Reinforcement Learning from Human Feedback without Reward Inference: Model-Free Algorithm and Instance-Dependent Analysis

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Abstract

In this paper, we study reinforcement learning from human feedback (RLHF) under an episodic Markov decision process with a general trajectory-wise reward model. We developed a model-free RLHF best policy identification algorithm, called BSAD, without explicit reward model inference, which is a critical intermediate step in the contemporary RLHF paradigms for training large language models (LLM). The algorithm identifies the optimal policy directly from human preference information in a backward manner, employing a dueling bandit sub-routine that constantly duels actions to identify the superior one. BSAD adopts a reward-free exploration and best-arm-identification-like adaptive stopping criteria to equalize the visitation among all states in the same decision step while moving to the previous step as soon as the optimal action is identifiable, leading to a provable, instance-dependent sample complexity $\tilde{\mathcal{O}}(c_{\mathcal{M}}SA^3H^3M\log\frac{1}{\delta})^1$ which resembles the result in classic RL, where $c_{\mathcal{M}}$ is the instance-dependent constant and M is the batch size. Moreover, BSAD can be transformed into an explore-then-commit algorithm with logarithmic regret and generalized to discounted MDPs using a frame-based approach. Our results show: (i) sample-complexity-wise, RLHF is not significantly harder than classic RL and (ii) end-to-end RLHF may deliver improved performance by avoiding pitfalls in reward inferring such as overfit and distribution shift.

1 Introduction

Reinforcement learning (RL), with a wide range of applications in gaming AIs (Bradley Knox & Stone, 2008; MacGlashan et al., 2017; Warnell et al., 2018), recommendation systems (Yang et al., 2024; Zeng et al., 2016; Kohli et al., 2013), autonomous driving (Wei et al., 2024; Schwarting et al., 2018; Kiran et al., 2022), and large language model (LLM) training (Wu et al., 2021; Nakano et al., 2021; Ouyang et al., 2022; Ziegler et al., 2019; Stiennon et al., 2020), has achieved tremendous success in the past decade. A typical reinforcement learning problem involves an agent and an environment, where at each step, the agent observes the state, takes a certain action, and then receives a reward signal. The state of the environment then transits to another state, and this process continues. However, most RL advances remain in the simulator environment where the data acquisition process heavily depends on the crafted reward signal, which limits RL from more realistic applications such as LLM, as defining a universal reward is generally difficult. In recent years, using human feedback as reward signals to train and fine-tune LLMs has delivered significant empirical successes for AI

¹we use $\mathcal{O}(\cdot)$ to hide instance-independent constants and use $\tilde{\mathcal{O}}(\cdot)$ to further hide logarithmic terms except $\log \frac{1}{\epsilon}$.

Setting	Algorithm	Sample Complexity	Space	Instance	Policy
RL	MOCA	$\mathcal{O}\left(rac{H^3SA\lograc{1}{\delta}}{\Delta_{\min}^2p_{\max}^m} ight) \ ilde{\mathcal{O}}\left(rac{H^4SA\lograc{1}{\delta}}{arepsilon^2} ight)$	model-based	dependent	Opt
	Q-Learning	$ ilde{\mathcal{O}}\left(rac{H^4SA\lograc{1}{\delta}}{arepsilon^2} ight)$	model-free	independent	$\varepsilon\text{-}\mathrm{Opt}$
RLHF	P2R-Q	$ ilde{\mathcal{O}}\left(rac{H^4SA\lograc{1}{\delta}}{arepsilon^2} ight)$	model-free	independent	$\varepsilon ext{-}\mathrm{Opt}$
	PEPS	$\tilde{\mathcal{O}}\left(\frac{H^4 SA \log \frac{1}{\delta}}{\varepsilon^2}\right) \\ \tilde{\mathcal{O}}\left(\frac{H^2 S^2 A \log \frac{1}{\delta}}{\varepsilon^2} + \frac{S^4 H^3 \log^3 \frac{1}{\delta}}{\varepsilon}\right)$	model-based	independent	$\varepsilon\text{-}\mathrm{Opt}$
	BSAD(Ours)	$\mathcal{O}\left(rac{H^3MSA^3\lograc{1}{\delta}}{(\overline{\Delta}_{\min}^Mp_{\max}^\pi)^2} ight)$	model-free	dependent	Opt

Table 1: Comparison of RL and RLHF algorithms with MOCA (Wagenmaker et al., 2022), Q-Learning (Jin et al., 2018), PEPS (Xu et al., 2020), and P2R (Wang et al., 2023) with Q-learning. S, A, and H are the number of states, actions, and planing steps. δ is confidence level, M is the batch size. Δ_{\min} is the minimum value function gap, $\overline{\Delta}_{\min}$ characterizes the preference probability gap (Def. 1), and p_{\max}^{π} characterizes the maximum state visitation probability (Def. 2).

alignment problems and produced dialog AIs such as the ChatGPT (Ouyang et al., 2022). This paradigm where the reward of the state and actions is inferred from real human preferences, instead of being handcrafted, is referred to as *Reinforcement Learning from Human Feedback* (RLHF). A typical RLHF algorithm on LLMs involves three steps: (i) pre-train a network with supervised learning, (ii) infer a reward model from human feedback, in the form of comparisons or rankings among trajectories (responses), and (iii) use classic RL algorithm to fine-tune the pre-trained model. An accurate reward model that aligns with human preferences is the key to the superiority of RLHF.

Pitfalls of Reward Inference: However, most reward models are trained on a maximum likelihood estimator (MLE) (Christiano et al., 2017; Wang et al., 2023; Saha et al., 2023) under Bradley-Terry model (Bradley & Terry, 1952). This paradigm exhibits pitfalls: (i) the reward models easily over-fit the dataset which produces in-distribution errors, and (ii) the reward models fail to measure out-of-distribution state-action pairs during fine-tuning. Even though attempts such as pessimistic estimations (Zhu et al., 2023; Zhan et al., 2023b;a) and regularity conditions are made to improve the accuracy and consistency of reward models, it remains a question of whether reward inference is indeed required. Can we develop a model-free RLHF algorithm without reward inference, which has provable instance-dependent sample complexity?

Contributions: We study an episodic RLHF problem with general trajectory rewards and propose a model-free algorithm called *Batched Sequential Action Dueling* (BSAD) which identifies the optimal action for each state backwardly using action dueling with batched trajectories to obtain human preferences. To equalize the state visitation of the same planning step, we adopt a reward-free exploration strategy and adaptive stopping criteria, which enables learning the exact optimal policy with an instance-dependent sample complexity (Theorem. 1) similar to classic RL with reward (Wagenmaker et al., 2022), as long as the batch size is chosen carefully. Moreover, our results only assume the existence of a uniformly optimal stationary policy and do not require the existence of a Condorcet winner, as we will show the optimal policy is the Condorcet winner when human preferences are obtained with large batch sizes. To the best of our knowledge, BSAD is the first RLHF algorithm with instance-dependent sample complexity, and a transformation of BSAD will provide the first model-free explore-then-commit RLHF algorithm with logarithmic regret.

Comparison to (Xu et al., 2020): From the best of our knowledge, the only algorithm with no reward inference (explicit/implicit) is PEPS (Xu et al., 2020). Our paper is different in (i) BSAD is model-free and takes $\mathcal{O}(SA^2)$ space complexity, while PEPS is model-based and takes $\mathcal{O}(S^2A^2)$ space complexity, (ii) BSAD employs adaptive stopping criteria which leads to an instance-dependent sample complexity with improved dependence in S and δ , while PEPS uses fixed exploration horizon and only has worst-case bounds, (iii) we assume the trajectory reward and require the existence

of uniformly deterministic optimal policy which slightly generalizes the classic reward, while PEPS requires the existence of Condorcet winner and stochastic triangle inequality, and (iv) we also generalize to discounted MDPs. The complete comparison of BSAD and related algorithms is summarized in Tab. 1, and a thorough review of related work is deferred to the appendix.

2 Preliminaries

Episodic MDP: An episodic Markov decision process (MDP) is a tuple $\mathcal{M} = (\mathcal{S}, \mathcal{A}, H, P, \mu_0)$, where \mathcal{S} is the state space with $|\mathcal{S}| = S$, \mathcal{A} is the action space with $|\mathcal{A}| = A$, H is the planning horizon, $P = \{P_h\}_{h=1}^H$ is the transition kernels, and μ_0 is the initial distribution. At each episode k, the agent chooses a policy π^k , which is a collection of H functions $\{\pi_h^k : \mathcal{S} \to \mathcal{A}\}_{h=1}^H$, and nature samples an initial state s_1^k from the initial distribution μ_0 . Then, at step h, the agent takes an action $a_h^k = \pi_h^k(s_h^k)$ after observing state s_h^k . The environment then moves to a new state s_{h+1}^k sampled from the distribution $P_h(\cdot|s_h^k, a_h^k)$ without revealing any feedback. After each episode, the trajectory of all state-action pairs is collected, which we use τ^k to denote, i.e., $\tau^k = \tau_{1:H}^k = \{(s_h^k, a_h^k)\}_{h=1}^H$.

Trajectory Reward Model: In this paper, we assume the expected reward of each trajectory τ is a general function $f(\tau)$ which maps trajectory to real values, a slight generalization of the cumulative reward structure. Let Ψ be the set of all partial or complete trajectories. Then, we assume there exists a function $f: \Psi \to [0, D]$ which is the expected reward of the MDP \mathcal{M} , where D is a positive constant. The reward of a certain trajectory may be random, but humans will evaluate trajectories based on the expected reward. The cumulative reward model is $f(\tau) = \sum_{h=1}^{H} r(s_h, a_h)$. Under the trajectory reward, we can formulate the Q-function as follows:

$$V_h^{\pi}(s) = \mathbb{E}^{\pi} \left[f(\tau_{h:H}) | s_h = s \right] = \mathbb{E} \left[f(\tau_{h:H}) | s_h = s, a_h = \pi(s), \tau_{h+1:H} \sim \pi \right],$$

$$Q_h^{\pi}(s, a) = \mathbb{E}^{\pi} \left[f(\tau_{h:H}) | s_h = s, a_h = a \right] = \mathbb{E} \left[f(\tau_{h:H}) | s_h = s, a_h = a, \tau_{h+1:H} \sim \pi \right].$$

The optimal policy π^* is defined as $\pi^* = \arg \max_{\pi} \mathbb{E}_{\mu_0}[V_1^{\pi}(x_1)]$. Without regularity on f, learning the π^* may fundamentally take $\Omega(A^H)$ samples. Therefore, we impose the following assumption:

Assumption 1 There exists a uniformly optimal deterministic stationary policy π^* for the MDP, i.e., $\pi^* = \arg \max_{\pi} V_h^{\pi}(s), \forall (h, s).$

Under the assumption, we define the value function gap for sub-optimal actions similar to classic MDPs as $\Delta_h(s,a) = V_h^*(s) - Q_h^*(s,a) = \max_{a'} Q_h^*(s,a') - Q_h^*(s,a)$. Let $\Delta_{\min} = \min_{h,s,a \neq \pi^*(s)} \Delta_h(s,a)$. For simplicity, we assume the optimal action $\pi_h^*(s)$ is unique for each (h,s). Otherwise, we can incorporate Δ_{\min} into the algorithm so that the duel between the two optimal actions will terminate in a finite time. As a special case, Convex MDPs (Zahavy et al., 2021), e.g., pure exploration (Hazan et al., 2019), apprenticeship learning (Abbeel & Ng, 2004), and adversarial RL (Rosenberg & Mansour, 2019), satisfy Assumption 1 when the optimal policy is deterministic.

Human Feedback: The agent has access to an oracle (a human expert) that evaluates the average quality (reward) of two trajectory batches. At the end of each episode, the agent has the opportunity to choose two sets of (partial) trajectories, denoted by \mathcal{D}_0 and \mathcal{D}_1 with cardinality M_0 and M_1 , to query the human for which has the higher average reward. We slightly abuse the notation τ to let τ_0^i and τ_1^i be the *i*-th (partial) trace in \mathcal{D}_0 and \mathcal{D}_1 respectively, i.e., $\mathcal{D}_0 = \{\tau_0^1, \tau_0^2, \cdots, \tau_0^{M_0}\}$, and $\mathcal{D}_1 = \{\tau_1^1, \tau_1^2, \cdots, \tau_1^{M_1}\}$. Each of them may contain only certain steps. After observing the two sets of trajectories, the oracle will give a one-bit feedback $\sigma \in \{0, 1\}$ to the agent to indicate the dataset he/she favors. For simplicity, let $\overline{f}(\mathcal{D}_1)$ and $\overline{f}(\mathcal{D}_0)$ denote the average trajectory reward of \mathcal{D}_1 and \mathcal{D}_0 . Existing works mostly assume the Bradley-Terry model for preference generalization, i.e., the preference probability is a logistic function of the reward difference, i.e.,

$$\mathbb{P}\left(\mathcal{D}_1 \succ \mathcal{D}_0\right) = u\left(\overline{f}(\mathcal{D}_1) - \overline{f}(\mathcal{D}_0)\right) = \frac{1}{1 + \exp\left(\overline{f}(\mathcal{D}_1) - \overline{f}(\mathcal{D}_0)\right)},$$

where $u : \mathbb{R} \to [0, 1]$ is referred to as the link function (Bengs et al., 2021) which characterizes the structure of preference models. Other link functions, such as linear function, probit function, cloglog

function, and cauchit function, have also been well-studied in dueling bandits (Ailon et al., 2014) and generalized linear models (Razzaghi, 2013; McCulloch, 2000), but not RLHF. In this paper, we use a 0-1 link function that indicates the favored set with higher reward, i.e.,

$$\sigma = \mathsf{HumanFeedback}(\mathcal{D}_0, \mathcal{D}_1) = \mathop{\arg\max}_{i \in \{0,1\}} \overline{f}(\mathcal{D}_i) = \mathop{\arg\max}_{i \in \{0,1\}} \frac{1}{M_i} \sum_{m=1}^{M_i} f(\tau_i^m).$$

Generalization to other link functions can be achieved through revising the probability gap definition below (Def. 1). Furthermore, we show in Fig. 1 that single trajectory preference may not align with the expected reward and thus batched comparison is necessary, and it may be easier for humans to identify a better response if the trajectory batches resemble each other with the same initial state, which motivates the comparison between partial and batched trajectories. Typically, in an LLM training setting, for each candidate policy, the human evaluator will look at multiple responses generated respectively and then assess which policy has a better average quality. Similarly for UAV training, humans will watch multiple UAV trajectories for each policy and declare which policy is better based on the average quality of the movement, i.e., success rate, stability, etc. When the batch sizes are not unbearably large, batched preference assessment of trajectories should not be essentially harder than single trajectory preference assessment.

Problem Formulation: Our goal is to design a learning algorithm to interact with the MDP and learn the optimal policy π^* from the human feedback as quickly as possible. A learning algorithm Alg consists of (i) a sampling rule which decides which policy to choose at each episode and whether to query the human agent, (ii) a stopping rule which decides a stopping time when the learner wishes to output an learned policy, and (iii) a decision rule which decides which policy $\hat{\pi}$ to output. We call an algorithm δ -PAC if it outputs an optimal policy with probability at least $1 - \delta$. Our goal is to design such an algorithm to minimize sample complexity K:

$$\min \mathbb{E}[K]$$
, such that $\mathbb{P}(\hat{\pi} = \pi^*) \ge 1 - \delta$.

3 Main Results for Episodic MDPs

In this paper, we focus on the instance-dependent performance. To characterize the structure of the MDPs under human feedback, we introduce the notion of probability gaps in Def. 1 for each state and sub-optimal action, which is a generalization of the calibrated pairwise preference probability considered in the dueling bandits literature (Yue et al., 2012; Yue & Joachims, 2011). We also define the state visitation probability $p_h^{\pi}(s)$ of a given policy π in Def. 2.

Definition 1 (Probability Gap) Given (h,s) and a sub-optimal action a, the probability gap $\overline{\Delta}_h^M(s,a)$ for comparison of two trajectory sets with cardinality both being M is defined as:

$$\overline{\Delta}_{h}^{M}(s,a) = \underbrace{\mathbb{P}\left(\sum_{m=1}^{M} f(\tau_{0}^{m}) > \sum_{m=1}^{M} f(\tau_{1}^{m}) \middle| \tau_{0}^{m} \sim \pi^{*}, \ \tau_{1}^{m} \sim \{a_{h} = a, \pi^{*}\}\right)}_{\overline{p}_{h}^{M}(s,a)} - \frac{1}{2},$$

where the traces $\{\tau_0^1,\cdots,\tau_0^M\}$ are independently sampled starting from state (h,s) using the optimal policy $\{\pi_k^*\}_{k=h}^H$, while $\{\tau_1^1,\cdots,\tau_1^M\}$ are independently sampled starting from state (h,s) using immediate action $a_h=a$ and the optimal policy $\{\pi_k^*\}_{k=h+1}^H$ afterwards. Let $\overline{\Delta}_{\min}^M=\min_{h,s,a}\overline{\Delta}_h^M(s,a)$.

Definition 2 (State Visitation Probability) Given $(h,s) \in [H] \times S$, the visitation probability (occupancy measure) of policy π is defined as follows:

$$p_h^{\pi}(s) = \mathbb{P}(s_h = s | s_0 \sim \mu_0, \ a_{h'} \sim \pi(s_{h'}), \ \forall h' < h).$$

Let $p_{\max}^{\pi} = \min_{h,s} \max_{\pi} p_h^{\pi}(s)$, and we assume it is positive. We will use both the probability gap and the state visitation probability to characterize our instance-dependent performance.

Algorithm 1: BASD for Episodic MDPs

```
initialize for all (h, s, a), J_h(s, a) \leftarrow 1, L_h(s, a) \leftarrow 0, M_h(s) \leftarrow 0, and l \leftarrow H, k \leftarrow 0;
initialize for all (h, s, a, a'), w_h(s, a, a') \leftarrow 0, N_h(s, a, a') \leftarrow 0, \hat{\pi}_h(s) = \mathcal{D}_h^0(s) = \mathcal{D}_h^1(s) = \emptyset;
define \iota \equiv c \log(\frac{SAHk}{\delta}), \beta_t = \sqrt{\frac{H\iota}{\max\{t,1\}}}, and \alpha_t = \frac{H+1}{H+t};
\hat{\sigma}_h(s,a,a') \equiv \frac{w_h(s,a,a')}{N_h(s,a,a')} \text{ or } \frac{1}{2} \text{ if } N_h(s,a,a') = 0, \ b_h(s,a,a') \equiv \sqrt{\frac{\iota}{\max\{N_h(s,a,a'),1\}}}, \ \forall (h,s,a,a') \ ;
while l \ge 1 do
      receive s_1, k = k + 1;
                                                                                                                     // reward-free exploration
      for step \ h = 1 : l - 1 \ do
            take action a_h \leftarrow \arg\max_a J_h(s_h, a) and observe s_{h+1}, L_h(s_h, a_h) \leftarrow L_h(s_h, a_h) + 1;
            W_{h+1}(s_{h+1}) \leftarrow \min\{1, \max_a J_{h+1}(s_{h+1}, a)\}\;;
           J_h(s_h, a_h) \leftarrow (1 - \alpha_t) J_h(s_h, a_h) + \alpha_t [W_{h+1}(s_{h+1}) + 2\beta_t] \text{ where } t = L_h(s_h, a_h) ;
      M_l(s_l) \leftarrow M_l(s_l) + 1. \ W_l(s_l) \leftarrow \min\{1, b_{M_l(s_l)}\}\ ;
      call action dueling sub-routine B-RUCB(l, s_l, M_l(s_l));
                                                                                                                                    // action dueling
      if \forall s, \exists a, \text{ such that } \forall a', \ \hat{\sigma}_l(s, a, a') - b_l(s, a, a') \geq 0.5 \text{ then}
            \forall s, \, \hat{\pi}_l(s) \in \{a | \forall a', \, \hat{\sigma}_l(s, a, a') - b_l(s, a, a') \ge 0.5\} \; ;
           l \leftarrow l-1. J_h(s,a) \leftarrow 1, L_h(s,a) \leftarrow 0, \forall (h,s,a), k \leftarrow 0;
                                                                                                                                  // backward search
return \hat{\pi}
```

Algorithm 2: B-RUCB: a batched dueling bandits sub-routine

```
Input: step h, state s, candidate policy \hat{\pi}, past visits M_h(s).
if M_h(s) \pmod{2M} \leq M then
     if M_h(s) \equiv 1 \pmod{M} then
                                                                                                            // select relative optimal arm
           C_h(s) = \{a | \forall a' : \hat{\sigma}_h(s, a, a') + b_h(s, a, a') \ge 0.5\}, \text{ sample } \hat{a}_s \text{ uniformly from } C_h(s);
        \mathcal{D}_h^0(s) \leftarrow \emptyset, \, \mathcal{D}_h^1(s) \leftarrow \emptyset;
     take action a_h \leftarrow \hat{a}_s and observe s_{h+1}, and use policy \hat{\pi} for steps afterwards;
     \mathcal{D}_{b}^{0}(s) = \mathcal{D}_{b}^{0}(s) \cup \{(s_{h}, a_{h}), \cdots, (s_{H}, a_{H})\};
else
     if M_h(s) \equiv 1 \pmod{M} then
                                                                                                   // select combating arm based on {\tt UCB}
       \tilde{a}_s = \arg\max_{a \neq \hat{a}_s} \{\hat{\sigma}_h(s, a, \hat{a}_s) + b_h(s, a, \hat{a}_s)\};
     take action a_h \leftarrow \tilde{a}_s and observe s_{h+1}, and use policy \hat{\pi} for steps afterwards;
     \mathcal{D}_h^1(s) = \mathcal{D}_h^1(s) \cup \{(s_h, a_h), \cdots, (s_H, a_H)\}\;;
if M_h(s) \equiv 0 \pmod{2M} then
                                                                                                         // query human every 2M episodes
     query feedback \sigma = \mathsf{HumanFeedback}\left(\mathcal{D}_h^0(s), \mathcal{D}_h^1(s)\right);
     w_h(s, \tilde{a}_s, \hat{a}_s) \leftarrow w_h(s, \tilde{a}_s, \hat{a}_s) + \sigma, w_h(s, \hat{a}_s, \tilde{a}_s) \leftarrow w_h(s, \hat{a}_s, \tilde{a}_s) + 1 - \sigma;
     N_h(s, \tilde{a}_s, \hat{a}_s) = N_h(s, \tilde{a}_s, \hat{a}_s) + 1;
return
```

3.1 Algorithm for Episodic RLHF

In this section, we propose an algorithm called BASD (Alg. 1) to solve the RLHF for episodic MDPs. The algorithm can be divided into two major modules: (i) an action dueling sub-routine generalizing the RUCB algorithm from the dueling bandits (Zoghi et al., 2014), and (ii) a reward-free exploration strategy to equalize the visitation probability of each state to minimize the overall sample complexity.

Backward Action Dueling: BSAD identifies the optimal policy for each state using a backward search. The backbone is to employ a batched version of the RUCB algorithm (Zoghi et al., 2014), called B-RUCB in Alg. 2, which is called in step l and controls the action selection policy from step l to H. Namely, it chooses the action a_l at step l using the RUCB dueling bandits principle and then uses the candidate optimal policy $\hat{\pi}$ for steps afterward. If the policy $\hat{\pi}$ is indeed the optimal

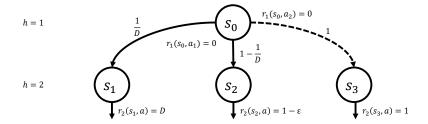


Figure 1: MDP where $\pi_h^*(s)$ is not the Condorcet winner: there are 3 states ($\{s_1, s_2, s_3\}$) at step 2 with 1 action, and 1 state s_0 in step 1 with 2 actions. With action a_1 , the state transits w.p. 1/D to state s_1 with reward D, and w.p. 1-1/D to state s_2 which gives reward $1-\varepsilon$, where $0 < \varepsilon < 1$. With action 2, the state transits deterministically to state s_3 with reward 1.

policy π^* , the average reward from step l to H constitutes an unbiased estimator of $Q_h^*(s_l, a_l)$, which resembles dueling bandits. Different from classic RUCB, we query human feedback every 2M episode with batches and we will show later that it allows the optimal action $\pi_h^*(s)$ to be the action favored by the human oracle (Condorcet winner). Moreover, we adopt a stopping rule for each (h, s) that if there exists one action a whose lower confidence bound of the preference probability estimation $\hat{\sigma}_h(s, a, a')$ is larger than half for all other actions, the optimal action is found. Specifically, we use $\mathcal{T}_h(s)$ to denote the stopping rule for state (h, s), i.e., $\mathcal{T}_h(s) = \{\exists a, \forall a', \hat{\sigma}_l(s, a, a') - b_l(s, a, a') \geq 0.5\}$. Then, the criteria for l to move from h to h-1 is equivalent to $\cap_{s=1}^S \mathcal{T}_h(s)$. Running B-RUCB with the stopping rule identifies the optimal action $\pi_l^*(s)$ for all states at step l with high probability.

Reward-free Exploration: To minimize the sample complexity, it is ideal that every state has a similar visitation probability so that action identification can be performed simultaneously for all the states. Our chosen model-free reward-free exploration between step 1 to step l-1 contributes towards this goal. We slightly adapted the UCBZero algorithm originally proposed in (Zhang et al., 2020) in our BSAD algorithm so that the overall algorithm is model-free. This strategic exploration policy will guarantee that we visit each state on step l proportional to the maximum visitation probability over all possible policy π starting from the initial distribution.

3.2 Theoretical Results

It is well-known from dueling bandits literature (Zoghi et al., 2014) that the RUCB algorithm only requires the existence of the Condorcet winner to identify the optimal action, where the Condorcet winner refers to an action that is preferred with probability larger than half when compared to any other action. Similar to the definition in dueling bandits, for any state (h, s) and any size M, we say the optimal action $\pi_h^*(s)$ is the Condorcet winner if the preference probability $\overline{p}_h^M(s, a)$ is larger than half for all other actions a. For any comparison-based algorithm to identify the optimal policy, the optimal policy must be the Condorcet winner. We will first characterize the existence of the Condorcet winner when human experts are queried with batch size M large enough.

Lemma 1 Given an MDP \mathcal{M} and for any (h, s), the action $\pi_h^*(s)$ associated with the optimal policy π^* is the Condorcet winner in the HumanFeedback comparison as long as $M = \Omega(D^2 \Delta_{\min}^{-2})$.

Existence of Condorcet Winner: In general, the optimal action $\pi_h^*(s)$, although it maximizes the expected reward, is not necessarily the Condorcet winner with arbitrary M. To see this, consider a two-step MDP with traditional cumulative reward as shown in Fig. 1. For state s_0 and D > 2 in step 1, the optimal action is a_1 which gives expected reward $1 + (1 - D^{-1})(1 - \varepsilon)$ larger than 1 given by action a_2 . However, if we choose M = 1 and query human feedback of the duel between action a_1 and a_2 , the human expert will only prefer action a_1 if the state transits to s_1 , which only occurs with probability 1/D and could be much less than half. Therefore, the optimal action a_1 for state s_0 is not the Condorcet winner. Similarly, it is also not hard to construct counter-examples with more

than three actions to show that the Condorcet winner does not exist. However, Lemma. 1 shows that the optimal action $\pi_h^*(s)$ is indeed the Condorcet winner at every state (h,s) as long as the batch size M is large enough. The bound is proportional to D^2 which characterizes the variance of reward for a single trajectory and inversely proportional to the square of the minimum value function gap Δ_{\min} , which characterizes the distinguishability among actions. The proof of Lemma. 1 is deferred to the appendix, where we apply concentration inequalities to lower bound the preference probability $\overline{p}_h^M(s,a)$. Next, we characterize the sample complexity of BSAD.

Theorem 1 Given an MDP \mathcal{M} , fix δ and suppose M is chosen large enough such that the optimal policy π^* is the Condorcet winner for all states (h,s). Then with probability at least $1 - \mathcal{O}(\delta)$, the BSAD algorithm terminates within K episodes and returns the optimal policy $\hat{\pi} = \pi^*$ with:

$$K = \tilde{\mathcal{O}}\left(\sum_{h=1}^{H} \frac{SA^3h^2M\log(\frac{1}{\delta})}{\min_{s,a} \max_{\pi} [\overline{\Delta}_h^M(s,a)p_h^{\pi}(s)]^2}\right).$$

Proof Roadmap: Our main Theorem. 1 conveys two messages: (i) BSAD is δ -PAC, and (ii) BSAD has provable instance-dependent sample complexity bound under general reward model. The proof of Theorem. 1 is deferred to appendix. To obtain the correctness guarantee, we decompose the probability of making a mistake into the sum of probabilities where the mistake is made on a certain step h. Then, using a backward induction argument, we show that the total mistake probability is small. To obtain the sample complexity bound, we fix (h, s) and then bound the number of comparisons between two actions. Next, we bound the total number of comparisons and the total number of episodes needed to identify the optimal action for this (h, s). This can be achieved by summing up the number of comparisons between all pairs of arms before the stopping criteria $\mathcal{T}_h(s)$ for that state is satisfied. Lemma. 2 characterizes the sample complexity for any state (h, s):

Lemma 2 Given an MDP \mathcal{M} , fix δ and suppose M is large enough. For fixed (h, s), the number of episodes with l = h and $s_h = s$ until the criteria $\mathcal{T}_h(s)$ is bounded with high probability by:

$$M_h(s) = \tilde{\mathcal{O}}\left(\sum_{i=2}^{A} \frac{i}{\overline{\Delta}_h^M(s, a_i)^2} M \log\left(\frac{1}{\delta}\right)\right) = \tilde{\mathcal{O}}\left(\frac{A^2 M \log\left(\frac{1}{\delta}\right)}{\min_a \overline{\Delta}_h^M(s, a)^2}\right),$$

where $\{a_1, a_2, \dots, a_A\}$ is a permutation of the action set \mathcal{A} such that a_1 is the optimal action and $\overline{\Delta}_h^M(s, a_2) \leq \overline{\Delta}_h^M(s, a_2) \leq \dots, \overline{\Delta}_h^M(s, a_A)$.

Notice that our bound in Lemma. 2 is different from the original RUCB algorithm provided in (Zoghi et al., 2014, Theorem 4) due to (i) we study a PAC setting while the vanilla RUCB focuses on regret minimization and (ii) we chose a larger confidence bonus so that our bound only have logarithmic dependence on δ . After bounding the sample complexity to identify the optimal action for each state, we need to relate $M_h(s)$ to the total number of episodes through reward-free exploration. We show in Lemma. 3 that the number of episodes spent for a step l=h is bounded by the number of visitations $M_h(s)$, which is analog to (Zhang et al., 2020, Theorem 3).

Lemma 3 Given an MDP \mathcal{M} , fix δ and suppose M is large enough. For a fixed (h, s), suppose we have l = h and $k = K_h$ in the current episode, we have:

$$\forall s, \ K_h \le \mathcal{O}\left(\frac{SAh^2M_h(s)}{\max_{\pi} p_h^{\pi}(s)^2}\right).$$

Combining both Lemma. 2 and Lemma. 3, we will be able to prove Theorem. 1:

$$K = \sum_{h=1}^{H} \max_{s} \mathcal{O}\left(\frac{SAh^2 M_h(s)}{\max_{\pi} p_h^{\pi}(s)^2}\right) = \tilde{\mathcal{O}}\left(\sum_{h=1}^{H} \frac{SA^3h^2 M \log(\frac{1}{\delta})}{\min_{s,a} \max_{\pi} [\overline{\Delta}_h^M(s,a) p_h^{\pi}(s)]^2}\right).$$

RLHF Algorithm with Logarithm Regret: It is very simple to adapt the BSAD algorithm to an explore-then-commit type algorithm for regret minimization by choosing $\delta = T^{-1}$. Then, the sample complexity bound will convert into a regret bound in the order of $\mathcal{O}(\log T)$. To the best of our knowledge, this is the first RLHF algorithm with logarithmic regret performance.

Instance Dependence and Connection to Classical RL: Our sample complexity bound in Theorem. 1 has a linear dependence on the number of states S, a polynomial on the number of actions A and the planning horizon H, and a logarithmic dependence on the inverse of confidence δ . Moreover, it characterizes how the sample complexity depends on fine-grained structures of the MDP \mathcal{M} itself. It is also inversely proportional to the square of the probability gap $\overline{\Delta}_h^M(s,a)$ which resembles the sample complexity or regret bounds in the dueling bandit literature, and also resembles the dependence of the value function gap $\Delta_h(s,a)$ in the sample complexity bounds for traditional tabular RL, e.g., (Wagenmaker et al., 2022, Theorem 2). Moreover, the inverse proportional dependence of the maximum state visitation probability over all policies also resembles the traditional RL. In fact, with M chosen in the same order as in Lemma. 1 and using concentration inequalities, the sample complexity bound can be converted depending on the value function gap as follows:

$$K = \tilde{\mathcal{O}}\left(\frac{SA^3H^3D^2\log(\frac{1}{\delta})}{\min_{h,s,a}\Delta_h(s,a)^2\max_{\pi}p_h^{\pi}(s)^2}\right).$$

This shows that RLHF is almost no harder than classic RL given the appropriate parameter, except for a polynomial factor on the number of actions A and the planning horizon H. This finding coincides with (Wang et al., 2023) and sheds light on the similarity between RLHF and classic RL. Notice that our result is derived from a general reward model where the Bellman equations do not hold. Therefore, our result also seemingly implies that the fundamental backbone of RL is the existence of uniformly optimal stationary policy instead of the Bellman equations.

4 Generalization to Discounted MDPs

In this section, we generalize the BSAD algorithm to discounted MDPs with the traditional state-action reward function $r(s,a) \in [0,1]$ and discount factor γ . Our approach is to segment the time horizon into frames with length $H = \Theta(\frac{1}{1-\gamma}\log\frac{1}{\varepsilon(1-\gamma)^2})$. Then, we run BSAD (Alg. 1) with horizon H on the discounted MDP, as if it is episodic. This frame-based adaptation delivers provable instance-dependent sample complexity shown in Theorem. 2. Discussions are deferred to the appendix.

Theorem 2 suppose M is chosen large enough. Then with probability $1 - \mathcal{O}(\delta)$, BSAD terminates within K episodes and returns an ε -optimal policy with:

$$K = \tilde{\mathcal{O}}\left(\frac{SA^3M\log(\frac{1}{\delta})\log^3(\frac{1}{\varepsilon})}{(1-\gamma)^3\min_{h,s,a}\overline{\Delta}_h^M(s,a)^2\max_{\pi}\min_{s'}p_h^{\pi}(s|s')^2}\right),\,$$

where $\overline{\Delta}_h^M(s,a)$ to be the probability gap for action a and trajectories of length H-h compared to the Condorcet winner of that state s, and $p_h^{\pi}(s|s')$ is the visitation probability of s after h steps starting from state s' with policy π . Both definitions are analog to the definitions in episodic MDPs.

5 Numerical Results

In this section, we study the empirical performance of BSAD on an MDP based on Fig. 1 with D=10. The only difference is we replicate two copies of s_0 in the first step with different initial distributions. For these states, the optimal policy is not the Condorcet winner under a single trajectory comparison but will become the Condorcet winner when the batch size increases. We compare BSAD to existing value-based model-free RLHF algorithms, with and without reward inference, where the performance is measured by the value function $\mathbb{E}_{\mu_0}[V_1^{\hat{\pi}}(s)]$ of the candidate policy evaluated on the true MDP. The baselines that we chose are (i) a model-free and batched adaptation of PEPS (Xu et al., 2020) (no

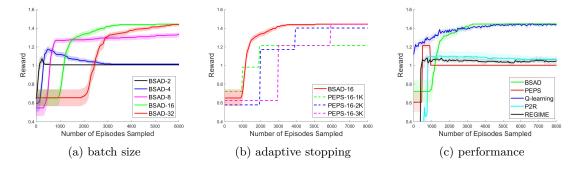


Figure 2: numerical experiment on a three-state two-step MDP: (a) shows the proposed BSAD algorithm with different batch sizes. (b) compares BSAD with adaptive stopping to batched version of PEPS with fixed exploration horizon. (c) compares BSAD to model-free RLHF and RL algorithms. Results are averaged over 100 trajectories and shaded areas represent bootstrap confidence intervals.

reward inference) which uses UCBZero (Zhang et al., 2020), (ii) Q-learning with P2R (Wang et al., 2023) (reward inference) where the candidate policy $\hat{\pi}$ is the greedy policy, and (iii) REGIME (Zhan et al., 2023b) (reward inference) with UCBZero and pessimistic Q-learning (Shi et al., 2022) as offline RL oracle, where each point is obtained through a 1k-episode offline RL algorithm. We also compare to classic RL algorithms, i.e., Q-learning (Jin et al., 2018).

Algorithm	BSAD(ours)	PEPS	Q-learning	P2R	REGIME
Running Time (ms)	171.21	179.23	1090.12	5898.30	4613.73

Table 2: running time comparisons on 1 CPU averaged over 50 trajectories.

Fig. 2a shows the effect of batch size. When using a small batch size, i.e., M = 2, 4, the Condorcet winner at h=1 is not optimal, and BSAD converges to a sub-optimal policy. When M is large, BSAD identifies the optimal policy, and the sample complexity displays a decrease-then-increase trend, which coincides with Theorem. 1. Specifically, when M increases, the probability gap in the denominator increases sharply, leading to reduced sample complexity, and as M continues to increase, M in the numerator starts to dominate. This justifies BSAD is adaptive to MDP instances. Fig. 2b shows the comparison of BSAD to a batched version of PEPS with different exploration horizons. The observation that the curve of BSAD lies uniformly above all PEPS curves shows the necessity of adaptive algorithm design. Specifically, our design of adaptive stopping criteria identifies the optimal policy earlier and adapts to the different distinguishability in different states. which results in improved regret performance. In Fig. 2c, we compare BSAD to Q-learning and RLHF algorithms with reward inference. First, we observe that BSAD has almost the same performance as Q-learning which uses the reward information, which shows RLHF is almost no harder than classic RL. However, our algorithm applies to the general trajectory reward function while Q-learning cannot be used anymore. BSAD exhibits superior performance than other RLHF algorithms also in running time as shown in Table. 2, because training reward models with MLE is difficult and takes much larger sample and computational complexity, let alone the best policy can only be obtained when the reward model is accurate enough. This observation somewhat justifies the reward model is unnecessary given it suffers from pitfalls like over-fitting and distribution shift.

6 Conclusion

We studied RLHF under both episodic MDPs with trajectory reward structure, a generalization of the classic cumulative reward. We propose an algorithm called BSAD which enjoys a provable instance-dependent sample complexity that resembles the result in classic RL with reward. We also

generalize our results to discounted MDPs. Our results show RLHF is almost no harder than classic RL, and the current dominating reward model training module in RLHF may be unnecessary.

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