{Model} \\ \theta \end{array} \end{array} \rightarrow z \in \mathbb{R} \xrightarrow{\text{Sigmoid } \sigma} \quad \mathscr{P}^{\star}(a^1 \succ a^2 \ x, a^1, a^2) = \sigma(z) \end{array}$

• The Preference Model is a *proxy* of the preference oracle with larger capacity:

• Value It doesn't impose the transitivity ($a^1 < a^2 \& a^2 < a^3 \Rightarrow a^1 < a^3$)



RLHF with General Preference

KL-Regularized Two-player Game:

$$(\pi^{\star}, \pi^{\star}) = \max_{\pi} \min_{\pi'} R^{\star}(\pi, \pi') - \eta \text{KL}(\pi || \pi_0) + \eta \text{KL}(\pi' || \pi_0)$$

With the KL terms, the regularized objective enjoy following benefits:

- The KL regularization can (potentially) mitigate reward hacking and guarantee the optimal policy to be stochastic (diverse)
- Nash equilibrium

Note: KL is not the only choice, other divergences may also be used (e.g., Jensen-Shannon). arXiv:2309.16240

• The objective becomes strongly concave-convex \rightarrow unique symmetric

Online Iterative RLHF with General Preference

Computation oracle: $\mathcal{O}(R, \pi_0, \eta) = \arg \max \arg \min R(\pi, \pi') - \eta \text{KL}(\pi || \pi_0) + \eta \text{KL}(\pi' || \pi_0)$

Initialized with $\mathcal{D} = \mathcal{O}$, for t=1,2,3,...

- Main agent: compute the MLE \hat{R}_i
- Choose the enhancer policy: $\pi_t^2 = \arg\min_{\pi^2 \in \Pi} \mathbb{E}_{a^1 \sim \pi_t^1, a^2 \sim \pi^2} \sup_{R \in \mathscr{R}} \frac{1}{\sqrt{\lambda + \frac{1}{\kappa}}}$
- Collect the m new samples $a_{t,i}^1, a_{t,i}^2$ *^v*,*J*

t on
$$\mathscr{D}$$
 and take $\pi_t^1 = \mathscr{O}(\hat{R}_t, \pi_0, \eta)$

Information ratio

$$R(x, \pi_t^1, \pi^2) - \hat{R}_t(x, \pi_1^t, \pi^2)$$

$$\frac{1}{m} \sum_{s=1}^{t-1} \sum_{j=1}^{m} (R(x_{s,j}, a_{s,j}^{1}, a_{s,j}^{2}) - \hat{R}_{t}(x_{s,j}, a_{s,j}^{1}, a_{s,j}^{2}))^{2}$$

$$\frac{2}{t,j} \sim (\pi_{t}^{1}, \pi_{t}^{2}), \qquad y_{t,j} \sim \mathscr{P}^{\star} \text{ into } \mathscr{D}.$$





Theorem 3: Guarantee for the Online Iterative RLHF with General Preference

- If we run the algorithm with batch size least $1 - \delta$, we can find a $t_0 \in [T]$ such that $J(\pi^{\star}, \pi^{\star}) - \min_{\pi'} J(\pi^{1}_{t_{0}}, \pi') = -\min_{\pi'} \left[R^{\star}_{t_{0}} \right]$
 - With small η, ϵ , the model consistently outperform any competing policy 1.

$$\min_{\pi'\in\Pi} \mathbb{E}_{x\sim d_0} \mathbb{E}_{a^1\sim\pi_{t_0}^1,a^2\sim\pi'} \mathcal{P}(a^1 \succ a^2 \ x,a^1,a^2) > 0.5.$$

3. With the BT model,

$$\mathbb{E}_{x \sim d_0} \mathbb{E}_{a^1 \sim \pi_{t_0}^1} \left[r^{\star}(x, a^1) - \eta \mathrm{KL}(\pi_{t_0}^1 \| \pi_0) \right]$$

$$e m = c \cdot \frac{d}{\epsilon^2}$$
 for $T = \tilde{\Omega}(d)$ times, w.p. at

$$f^{\star}(x, a^1, a^2) - \eta \text{KL}(\pi_{t_0}^1 || \pi_0) + \eta \text{KL}(\pi' || \pi_0)] \le \epsilon$$

$\geq \max_{x \sim d_0} \mathbb{E}_{x \sim d_0} \mathbb{E}_{a^2 \sim \pi'} \left[r^*(x, a^2) - \eta \mathrm{KL}(\pi' \| \pi_0) \right] - \epsilon \,.$ $\pi' \in \Pi$

Ye C, Xiong W, Zhang Y, et al., Iterative reinforcement learning from human feedback with general preference: from theory to algorithm

On-going Challenges and Future Directions

Challenge 1: Preference Conflict

- The agreement rate among humans is only 70%;
- Even the LLMs have different preferences.

Peering Through Preferences: Unraveling Feedback Acquisition for Aligning Large Language Models HELM Instruct: A Multidimensional Instruction Following Evaluation Framework with Absolute Ratings

Helpfulness					Understandability			
	MTurk	Scale	GPT4	Claude		MTurk	Scale	GPT4
MTurk	1.00				MTurk	1.00		
Scale	0.53	1.00			Scale	0.31	1.00	
GPT4	0.59	0.48	1.00		GPT4	0.36	0.28	1.00
Claude	0.41	0.36	0.50	1.00	Claude	0.37	0.30	0.65
Conciseness					Harmlessness			
	MTurk	Scale	GPT4	Claude		MTurk	Scale	GPT4
MTurk	MTurk 1.00	Scale	GPT4	Claude	MTurk		Scale	GPT4
MTurk Scale		Scale	GPT4	Claude	MTurk Scale	MTurk	Scale	GPT4
	1.00		GPT4 1.00	Claude		MTurk 1.00		GPT4



Challenge 2: Insufficiency of Scalar Reward

Human possesses *intricate* and even *contradictory* targets

helpfulness

Attribute

HelpSteer: Multi-attribute Helpfulness Dataset for SteerLM



Multi-objective Reward

- Reward Modeling: multi-objective rewards $\vec{r} = (r_1, r_2, \dots, r_k)$ 1.
 - Good performance 1.
 - Multi-head + Mixture of Expert 2. $f(x,a) = \sum_{i=1}^{k} g(x)_{i} \cdot r_{i}(x,a)$ i=1

Nathan Lambert et al., RewardBench: Evaluating Reward Models for Language Modeling

Mixture of Experts Layer



User-preference-aware Alignment

User-preference-aware objective 1.

$$J(\pi) = \mathbb{E}_{\nu \sim d_{\nu}} \Big[\mathbb{E}_{x \sim d_{0}, a \sim \pi(\cdot \nu, x)} f(\nu, x, a) \Big]$$

Traditional RLHF

•



Wang H, Lin Y, Xiong W, et al. Arithmetic Control of LLMs for Diverse User Preferences: Directional Preference Alignment with Multi-Objective Rewards

$$f(\nu, x, a) = \sum_{i=1}^{k} g(\nu, x)_{i} \cdot r_{i}(x, a)$$

Ours

End Note

Central problem: how to model the preference signal

- Offline learning: pessimism; 1.
- 2. Online iterative learning: collecting new online data;
- 3. Use more general preference modeling:
 - General preference 1.
 - Multi-objective reward 2.
 - User-dependent preference 3.
- 4. Structured problem: math, coding, and agent...

Thanks for listening!