THE PERILS OF OPTIMIZING LEARNED REWARD FUNCTIONS: LOW TRAINING ERROR DOES NOT GUARANTEE LOW REGRET

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For reviewers:
Red parts are from the original submission and will be removed for the camera-ready version.
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ABSTRACT

In reinforcement learning, specifying reward functions that capture the intended task can be very challenging. Reward learning aims to address this issue by *learning* the reward function. However, a learned reward model may have a low error on the data distribution, and yet subsequently produce a policy with large regret. We say that such a reward model has an *error-regret mismatch*. The main source of an error-regret mismatch is the distributional shift that commonly occurs during policy optimization. In this paper, we mathematically show that a sufficiently low expected test error of the reward model guarantees low worst-case regret, but that for any *fixed* expected test error, there exist realistic data distributions that allow for error-regret mismatch to occur. We then show that similar problems persist even when using policy regularization techniques, commonly employed in methods such as RLHF. Our theoretical results highlight the importance of developing new ways to measure the quality of learned reward models. We hope our results stimulate the theoretical and empirical study of improved methods to learn reward models, and better ways to reliably measure their quality.

1 INTRODUCTION

To solve a sequential decision problem with reinforcement learning (RL), we must first formalize that decision problem using a *reward function* (Sutton & Barto, 2018). However, for complex tasks, reward functions are often hard to specify correctly. To solve this problem, it is increasingly popular to *learn* reward functions with *reward learning algorithms*, instead of specifying the reward functions manually. There are many different reward learning algorithms (e.g., Ng & Russell, 2000; Tung et al., 2018; Brown & Niekum, 2019; Palan et al., 2019), with one of the most popular being *reward learning from human feedback* (RLHF) (Christiano et al., 2017; Ibarz et al., 2018).

For any learning algorithm, it is a crucial question whether or not that learning algorithm is guaranteed to converge to a "good" solution. For example, in the case of supervised learning for classification, it can be shown that a learning algorithm that produces a model with a low *empirical error* (i.e., training error) is likely to have a low *expected error* (i.e., test error), given a sufficient amount of training data and assuming that both the training data and the test data is drawn i.i.d. from a single stationary distribution (Kearns & Vazirani, 1994). In the case of normal supervised learning and standard assumptions, we can therefore be confident that a learning algorithm will converge to a good model, provided that it is given a sufficient amount of training data.

Since reward models are also typically learned by supervised learning, we might assume that classical learning-theoretic guarantees carry over. However, these guarantees only ensure that the reward model is approximately correct *relative to the training distribution*. But after reward learning, we optimize a policy to maximize the learned reward, which effectively leads to a *distributional shift*. This raises the worry that the trained policy can exploit regions of the state space with abnormally

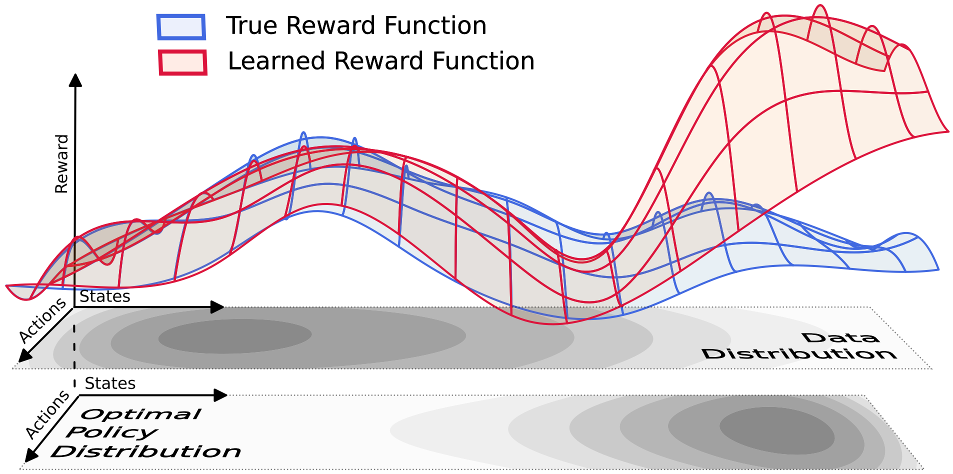

Figure 1: Reward models (red function) are commonly trained by supervised learning to approximate some latent, true reward (blue function). Given enough data, one can hope that the reward model is close to the true reward function on average over the data distribution (upper gray layer) — the expected *error* is low. However, low expected error only guarantees a good approximation to the true reward function in areas with high coverage by the data distribution! On the other hand, optimizing an RL policy to maximize the learned reward model induces a distribution shift which can lead the policy to exploit uncertainties of the learned reward model in low-probability areas of the transition space (lower gray layer). This may then lead to high *regret*. We refer to this phenomenon as *error-regret mismatch*.

high learned rewards if those regions have a low data coverage during training. In this case, we can have reward models that have both a low error on the training distribution and an optimal policy with large regret, a phenomenon we call *error-regret mismatch*. We visualize this concern in Figure 1.

To single out the issue of error-regret mismatch in our analysis, we take the goals of classical learning theory as a given and show that *they are not enough to ensure low regret*. More precisely, in probably approximately correct (PAC) learning (Kearns & Vazirani, 1994) the goal is to derive a sample size that guarantees a certain likelihood (“P”) of an approximately correct (“AC”) model on new data points sampled from the training distribution. In our results, we assume that we *already have* an approximately correct reward model on a data distribution, and then investigate what we can or can not conclude about the regret of policies trained to maximize the modeled reward.

Our theoretical analysis shows that guarantees in policy regret are very sensitive to the data distribution used to train the reward model, leading to our notions of *safe* and *unsafe data distributions*. Moreover, we find evidence that some MDPs are in a certain sense “too large” to allow for safe data distributions relative to a reasonable reward model error and desired regret bound. We establish for general MDPs:

1. As the error of a learned reward model on a data distribution goes to zero, the worst-case regret of optimizing a policy according to that reward model also goes to zero (Propositions 3.1 and 3.2)

2. However, for any $\epsilon > 0$, whenever a data distribution has sufficiently low coverage of some bad policy, it is *unsafe*; in other words, there exists a reward model that achieves an expected error of ϵ but has a high-regret optimal policy (Proposition 3.3), a case of error-regret mismatch.

3. As a consequence, when an MDP has a large number of independent bad policies, *every* data distribution is unsafe (Corollary 3.4).

4. More precisely, we derive a set of linear constraints that precisely characterize the safe data distributions for a given MDP (Theorem 3.5).

We then investigate the case of *regularized* policy optimization (including KL-regularized policy optimization, which is commonly used in methods such as RLHF). We derive regularized versions of Propositions 3.1 and 3.3 in Proposition 4.1 and Theorem 4.2. This shows that regularization alone is no principled solution to error-regret mismatch.

We then develop several generalizations of our results for different types of data sources for reward model training, such as preferences over trajectories (Propositions 5.2 and 5.3), and trajectory scoring (Proposition 5.1). Lastly, motivated by the recent success of large language models (OpenAI, 2022; Gemini Team, 2023; Anthropic, 2023), we provide an analysis for the special case of RLHF in the contextual bandit case where we prove a stronger version (Theorem 6.1) of the failure mode already discussed in Theorem 4.2 for general MDPs.

1.1 Related work

Note: We provide a more extensive related work section in Appendix A

Reward Learning Reward learning is a key concept in reinforcement learning that involves learning the reward function for complex tasks with latent and difficult-to-specify reward functions. Many methods have been developed to incorporate various types of human feedback into the reward learning process (Wirth et al., 2017; Ng et al., 2000; Bajcsy et al., 2017; Jeon et al., 2020).

Challenges in Reward Learning Reward learning presents several challenges (Casper et al., 2023; Lang et al., 2024b; Skalse & Abate, 2023; 2024), such as *reward misgeneralization*, where a learned reward model performs well on in-distribution data but misgeneralizes on out-of-distribution data (Skalse et al., 2023). This can lead to unintended consequences in real-world applications.

Reward misgeneralization can also result in *reward hacking* (Krakovna, 2020), a consequence of Goodhart's law (Goodhart, 1984; Zhuang & Hadfield-Menell, 2020; Hennessy & Goodhart, 2023; Strathern, 1997; Karwowski et al., 2023). Reward hacking has been extensively studied both theoretically (Skalse et al., 2022; 2024; Zhuang & Hadfield-Menell, 2020) and empirically (Zhang et al., 2018; Farebrother et al., 2018; Cobbe et al., 2019; Krakovna, 2020; Gao et al., 2023; Tien et al., 2022).

Distributional Shifts in policy learning During policy optimization, a distribution shift occurs where the policy under training can explore areas of the input space that are outside of the reward model's training distribution. This might lead to large regret in case that the reward model is misgeneralized. To address issues with distributional shifts in reward learning specifically, prior work has proposed many different methods, such as ensembles of conservative reward models (Coste et al., 2023), averaging weights of multiple reward models (Ramé et al., 2024), iteratively updating training labels (Zhu et al., 2024), on-policy reward learning (Lang et al., 2024a), and distributionally robust planning (Zhan et al., 2023).

Worst-case regret studies Several prior works perform theoretical investigations of policy regret under a worst-case MDP in settings involving imitation learning (Ross et al., 2011), offline RL (Kim et al., 2024; Jin et al., 2021; Zhang et al., 2022), and other RL settings (Lu et al., 2024; Laidlaw et al., 2024; Kwa et al., 2024). Furthermore, additional work performs analyses of RLHF (Cen et al., 2024; Xiong et al., 2024; Zhu et al., 2023; Ji et al., 2023; Mehta et al., 2023) and reward learning in general (Agarwal et al., 2012; Foster et al., 2020) in the contextual bandit setting.

Our work is most closely related to (Zhu et al., 2024; Nika et al., 2024; Cen et al., 2024), which provide examples of high regret and regret bounds specifically for different RLHF settings. We contrast ourselves from their work by focusing on theoretically analyzing the guarantees from errors with respect to data distributions on the regret of the final policy. We thus narrow down and illuminate issues that are unique to RL with policy learning compared to supervised learning. In doing so, we assume *arbitrary* MDPs and investigate the regret a policy might attain for a worst-case reward model (instead of a worst-case MDP).

2 Preliminaries

A *Markov Decision Process* (MDP) is a tuple $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ where $\mathcal{S}$ is a set of *states*, $\mathcal{A}$ is a set of *actions*, $\tau : \mathcal{S} \times \mathcal{A} \to \Delta(\mathcal{S})$ is a *transition function*, $\mu_0 \in \Delta(S)$ is an *initial state distribution*,

$R : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ is a *reward function*, and $\gamma \in (0, 1)$ is a *discount rate*. We define the *range* of a reward function R as $\operatorname{range} R \coloneqq \max_{(s,a) \in \mathcal{S} \times \mathcal{A}} R(s, a) - \min_{(s,a) \in \mathcal{S} \times \mathcal{A}} R(s, a)$.

A *policy* is a function $\pi : \mathcal{S} \to \Delta(\mathcal{A})$. We denote the set of all policies by Π. A *trajectory* $\xi = \langle s_0, a_0, s_1, a_1, ... \rangle$ is a possible path in an MDP. The *return function* G gives the cumulative discounted reward of a trajectory, $G(\xi) = \sum_{t=0}^{\infty} \gamma^t R(s_t, a_t)$, and the *evaluation function* J gives the expected trajectory return given a policy, $J(\pi) = \mathbb{E}_{\xi \sim \pi} [G(\xi)]$. A policy maximizing J is an *optimal policy*. We define the *regret* of a policy π with respect to reward function R as

$$\operatorname{Reg}^R (\pi) \coloneqq \frac{\max_{\pi' \in \Pi} J_R(\pi') - J_R(\pi)}{\max_{\pi' \in \Pi} J_R(\pi') - \min_{\pi' \in \Pi} J_R(\pi')} \in [0, 1].$$

Here, J_R is the policy evaluation function for R.

In this paper, we assume that $\mathcal{S}$ and $\mathcal{A}$ are finite, and that all states are reachable under τ and μ_0. We also assume that $\max J_R - \min J_R \neq 0$ (since the reward function would otherwise be trivial). Note that this implies that $\operatorname{range} R > 0$, and that $\operatorname{Reg}^R (\pi)$ is well-defined.

The *state-action occupancy measure* is a function $\eta : \Pi \to \mathbb{R}^{|\mathcal{S} \times \mathcal{A}|}$ mapping each policy $\pi \in \Pi$ to the corresponding "state-action occupancy measure", describing the discounted frequency that each state-action tuple is visited by a policy. Formally, $\eta(\pi)(s, a) = \eta^\pi(s, a) = \sum_{t=0}^{\infty} \gamma^t \cdot P(s_t = s, a_t = a \mid \xi \sim \pi)$. Note that by writing the reward function R as a vector $\vec{R} \in \mathbb{R}^{|\mathcal{S} \times \mathcal{A}|}$, we can split J into a function that is linear in R: $J(\pi) = \eta^\pi \cdot \vec{R}$. By normalizing a state-action occupancy measure η^π we obtain a *policy-induced distribution* $D^\pi \coloneqq (1 - \gamma) \cdot \eta^\pi$.

2.1 Problem formalization of RL with reward learning

In RL with reward learning, we assume that we have an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ where the reward function R is unknown. We may also assume that τ and μ_0 are unknown, as long as we can sample from them (though $\mathcal{S}$, $\mathcal{A}$, and γ must generally be known, at least implicitly). We then first learn a reward model $\hat{R}$ that approximates the true reward R and then optimize a policy $\hat{\pi}$ to maximize $\hat{R}$. The aim of this two-step procedure is for $\hat{\pi}$ to achieve low regret under the true reward function R. We now formalize these aspects in detail for our theoretical analysis, with a visualization provided in Figure 2:

Reward learning We first learn a reward model $\hat{R}$ from data. There are many possible data sources for reward learning, like demonstrations (Ng & Russell, 2000), preferences over trajectories (Christiano et al., 2017), or even the initial environment state (Shah et al., 2019); a taxonomy can be found in (Jeon et al., 2020). Since we are concerned with problems that remain even when the reward model is already *approximately correct*, we abstract away the data sources and training procedures and assume that we learn a reward model $\hat{R}$ which satisfies

$$\mathbb{E}_{(s,a) \sim D} \left[\frac{|\hat{R}(s, a) - R(s, a)|}{\operatorname{range} R} \right] \leq \epsilon \tag{1}$$

for some $\epsilon > 0$ and stationary distribution D over transitions $\mathcal{S} \times \mathcal{A}$. Note that this is the true expectation under D, rather than an estimate of this expectation based on some finite sample. We divide by $\operatorname{range} R$, since the absolute error ϵ is only meaningful relative to the overall scale of the reward R.

To be clear, most reward learning algorithms *cannot guarantee* a bound as in Equation (1) since most realistic data sources do not determine the true reward function, even for infinite data (Skalse et al., 2023). Instead, we choose Equation (1) because it serves as an *upper bound* to many common reward learning training objectives (see Appendix C.5). Thus, when we show in later sections that high regret is possible even when this inequality holds, then this problem can be expected to generalize to other data sources. We make this generalization precise for some data sources in Section 5. In particular, we will show that Equation (1) implies a low cross-entropy error between the choice distributions of the true reward function and the reward model, as is commonly used for RLHF, e.g. in the context of language models (Ziegler et al., 2019).

Policy optimization Given $\hat{R}$, we then learn a policy $\hat{\pi}$ by solving the MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, \hat{R}, \gamma \rangle$. In the most straightforward case, we do this by simply finding a policy that is optimal according

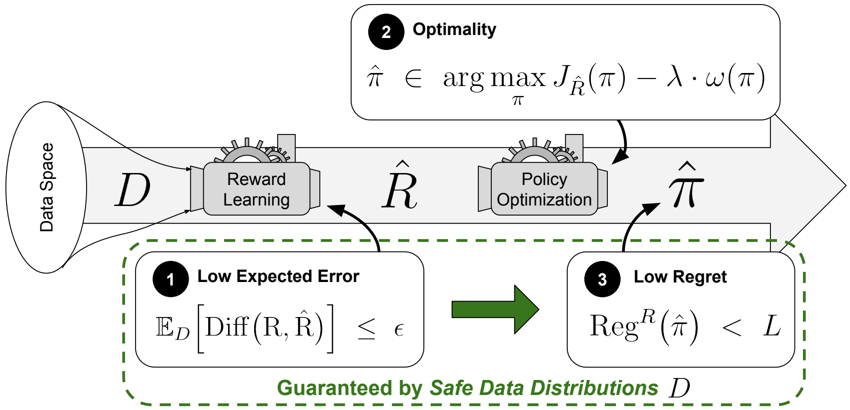

Figure 2: An abstract model of the classical reward learning pipeline. A reward model $\hat{R}$ is trained to approximate the true reward function R under some data distribution D. The training process converges when $\hat{R}$ is similar to R in expectation (see 1). In the second step, a policy $\hat{\pi}$ is trained to achieve high learned reward, possibly involving a regularization (see 2). We are interested in the question of when exactly this training process guarantees that $\hat{\pi}$ has low regret. More formally, we call a data distribution D *safe* whenever the implication 1 $\Longrightarrow$ 3 holds for all reward models $\hat{R}$ that satisfy 1.

to $\hat{R}$. However, it is also common to perform *regularized optimization*. In that case, we make use of an additional regularization function $\omega : \Pi \to \mathbb{R}$, with $\omega(\pi) \geq 0$ for all $\pi \in \Pi$. Given $\hat{R}$, a regularization function ω, and a regularization weight $\lambda \in [0, \infty)$, we say that $\hat{\pi}$ is (λ, ω)-optimal if

$$\hat{\pi} \in \arg\max_{\pi} J_{\hat{R}}(\pi) - \lambda\omega(\pi). \tag{2}$$

Typically, λ punishes large deviations from some reference policy π_{ref}, e.g. with the regularization function given by the KL-divergence $\omega(\pi) = \mathbb{D}_{\text{KL}}\left(\pi || \pi_{\text{ref}}\right)$. π_{ref} may also be used to collect training data for the reward learning algorithm, in which case we may assume $D = D^{\pi}$ in Equation (1). Most of our results to not depend on these specific instantiations, however.

Regret minimization The aim of the previous two steps is for the policy $\hat{\pi}$ to have low regret $\mathrm{Reg}^R(\hat{\pi})$ under the true reward function R. Our question is thus if and when it is sufficient to ensure that $\hat{R}$ satisfies Equation 1, in order to guarantee that a policy $\hat{\pi}$ optimal according to Equation (2) has low regret $\mathrm{Reg}^R(\hat{\pi})$.

2.2 Safe data distributions

We now make the elaborations from the previous subsections more concrete by providing a formal definition of a *safe data distribution*. In particular, we say that a data distribution D is safe, whenever it holds that for every reward model $\hat{R}$ that satisfies Equation (1) for D, all optimal policies of $\hat{R}$ have low regret. We provide a visualization of this concept in Figure 2 and a formal definition in Definition 2.1.

Definition 2.1 (Safe- and unsafe data distributions)**.** For a given MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, let $\epsilon > 0$, $L \in [0, 1]$, and $\lambda \in [0, \infty)$. Let ω be a continuous function with $\omega(\pi) \geq 0$ for all $\pi \in \Pi$. Then the set of *safe data distributions* $\mathbf{safe}(R, \epsilon, L, \lambda, \omega)$ is the set of all distributions $D \in \Delta(\mathcal{S} \times \mathcal{A})$ such that for all possible reward models $\hat{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ and policies $\hat{\pi} : \mathcal{S} \to \Delta(\mathcal{A})$ that satisfy the following two properties:

1. **Low expected error:** $\hat{R}$ is ϵ-close to R under D, i.e., $\mathbb{E}_{(s,a) \sim D}\left[\frac{|\hat{R}(s,a) - R(s,a)|}{\text{range } R}\right] \leq \epsilon$.

2. **Optimality:** $\hat{\pi}$ is (λ, ω)-optimal with respect to $\hat{R}$, i.e. $\hat{\pi} \in \arg\max_{\pi} J_{\hat{R}}(\pi) - \lambda\omega(\pi)$.

we can guarantee that $\hat{\pi}$ has regret smaller than L, i.e.:

3. **Low regret:** $\hat{\pi}$ has a regret smaller than L with respect to R, i.e., $\text{Reg}^R(\hat{\pi}) < L$.

Similarly, we define the set of *unsafe data distributions* to be the complement of $\mathbf{safe}(R, \epsilon, L, \lambda, \omega)$:

$$\mathbf{unsafe}(R, \epsilon, L, \lambda, \omega) \quad := \quad \{\, D \in \Delta(\mathcal{S} \times \mathcal{A}) \mid D \notin \mathbf{safe}(R, \epsilon, L, \lambda, \omega)\}.$$

Thus, $\mathbf{unsafe}(R, \epsilon, L, \lambda, \omega)$ consists of the data distributions D for which there *exists* a reward model $\hat{R}$ that is ϵ-close to R and a policy $\hat{\pi}$ that is (λ, π)-optimal with respect to $\hat{R}$, but such that $\hat{\pi}$ has large regret $\text{Reg}^R(\hat{\pi}) \geq L$. In this sense, we are operating under a worst-case framework for the reward model and policy learned by our training algorithms. Lastly, whenever we consider the unregularized case ($\lambda = 0$ or $\omega = 0$), we drop the λ and ω to ease the notation and just use $\mathbf{safe}(R, \epsilon, L)$ and $\mathbf{unsafe}(R, \epsilon, L)$ instead.

Note: Throughout this paper, we will use the terminology that a data distribution D "allows for error-regret mismatch" as a colloquial term to express that $D \in \mathbf{unsafe}(R, \epsilon, L, \lambda, \omega)$.

3 Error-regret mismatch for unregularized policy optimization

In this section, we investigate the case where no regularization is used in the policy optimization stage. We seek to determine if it is sufficient for a reward model to be close to the true reward function on a data distribution in order to ensure low regret for the learned policy.

In our first result, we show that under certain conditions, a low expected error ϵ does indeed guarantee that policy optimization will yield a policy with low regret.

Proposition 3.1. *Let $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be an arbitrary MDP, let $L \in (0, 1]$, and let $D \in \Delta(\mathcal{S} \times \mathcal{A})$ be a* positive *data distribution (i.e., a distribution such that $D(s, a) > 0$ for all $(s, a) \in \mathcal{S} \times \mathcal{A}$). Then there exists an $\epsilon > 0$ such that $D \in \mathbf{safe}(R, \epsilon, L)$.*

The proof of Proposition 3.1 can be found in Appendix D.1 (see Corollary D.7) and is based on an application of Berge's maximum theorem (Berge, 1963), and the fact that the expected distance between the true reward function and the learned reward model under D is induced from a norm. See Theorem 6.1 for a similar result in which the expected error in rewards is replaced by an expected error in choice probabilities.

One might be inclined to conclude that the guarantee of Proposition 3.1 allows one to practically achieve low regret by ensuring a low error ϵ (as measured by Equation 1). However, in the following result we provide a more detailed analysis that shows that low regret requires a prohibitively low ϵ:

Proposition 3.2. *Let the setting be as in Proposition 3.1. If $\epsilon > 0$ satisfies*

$$\epsilon < \frac{1-\gamma}{\sqrt{2}} \cdot \frac{\text{range } J^R}{\text{range } R} \cdot \min_{(s,a) \in \mathcal{S} \times \mathcal{A}} D(s, a) \cdot L$$

then $D \in \mathbf{safe}(R, \epsilon, L)$.

The proof can be found in Theorem D.11, Appendix D.2. Example D.13 shows that the bound on ϵ is tight up to a factor of $\sqrt{2}$. This result is problematic in practice due to the dependence on the minimum of D. Realistic MDPs usually contain a massive amount of states and actions, which necessarily requires D to give a very small support to at least some transitions. The dependence of the upper bound on D also shows that there is no ϵ for which every distribution D is guaranteed to be safe, as $\min_{(s,a) \in D} D(s, a)$ can be arbitrarily small. We concretize this intuition by showing that in every MDP and for every $\epsilon > 0$, there exist weak assumptions for which a data distribution allows for a large error-regret mismatch.

Proposition 3.3. *Let $M = \langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be an MDP, $D \in \Delta(\mathcal{S} \times \mathcal{A})$ a data distribution, $\epsilon > 0$, and $L \in [0, 1]$. Assume there exists a policy $\hat{\pi}$ with the property that $\text{Reg}^R(\hat{\pi}) \geq L$ and $D(\text{supp } D^{\hat{\pi}}) < \epsilon$, where $\text{supp } D^{\hat{\pi}}$ is defined as the set of state-action pairs $(s, a) \in \mathcal{S} \times \mathcal{A}$ such that $D^{\hat{\pi}}(s, a) > 0$. In other words, there is a "bad" policy for R that is not very supported by D. Then, D allows for error-regret mismatch to occur, i.e., $D \in \mathbf{unsafe}(R, \epsilon, L)$.*

The proof of Proposition 3.3 can be found in Appendix C.2 (see Proposition C.5). The intuition is straightforward: There exists a reward model $\hat{R}$ that is very similar to the true reward function R

outside the support of $D^{\hat{\pi}}$ but has very large rewards for the support of $D^{\hat{\pi}}$. Because $D(\text{supp } D^{\hat{\pi}})$ is very small, this still allows $\hat{R}$ to have a very small expected error w.r.t. to D, while $\hat{\pi}$, the optimal policy for $\hat{R}$, will have regret at least L. To avoid confusions, we show in Proposition C.7 that the assumptions on ϵ in Proposition 3.2 and Proposition 3.3 cannot hold simultaneously. This is as expected since otherwise the *conclusions* of these propositions would imply that a data distribution can be both safe and unsafe.

Note that the conditions for unsafe data distributions in Proposition 3.3 also cover positive data distributions (that we showed to be eventually safe for small enough ϵ in Proposition 3.1). Furthermore, especially in very large MDPs, it is very likely that the data distribution will not sufficiently cover large parts of the support of some policies, especially since the number of (deterministic) policies grows exponentially with the number of states. Sometimes, this can lead to *all* data distributions being unsafe, as we show in the following corollary:

Corollary 3.4. *Let $M = \langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be an MDP, $\epsilon > 0$, and $L \in [0, 1]$. Assume there exists a set of policies Π_L with:*

- $\text{Reg}^R(\pi) \geq L$ *for all* $\pi \in \Pi_L$*;*
- $\text{supp } D^{\pi} \cap \text{supp } D^{\pi'} = \emptyset$ *for all* $\pi, \pi' \in \Pi_L$*; and*
- $|\Pi_L| \geq 1/\epsilon$.

Then $\mathbf{unsafe}(R, \epsilon, L) = \Delta(\mathcal{S} \times \mathcal{A})$*, i.e.: all distributions are unsafe.*

The proof of Corollary 3.4 can be found in Appendix C.2 (see Corollary C.6).

Corollary 3.4 outlines sufficient conditions for a scenario where all possible data distributions are unsafe for a given MDP. This happens when there exist *many* different policies with large regret and disjoint support, which requires there to be a large action space. This could for example happen in the case of a language model interacting with a user. There are some ways to interact with the user that have large regret $\geq L$, e.g., by providing instructions for building weapons. Now consider that for a single such policy, we can easily imagine many adaptations that all behave in essentially the same way, but have individually consistent and mutually distinct writing styles or idiosyncratic differences in word choice. The set of all these variations Π_L will then be large ($|\Pi_L| > 1/\epsilon$) and consist of policies with high regret $\geq L$ that have mutually disjoint support since their actions, i.e. responses, consistently differ in style.

An example of such an MDP is the natural language environment, where the state space is a sequence of user-prompts and assistant responses. Therefore, while Proposition 3.1 shows that for every data distribution D there exists a test error ϵ small enough such that D becomes safe, Corollary 3.4 shows that in some settings ϵ might need to be extremely small in order to allow for safety.

We conclude by stating the main result of this section, which unifies all previous results and derives the most general conditions, i.e. *necessary and sufficient* conditions, for when exactly a data distribution allows for error-regret mismatch to occur:

Theorem 3.5. *For all MDPs $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ and $L \in [0, 1]$, there exists a matrix M such that for all $\epsilon > 0$ and $D \in \Delta(\mathcal{S} \times \mathcal{A})$ we have:*

$$D \in \mathbf{safe}(R, \epsilon, L) \quad \Longleftrightarrow \quad M \cdot D > \epsilon \cdot \text{range } R \cdot \mathbf{1}, \tag{3}$$

where we use the vector notation of D, and $\mathbf{1}$ is a vector containing all ones.

The proof of Theorem 3.5 can be found in Appendix C.3 (see Theorem C.16) and largely relies on geometric arguments that arise from comparing the set of unsafe reward models and the set of reward models that are close to the true reward function. Interestingly, this means that the set of *safe* data distributions resembles a polytope, in the sense that it is a convex set and is defined by the intersection of an open polyhedral set (defined by the system of strict inequalities $M \cdot D > \epsilon \cdot \text{range } R \cdot \mathbf{1}$), and the closed data distribution simplex.

While Theorem 3.5 only proves the existence of such a matrix M, we provide further results and analyses in the appendix, namely:

1. In Appendix C.3.2 we derive closed-form expressions of the rows of matrix M, and show that its entries depend on multiple factors, such as the original reward function R, the state transition distribution τ, and the set of deterministic policies that achieve regret at least L.
2. In Appendix C.3.3 we provide an algorithm to compute matrix M.
3. In Appendix C.3.4 we provide a worked example of computing and visualizing the set of safe distributions for a toy example.

Lastly, we note that M does not depend on ϵ, and M only contains non-negative entries (see Appendix C.3.2). This allows us to recover Proposition 3.1, since by letting ϵ approach zero, the set of data distributions that fulfill the conditions in Equation (3) approaches the entire data distribution simplex. On the other hand, the dependence of M on the true reward function and the underlying MDP implies that computing M is infeasible in practice since many of these components are not known, restricting the use of M to theoretical analysis.

4 Error-regret mismatch for regularized policy optimization

In this section, we investigate the error-regret mismatch for regularized policy optimization. We begin by showing that there are conditions under which a low expected error ϵ guarantees that a provided data distribution is safer than an initial reference policy: First, we prove that for almost any reference policy π_{ref} that achieves regret L and minimizes the regularization term ω, there exists a sufficiently small ϵ such that reward learning within ϵ of the true reward function preserves the regret bound L.

Proposition 4.1. *Let $\lambda \in (0, \infty)$, let $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be any MDP, and let $D \in \mathcal{S} \times \mathcal{A}$ be any data distribution that assigns positive probability to all transitions. Let $\omega : \Pi \to \mathbb{R}$ be a continuous regularization function that has a reference policy π_{ref} as a minimum.*[1] *Assume that π_{ref} is* not *(λ, ω)-optimal for R and let $L = \text{Reg}^R(\pi_{\text{ref}})$. Then there exists $\epsilon > 0$ such that $D \in \textbf{safe}(R, \epsilon, L, \lambda, \omega)$.*

The proof of Proposition 4.1 can be found in Appendix D.4 (see Theorem D.21) and is again an application of Berge's theorem (Berge, 1963). Note that the regret bound L is defined as the regret of the reference policy. This makes intuitively sense, as regularized policy optimization constrains the policy under optimization $\hat{\pi}$ to not deviate too strongly from the reference policy π_{ref}, which will also constrain the regret of $\hat{\pi}$ to stay close to the regret of π_{ref}. Under the conditions of Proposition 4.1, the regret of π_{ref} serves as an upper regret bound because for small enough ϵ the learned reward $\hat{R}$ and the true reward R are close enough such that maximizing $\hat{R}$ also improve reward with respect to R. Furthermore, we note that it is also possible to derive a version of the theorem in which the expected error in rewards is replaced by a KL divergence in choice probabilities, similar to Proposition D.14, by combining the arguments in that proposition with the arguments in Berge's theorem. A full formulation and proof of the result can be found in Theorem D.22.

Similar to Proposition 3.1, Proposition 4.1 does not guarantee the existence of a universal ϵ such that all data distributions D are in $\textbf{safe}(R, \epsilon, L, \lambda, \omega)$. In our next result, we show that such an ϵ does not exist, since for each ϵ, there is a nontrivial set of data distributions that allows for error-regret mismatch to occur:

Theorem 4.2. *Let $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be an arbitrary MDP, $\lambda \in (0, \infty)$, $L \in (0, 1)$, and $\omega : \Pi \to \mathcal{R}$ be a regularization function. Furthermore, let π_* be a determinstic worst-case policy for R, meaning that $\text{Reg}^R(\pi_*) = 1$. Let $C := C(\mathcal{M}, \pi_*, L, \lambda, \omega) < \infty$ be the constant defined in Equation* (98) *in the appendix. Let $\epsilon > 0$. Then for all data distributions $D \in \Delta(\mathcal{S} \times \mathcal{A})$ with*

$$D(\text{supp } D^{\pi_*}) \leq \frac{\epsilon}{1 + C}, \tag{4}$$

we have $D \in \textbf{unsafe}(R, \epsilon, L, \lambda, \omega)$.

The proof of Theorem 4.2 can be found in Appendix C.5 (see Theorem C.38). The general idea is as follows: To prove that D is unsafe, define $\hat{R}$ to be equal to R outside of supp D^{π_*}, and very large in supp D^{π_*}. If it is sufficiently large in this region, then regularized optimization leads to a policy $\hat{\pi}$

[1] E.g., if $\pi_{\text{ref}}(a \mid s) > 0$ for all $(s, a) \in \mathcal{S} \times \mathcal{A}$ and $\omega(\pi) := \mathbb{D}_{\text{KL}}(\pi || \pi_{\text{ref}})$, then the minimum is π_{ref}.

with $\mathrm{Reg}^R(\hat{\pi}) \geq L$. Finally, the condition that $D(\mathrm{supp}\ D^{\pi_*}) \leq \frac{\epsilon}{1+C}$ ensures that $\hat{R}$ has a reward error bounded by ϵ.

Note that Theorem 4.2 is very general and covers a large class of different regularization methods. In Corollary C.40 we provide a specialized result for the case of KL-regularized policy optimization, and in Section 6 we investigate error-regret mismatch in the RLHF framework.

5 Generalization of the error measurement

Our results have so far expressed the error of the learned reward $\hat{R}$ in terms of Equation (1), i.e., in terms of the expected error of individual transitions. In this section, we show that many common reward learning training objectives can be upper-bounded in terms of the expected error metric defined in Equation (1). This in turn means that our negative results generalize to reward learning algorithms that use these other training objectives. We state all upper bounds for MDPs with finite time horizon T (but note that these results directly generalize to MDPs with infinite time horizon by taking the limit of $T \to \infty$).

In the finite horizon setting, trajectories are defined as a finite list of states and actions: $\xi = s_0, a_0, s_1, ..., a_{T-1}$. We use Ξ for the set of all trajectories of length T. As in the previous sections, $G : \Xi \to \mathbb{R}$ denotes the trajectory return function, defined as $G(\xi) = \sum_{t=0}^{T-1} \gamma^t \cdot R(s_t, a_t)$. We start by showing that low expected error in transitions implies low expected error in trajectory returns:

Proposition 5.1. *Given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, a data sampling policy $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ an its resulting data distribution $D^\pi = \frac{1-\gamma}{1-\gamma^T} \cdot \eta^\pi$ and a second reward function $\hat{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, we can upper bound the expected difference in trajectory evaluation as follows:*

$$\mathbb{E}_{\xi \sim \pi}\left[|G_R(\xi) - G_{\hat{R}}(\xi)|\right] \;\leq\; \frac{1-\gamma^T}{1-\gamma} \cdot \mathbb{E}_{(s,a)\sim D^\pi}\left[|R(s,a) - \hat{R}(s,a)|\right].$$

The proof of Proposition 5.1 can be found in Appendix C.4.1 (see Proposition C.24). Furthermore, a low expected error of trajectory returns implies a low expected error of choice distributions (a distance metric commonly used as the loss in RLHF (Christiano et al., 2017)). Namely, given a reward function R, define the probability of trajectory ξ_1 being preferred over ξ_2 to be $p_R(\xi_1 \succ \xi_2) = \sigma(G_R(\xi_1) - G_R(\xi_2)) = \frac{\exp(G_R(\xi_1))}{\exp(G_R(\xi_1)) + \exp(G_R(\xi_2))}$. We then have:

Proposition 5.2. *Given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, a data sampling policy $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ and a second reward function $\hat{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, we can upper bound the expected KL divergence over trajectory preference distributions as follows:*

$$\mathbb{E}_{\xi_1, \xi_2 \sim \pi \times \pi}\left[\mathbb{D}_{KL}\left(p_R(\cdot|\xi_1, \xi_2) || p_{\hat{R}}(\cdot|\xi_1, \xi_2)\right)\right] \;\leq\; 2 \cdot \mathbb{E}_{\xi \sim \pi}\left[|G_R(\xi) - G_{\hat{R}}(\xi)|\right].$$

The proof of Proposition 5.2 can be found in Appendix C.4.1 (see Proposition C.25).

Finally, in some RLHF scenarios, for example in RLHF with prompt-response pairs, one prefers to only compare trajectories with a common starting state. In the following proposition, we upper-bound the expected error of choice distributions with trajectories that share a common starting state by the expected error of choice distributions with arbitrary trajectories:

Proposition 5.3. *Given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, a data sampling policy $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ and a second reward function $\hat{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, we can upper bound the expected KL divergence of preference distributions over trajectories with a common starting state as follows:*

$$\mathop{\mathbb{E}}_{\substack{s_0 \sim \mu_0, \\ \xi_1, \xi_2 \sim \pi(s_0)}}\left[\mathbb{D}_{KL}\left(p_R(\cdot|\xi_1, \xi_2) || p_{\hat{R}}(\cdot|\xi_1, \xi_2)\right)\right] \;\leq\; \frac{\mathbb{E}_{\xi_1, \xi_2 \sim \pi \times \pi}\left[\mathbb{D}_{KL}\left(p_R(\cdot|\xi_1, \xi_2) || p_{\hat{R}}(\cdot|\xi_1, \xi_2)\right)\right]}{\min_{s' \in \mathcal{S}, \mu_0(s') > 0} \mu_0(s')}.$$

The proof of Proposition 5.3 can be found in Appendix C.4.1 (see Proposition C.26).

6 Error-regret mismatch in RLHF

In this section we use the generalization results from Section 5 to extend our results to reinforcement learning from human feedback (RLHF). We provide more general results about the class of KL-regularized optimization policy optimization methods in Appendix C.4.5.

RLHF, especially in the context of large language models, is usually modeled in a *contextual bandit* setting (Ziegler et al., 2019; Stiennon et al., 2020; Bai et al., 2022; Ouyang et al., 2022; Rafailov et al., 2023). A *contextual bandit* $\langle \mathcal{S}, \mathcal{A}, \mu_0, R \rangle$ is defined by a set of states $\mathcal{S}$, a set of actions $\mathcal{A}$, a data distribution $\mu_0 \in \Delta(\mathcal{S})$, and a reward function $R : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$. The goal is to learn a policy $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ that maximizes the expected return $J(\pi) = \mathbb{E}_{s \sim \mu_0, a \sim \pi(\cdot|s)}[R(s,a)]$. In the context of language models, $\mathcal{S}$ is usually called the set of *prompts* or *contexts*, and $\mathcal{A}$ the set of *responses*.

We state the following theorem using a more precise version of Definition 2.1 tailored to the RLHF setting. In particular, we replace the similarity metric (property 1. of Definition 2.1) with the expected similarity in choice probabilities. A precise mathematical definition can be found in Appendix C.4.3. We denote the resulting sets of safe- and unsafe data distributions by $\mathbf{safe}^{\mathrm{RLHF}}\big(R, \epsilon, L, \lambda, \mathbb{D}_{\mathrm{KL}}(\cdot || \pi_{\mathrm{ref}})\big)$ and $\mathbf{unsafe}^{\mathrm{RLHF}}\big(R, \epsilon, L, \lambda, \mathbb{D}_{\mathrm{KL}}(\cdot || \pi_{\mathrm{ref}})\big)$.

By making use of the specifics of this setting, we can derive more interpretable and stronger results. In particular, we specify a set of reference distributions for which performing KL-regularized policy optimization allows for error-regret mismatch to occur.

Theorem 6.1. *Let $\langle \mathcal{S}, \mathcal{A}, \mu_0, R \rangle$ be a contextual bandit. Given $L \in [0,1)$, we define for every state $s \in \mathcal{S}$ the reward threshold:$R_L(s) := (1-L) \cdot \max_{a \in \mathcal{A}} R(s,a) + L \cdot \min_{a \in \mathcal{A}} R(s,a)$. Lastly, let $\pi_{\mathrm{ref}} : \mathcal{S} \to \mathcal{A}$ be an arbitrary reference policy for which it holds that for every $(s,a) \in \mathcal{S} \times \mathcal{A}$, $\pi_{\mathrm{ref}}(a|s) > 0$, and there exists at least one action $a_s \in \mathcal{A}$ such that $R(s, a_s) < R_L(s)$ and $\pi_{\mathrm{ref}}(a_s|s)$ satisfies the following inequality:*

$$\pi_{\mathrm{ref}}(a_s|s) \ \leq \ \frac{(R_L(s) - R(s,a_s))}{L} \cdot \frac{\mathrm{range}\, R}{\exp\left(\frac{1}{\lambda} \cdot \mathrm{range}\, R\right)} \cdot \frac{\epsilon^2}{4 \cdot \lambda^2}.$$

Let $D^{\mathrm{ref}}(s,a) := \mu_0(s) \cdot \pi_{\mathrm{ref}}(a|s)$. Then $D^{\mathrm{ref}} \in \mathbf{unsafe}^{\mathrm{RLHF}}\big(R, 2 \cdot \epsilon, L, \lambda, \mathbb{D}_{KL}(\cdot || \pi_{\mathrm{ref}})\big)$

The proof of Theorem 6.1 can be found in Appendix C.4.4 (see Propositions C.31 and C.32). We expect the conditions on the reference policy π_{ref} to be likely to hold in real-world cases as the number of potential actions (or responses) is usually very large, and language models typically assign a large portion of their probability mass to only a tiny fraction of all responses. This means that for every state/prompt s, a huge majority of actions/responses a have a very small probability $\pi_{\mathrm{ref}}(a \mid s)$.

7 Discussion

We have contributed to building up the foundations for the learning theory of general reward learning in arbitrary MDPs by studying the relationship between the expected error of a learned reward function on some data distribution and the extent to which optimizing that reward function is guaranteed to produce a policy with low regret according to the true reward function. We showed that as the expected error ϵ of a reward model $\hat{R}$ goes to zero, the worst-case regret of a policy that is optimal under $\hat{R}$ (with or without regularization) also goes to zero (Propositions 3.1 and 4.1). However, in Proposition 3.2 we also showed that ϵ, in general, must be extremely small to ensure that $\hat{R}$'s optimal policies have a low worst-case regret. In particular, this value depends on the smallest probability that the data distribution D assigns to any transition in the underlying MDP, which means that it shrinks very quickly for large MDPs. Consequently, there exists no ϵ that can universally ensure low regret.

More generally, low expected error does *not* ensure low regret for all realistic data distributions (Proposition 3.3, Theorem 4.2 and Theorem 6.1). We refer to this phenomenon as *error-regret mismatch*. This is due to policy optimization (typically) involving a *distributional shift* from the data distribution that is used to train the reward model; a reward model that is accurate on the data distribution may fail to be accurate after this distributional shift. Moreover, we find evidence that some MDPs with very large action spaces do not allow for *any* safe data distributions relative to a reasonable reward model error and desired regret bound (Corollary 3.4). We also showed that our results generalize to various different data sources, such as preferences over trajectories (Propositions 5.2 and 5.3) and trajectory scores (Proposition 5.1), supporting the conclusion that this issue is a fundamental problem of reward learning.

Lastly, for the case of unregularized optimization, we derive a set of *necessary and sufficient* conditions that allow us to determine the set of safe and unsafe data distributions for arbitrary MDPs, thereby completely answering the question of when exactly a data distribution is safe (Theorem 3.5).

Our results highlight the challenge of deriving useful PAC-like generalization bounds for current reward learning algorithms. While there do exist bounds (Nika et al., 2024; Cen et al., 2024), they depend on some form of data coverage of (bad) policies. As we have shown, in practical situations, we should expect the coverage to be so low that the regret will be large. Our results highlight the challenge of deriving useful PAC-like generalization bounds for current reward learning algorithms. While this is possible (and has been done, see (Nika et al., 2024; Cen et al., 2024)), we showed that realistic bounds on the error in the learned reward function do not provide meaningful guarantees. By focusing on the propagation of reward function error to regret in policy optimization, our work provides an insightful analysis that disentangles a key obstacle specific to reward learning from classical learning theory challenges.

Our results also highlight the importance of researching ways for evaluating reward functions using methods other than evaluating them on a test set, e.g. by using interpretability methods (Michaud et al., 2020; Jenner & Gleave, 2022) or finding better ways to quantify reward function distance (Gleave et al., 2020; Skalse et al., 2024)). These are largely unsolved research efforts that would profit from further engagement.

7.1 Limitations and future work

Our work focuses on the question of whether there *exists* a reward model $\hat{R}$ that is compatible with the true reward function on a data distribution, such that there *exists* a policy $\hat{\pi}$ that is optimal under $\hat{R}$, but which has high regret. In practice, it may be that the inductive bias of the reward learning algorithm or the policy optimization algorithm avoids the most pathological cases. Our analysis could therefore be extended by attempting to take the inductive bias into account. Furthermore, our analyses assume that we are able to find optimal policies, but in practice, this is rarely the case. Generalizing our results to non-optimal policies therefore constitutes an important direction for further research. Finally, one could attempt to analyze the *likelihood* of a high-regret training outcome of reward learning and policy optimization instead of analyzing the worst-case.

Furthermore, it is important to theoretically analyze improved reward learning and policy optimization procedures. There is already some empirical work on using reward model ensembles (Coste et al., 2023) or weight averaged reward models (Ramé et al., 2024) to overcome problems of reward model overoptimization. In the special case of multi-armed bandits, iterated data-smoothing has been proposed and analyzed theoretically and empirically (Zhu et al., 2024). Very recent work also considers learning reward models on online data for mitigating distribution shifts and thus reward overoptimization (Lang et al., 2024a) or even theoretically analyzes such a setting for the special case of linear reward functions (Song et al., 2024). We hope that a careful theoretical analysis of all these settings in similar generality as our work can identify reliable ways to improve upon the "theoretical baseline" established by our work.

In addition to improving the theory and practice of reward learning itself, there are other ways to improve the safety of the resulting policies after training. We are excited about efforts to evaluate policies for dangerous capabilities (Phuong et al., 2024), red-teaming (Perez et al., 2022), safety cases (Clymer et al., 2024), shields (Alshiekh et al., 2018), and a numerous suite of other approaches (Anwar et al., 2024).

Moreover, there are numerous opportunities to identify more necessary and/or sufficient conditions when a data distribution (dis)allows error-regret mismatch. In general, it would be interesting to find more interpretable and practical conditions that guarantee a data distribution is safe or unsafe, i.e., conditions that do not rely on knowledge about the true reward function or the transition distribution.

For the purposes of communicating our paper updates in the rebuttal, we made additions to the paper that address some of the reviewer's concerns. They temporarily increase the page number above the limit. We will make sure to fit everything within the page limit for the camera-ready version.

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APPENDIX

This appendix develops the theory outlined in the main paper in a self-contained and complete way, including all proofs. In Appendix B, we present the setup of all concepts and the problem formulation, as was already contained in the main paper. In Appendix C, we present all "negative results". Conditional on an error threshold in the reward model, these results present conditions for the data distribution that allow reward models to be learned that allow for error-regret mismatch. That section also contains Theorem C.16 which is an equivalent condition for the absence of error-regret mismatch but could be considered a statement about error-regret mismatch by negation. In Appendix D, we present sufficient conditions for *safe optimization* in several settings. Typically, this boils down to showing that given a data distribution, a *sufficiently small* error in the reward model guarantees that its optimal policies have low regret.

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A Extended related work

Reward Learning Reward learning is a key concept in reinforcement learning that involves learning the reward function for complex tasks with latent and difficult-to-specify reward functions. Many methods have been developed to incorporate various types of human feedback into the reward learning process (Wirth et al., 2017; Ng et al., 2000; Bajcsy et al., 2017; Jeon et al., 2020).

Challenges in Reward Learning Reward learning presents several challenges (Casper et al., 2023; Lang et al., 2024b; Skalse & Abate, 2023; 2024), such as *reward misgeneralization*, where the reward model learns a different reward function that performs well on in-distribution data but differs strongly on out-of-distribution data (Skalse et al., 2023). This can lead to unintended consequences in real-world applications.

Reward misgeneralization can also result in *reward hacking* (Krakovna, 2020), a consequence of Goodhart's law (Goodhart, 1984; Zhuang & Hadfield-Menell, 2020; Hennessy & Goodhart, 2023; Strathern, 1997; Karwowski et al., 2023). Reward hacking has been extensively studied both theoretically (Skalse et al., 2022; 2024; Zhuang & Hadfield-Menell, 2020) and empirically (Zhang et al., 2018; Farebrother et al., 2018; Cobbe et al., 2019; Krakovna, 2020; Gao et al., 2023; Tien et al., 2022).

How we complement prior work Over the past few years, several works have observed and investigated distribution shifts in RL empirically (Wiles et al., 2021; Fujimoto et al., 2024; Mann et al., 2021; Ajay et al., 2022; Kumar et al., 2020). These studies provide valuable insights into the impact of distribution shifts on RL performance, but there remain gaps in our understanding of this phenomenon.

We are interested in theoretically analyzing the impact that the initial *data distribution*, used to train the reward model, has on the regret of the final policy. In particular, we assume arbitrary MDPs and investigate the regret a policy might attain for a worst-case reward model, that might be trained during reward learning. Our work thereby nicely extends and complements theoretical work that investigates policy regret under a worst-case MDP in settings such as imitation learning (Ross et al., 2011), offline RL (Kim et al., 2024; Jin et al., 2021; Zhang et al., 2022), and other RL settings (Lu et al., 2024; Laidlaw et al., 2024; Kwa et al., 2024)

Furthermore, we try to remain as general in our results as possible by letting all our results in Sections 3 and 4 hold for arbitrary MDPs without any additional restrictions. In contrast, (Jin et al., 2021; Zhang et al., 2022; Nika et al., 2024) choose to investigate results in linear MDPs, whereas (Zhu et al., 2024) focus their analysis to multi-armed bandits.

In terms of new results, we develop precise conditions (i.e., necessary and sufficient) for when exactly a given data distribution is safe for some fixed MDP (Theorem 3.5) for unregularized policy optimization. To the best of our knowledge, we are the first to develop such results and point out the surprisingly regular shape of the set of safe data distributions. We hope this can act as a "theoretical baseline" for theoretical investigations of improved reward learning methods and their "safe starting conditions".

Lastly, we demonstrate that without additional assumptions, a wide range of reward learning methods are not guaranteed to be safe, i.e., there exist reasonable conditions under which RL with reward learning might yield a policy that behaves very badly. Importantly, straightforward fixes such as policy regularization do not fix this issue (Theorem 4.2) and we show in Section 6 that our results directly apply to the standard RLHF setting as well. This means that the most widely used LLM safety technique is not safe, without additional assumptions. In contrast to the works Zhu et al. (2024); Nika et al. (2024) we again show this for non-adversarial MDPs, as well as less simplified/constraint settings

Advancements in Addressing Distribution Shifts Several approaches have been proposed to address the issue of out-of-distribution robustness in reward learning, such as ensembles of conservative reward models (Coste et al., 2023), averaging weights of multiple reward models (Ramé et al., 2024), iteratively updating training labels (Zhu et al., 2024), on-policy reward learning (Lang et al., 2024a), and distributionally robust planning (Zhan et al., 2023).

Our work further emphasizes the usefulness of exploring additional assumptions or methods to mitigate the perils of distribution shift, as we show that without any additional assumptions, there are next to no guarantees. We therefore hope that our work can serve as a theoretical baseline, that people can use to express and analyze their new assumptions or methods.

In classical machine learning, research in out-of-distribution generalization has a long history, and a rich literature of methods exists (Li et al., 2022; Zhou et al., 2022; Wang et al., 2022; Liu et al., 2021; Li et al., 2023; Yoon et al., 2023). These methods could potentially be adapted to address distribution shift challenges in reinforcement learning.

Contextual Bandits In Section 6 we work in the contextual bandit setting and derive variants of our results for RLHF. Several theoretical results have been developed that investigate the challenge of RLHF (Xiong et al., 2024; Zhu et al., 2023; Ji et al., 2023; Mehta et al., 2023) and reward learning in general, (Agarwal et al., 2012; Foster et al., 2020) in the contextual bandit setting. Compared to this prior work, we focus on the offline setting where the data distribution D has been pre-generated by a reference policy.

B INTRODUCTION

B.1 PRELIMINARIES

A *Markov Decision Process* (MDP) is a tuple $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ where $\mathcal{S}$ is a set of *states*, $\mathcal{A}$ is a set of *actions*, $\tau : \mathcal{S}{\times}\mathcal{A} \to \Delta(\mathcal{A})$ is a *transition function*, $\mu_0 \in \Delta(S)$ is an *initial state distribution*, $R : \mathcal{S}{\times}\mathcal{A} \to \mathbb{R}$ is a *reward function*, and $\gamma \in (0, 1)$ is a *discount rate*. A *policy* is a function $\pi : \mathcal{S} \to \Delta(\mathcal{A})$. A *trajectory* $\xi = \langle s_0, a_0, s_1, a_1, ... \rangle$ is a possible path in an MDP. The *return function* G gives the cumulative discounted reward of a trajectory, $G(\xi) = \sum_{t=0}^{\infty} \gamma^t R(s_t, a_t, s_{t+1})$, and the *evaluation function* J gives the expected trajectory return given a policy, $J(\pi) = \mathbb{E}_{\xi \sim \pi}[G(\xi)]$. A policy maximizing J is an *optimal policy*. The *state-action occupancy measure* is a function $\eta : \Pi \to \mathbb{R}^{|\mathcal{S}\times\mathcal{A}|}$ which assigns each policy $\pi \in \Pi$ a vector of occupancy measure describing the discounted frequency that a policy takes each action in each state. Formally, $\eta(\pi)(s, a) = \eta^\pi(s, a) = \sum_{t=0}^{\infty} \gamma^t \cdot P(s_t = s, a_t = a \mid \xi \sim \pi)$. Note that by writing the reward function R as a vector $\vec{R} \in \mathbb{R}^{|\mathcal{S}\times\mathcal{A}|}$, we can split J into a linear function of π: $J(\pi) = \eta^\pi \cdot \vec{R}$. The *value function* V of a policy encodes the expected future discounted reward from each state when following that policy. We use $\mathcal{R}$ to refer to the set of all reward functions. When talking about multiple rewards, we give each reward a subscript R_i, and use J_i, G_i, and V_i^π, to denote R_i's evaluation function, return function, and π-value function.

B.2 PROBLEM FORMALIZATION

The standard RL process using reward learning works roughly like this:

1. You are given a dataset of transition-reward tuples $\{(s_i, a_i, r_i)\}_{i=0}^n$. Here, each $(s_i, a_i) \in \mathcal{S}{\times}\mathcal{A}$ is a transition from some (not necessarily known) MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ that has been sampled using some distribution $D \in \Delta(\mathcal{S}{\times}\mathcal{A})$, and $r_i = R(s_i, a_i)$. The goal of the process is to find a policy $\hat{\pi}$ which performs roughly optimally for the unknown true reward function R. More formally: $J_R(\hat{\pi}) \approx \max_{\pi\in\Pi} J_R(\pi)$.
2. Given some error tolerance $\epsilon \in \mathbb{R}$, a reward model $\hat{R} : \mathcal{S}{\times}\mathcal{A} \to \mathbb{R}$ is learned using the provided dataset. At the end of the learning process $\hat{R}$ satisfies some optimality criterion such as: $\mathbb{E}_{(s,a)\sim D}\left[|\hat{R}(s, a) - R(s, a)|\right] < \epsilon$
3. The learned reward model $\hat{R}$ is used to train a policy $\hat{\pi}$ that fulfills the following optimality criterion: $\hat{\pi} = \arg\max_{\pi\in\Pi} J_{\hat{R}}(\pi)$.

The problem is that training $\hat{\pi}$ to optimize $\hat{R}$ effectively leads to a distribution shift, as the transitions are no longer sampled from the original data distribution D but some other distribution $\hat{D}$ (induced by the policy $\hat{\pi}$). Depending on the definition of D, this could mean that there are no guarantees about how close the expected error of $\hat{R}$ to the true reward function R is (i.e., $\mathbb{E}_{(s,a)\sim\hat{D}}\left[|\hat{R}(s,a) - R(s,a)|\right]$ could not be upper-bounded).

This means that we have no guarantee about the performance of $\hat{\pi}$ with respect to the original reward function R, so it might happen that $\hat{\pi}$ performs arbitrarily bad under the true reward R: $J_R(\hat{\pi}) \ll \max_\pi J_R(\pi)$.

If for a given data distribution D there exists a reward model $\hat{R}$ such that $\hat{R}$ is close in expectation to the true reward function R but it is possible to learn a policy that performs badly under J_R despite being optimal for $\hat{R}$, we say that D *allows for error-regret mismatch* and that $\hat{R}$ *has an error-regret mismatch*.

C Existence of error-regret mismatch

In this section, we answer the question under which circumstances error-regret mismatch could occur. We consider multiple different settings, starting from very weak statements, and then steadily increasing the strength and generality.

C.1 Assumptions

For every MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ that we will define in the following statements, we assume the following properties:

- **Finiteness:** Both the set of states $\mathcal{S}$ and the set of actions $\mathcal{A}$ are finite
- **Reachability:** Every state in the given MDP's is reachable, i.e., for every state $s \in S$, there exists a path of transitions from some initial state s_0 (s.t. $\mu_0(s_0) > 0$) to s, such that every transition (s, a, s) in this path has a non-zero probability, i.e., $\tau(s'|s,a) > 0$. Note that this doesn't exclude the possibility of some transitions having zero probability in general.

C.2 Intuitive unregularized existence statement

Definition C.1 (Regret)**.** We define the *regret* of a policy π with respect to reward function R as

$$\mathrm{Reg}^R(\pi) := \frac{\max J_R - J_R(\pi)}{\max J_R - \min J_R} \in [0,1].$$

Here, J is the policy evaluation function corresponding to R.

Definition C.2 (Policy-Induced Distribution)**.** Let π be a policy. Then we define the *policy-induced distribution* D^π by

$$D^\pi := (1-\gamma)\cdot\eta^\pi.$$

Definition C.3 (Range of Reward Function)**.** Let R be a reward function. Its *range* is defined as

$$\mathrm{range}\, R := \max R - \min R.$$

Lemma C.4. *for any policy π, D^π is a distribution.*

Proof. This is clear. □

Proposition C.5. *Let $M = \langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be an MDP, $D \in \Delta(\mathcal{S}\times\mathcal{A})$ a data distribution, and $\epsilon > 0$, $L \in [0,1]$. Assume there exists a policy $\hat{\pi}$ with the property that $\mathrm{Reg}^R(\hat{\pi}) \geq L$ and $D(\mathrm{supp}\, D^{\hat{\pi}}) < \epsilon$, where $\mathrm{supp}\, D^{\hat{\pi}}$ is defined as the set of state-action pairs $(s,a) \in \mathcal{S}\times\mathcal{A}$ such that $D^{\hat{\pi}}(s,a) > 0$. In other words, there is a "bad" policy for R that is not very supported by D. Then, D allows for error-regret mismatch to occur, i.e., $D \in \mathbf{unsafe}(R, \epsilon, L)$.*

Proof. We will show that whenever there exists a policy $\hat{\pi}$ with the following two properties:

- $\mathrm{Reg}^R(\hat{\pi}) \geq L$;
- $D(\mathrm{supp}\, D^{\hat{\pi}}) < \epsilon$.

Then there exists a reward function $\hat{R}$ for which $\hat{\pi}$ is optimal, and such that

$$\mathbb{E}_{(s,a)\sim D}\left[\frac{|R(s,a)-\hat{R}(s,a)|}{\text{range } R}\right] \leq \epsilon.$$

Define

$$\hat{R}(s,a) := \begin{cases} R(s,a), & (s,a) \notin \text{supp } D^{\hat{\pi}}; \\ \max R, & \text{else.} \end{cases}$$

Then obviously, $\hat{\pi}$ is optimal for $\hat{R}$. Furthermore, we obtain

$$\begin{aligned}
\mathbb{E}_{(s,a)\sim D}\left[\frac{|R(s,a)-\hat{R}(s,a)|}{\text{range } R}\right] &= \sum_{(s,a)} D(s,a)\frac{|R(s,a)-\hat{R}(s,a)|}{\text{range } R} \\
&= \sum_{(s,a)\in \text{supp } D^{\hat{\pi}}} D(s,a)\frac{\max R - R(s,a)}{\text{range } R} \\
&\leq \sum_{(s,a)\in \text{supp } D^{\hat{\pi}}} D(s,a) \\
&= D(\text{supp } D^{\hat{\pi}}) \\
&\leq \epsilon.
\end{aligned}$$

That was to show. $\square$

Corollary C.6. *Let $M = \langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be an MDP, $\epsilon > 0$, and $L \in [0,1]$. Assume there exists a set of policies Π_L with:*

- $\text{Reg}^R(\pi) \geq L$ *for all* $\pi \in \Pi_L$*;*
- $\text{supp } D^{\pi} \cap \text{supp } D^{\pi'} = \emptyset$ *for all* $\pi, \pi' \in \Pi_L$*; and*
- $|\Pi_L| \geq 1/\epsilon$.

Then $\textbf{unsafe}(R, \epsilon, L) = \Delta(\mathcal{S} \times \mathcal{A})$*, i.e.: all distributions are unsafe.*

Proof. Let $D \in \Delta(\mathcal{S} \times \mathcal{A})$. Let $\pi \in \arg\min_{\pi' \in \Pi_L} D(\text{supp } D^{\pi'})$. We obtain

$$|\Pi_L| \cdot D(\text{supp } D^{\pi}) \leq \sum_{\pi' \in \Pi_L} D(\text{supp } D^{\pi'}) = D\left(\bigcup_{\pi' \in \Pi_L} \text{supp } D^{\pi'}\right) \leq 1,$$

and therefore $D(\text{supp } D^{\pi}) \leq 1/|\Pi_L| < \epsilon$. The result follows from Proposition 3.3. $\square$

Proposition C.7. *The assumptions on ϵ in Proposition 3.2 and Proposition 3.3 cannot hold simultaneously.*

Proof. If they *would* hold simultaneously, we would get:

$$\min_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a) \leq D\big(\text{supp} D^{\hat{\pi}}\big) < \epsilon < \frac{1-\gamma}{\sqrt{2}} \cdot \frac{\text{range} J_R}{\text{range} R} \cdot \min_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a) \cdot L.$$

Here, the first step is clear, the second step is the assumption from Proposition 3.3, and the third step is the assumption from Proposition 3.2. We now show that this leads to a contradiction.

Dividing by the minimum on both sides, we obtain

$$1 < \frac{L}{\sqrt{2}} \cdot \frac{(1-\gamma)\text{range} J_R}{\text{range} R}. \tag{5}$$

Clearly, we have $L/\sqrt{2} < 1$. We also claim that the second fraction is smaller or equal to 1, which then leads to the desired contradiction. Indeed, let π^* and π_* be an optimal and a worst-case policy, respectively. Then we have

$$\begin{aligned}
(1-\gamma)\text{range}J_R &= (1-\gamma)(J_R(\pi^*) - J_R(\pi_*)) \\
&= (1-\gamma)\eta^{\pi^*} \cdot \vec{R} - (1-\gamma)\eta^{\pi_*} \cdot \vec{R} \\
&= D^{\pi^*} \cdot \vec{R} - D^{\pi_*} \cdot \vec{R} \\
&= \sum_{(s,a)\in\mathcal{S}\times\mathcal{A}} D^{\pi^*}(s,a)R(s,a) - \sum_{(s,a)\in\mathcal{S}\times\mathcal{A}} D^{\pi_*}(s,a)R(s,a) \\
&\leq \max_{(s,a)\in\mathcal{S}\times\mathcal{A}} R(s,a) - \min_{(s,a)\in\mathcal{S}\times\mathcal{A}} R(s,a) \\
&= \text{range}R.
\end{aligned}$$

Here, we used the formulation of the policy evaluation function in terms of the occupancy measure η, and then that $1-\gamma$ is a normalizing factor that transforms the occupancy measure into a distribution. Overall, this means that $(1-\gamma)\text{range}J_R/\text{range}R \leq 1$, contradicting (5). Consequently, the assumptions of Proposition 3.2 and Proposition 3.3 cannot hold simultaneously. $\square$

C.3 General existence statements

We start by giving some definitions:

Definition C.8 (Minkowski addition)**.** Let A, B be sets of vectors, then the Minkowski addition of A, B is defined as:

$$A + B \coloneqq \{a + b \mid a \in A,\ b \in B\}.$$

(Karwowski et al., 2023) showed in their proposition 1, that for every MDP, the corresponding occupancy measure space Ω forms a convex polytope. Furthermore, for each occupancy measure $\eta \in \Omega$ there exists at least one policy π^η such that $\forall (s,a) \in \mathcal{S}\times\mathcal{A},\ \eta^\pi(s,a) = \eta(s,a)$ (see Theorem 6.9.1, Corollary 6.9.2, and Proposition 6.9.3 of (Puterman, 1994)). In the following proofs, we will refer multiple times to vertices of the occupancy measure space Ω whose corresponding policies have high regret. We formalize this in the following definition:

Definition C.9 (High regret vertices)**.** Given a lower regret bound $L \in [0,1]$, an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma\rangle$ and a corresponding occupancy measure Ω, we define the set of high-regret vertices of Ω, denoted by V_R^L, to be the set of vertices v of Ω for which $\text{Reg}^R(\pi^v) \geq L$

Definition C.10 (Active inequalities)**.** Let $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma\rangle$ be an MDP with corresponding occupancy measure space Ω. For every $\eta \in \Omega$, we define the set of transitions (s,a) for which $\eta(s,a) = 0$ by $zeros(\eta)$.

Definition C.11 (Normal cone)**.** The normal cone of a convex set $C \subset \mathbb{R}^n$ at point $x \in C$ is defined as:

$$N_C(x) \ \coloneqq\ \{n \in \mathbb{R}^n \mid n^T \cdot (x' - x) \leq 0 \ \text{ for all } x' \in C\} \tag{6}$$

We first state a theorem from prior work that we will use to prove some lemmas in this section:

Theorem C.12 ((Schlaginhaufen & Kamgarpour, 2023))**.** *Let $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, \gamma\rangle$ be an MDP without reward function and denote with Ω its corresponding occupancy measure space. Then, for every reward function R and occupancy measure $\eta \in \Omega$, it holds that:*

$$\eta \textit{ is optimal for } R \quad\Longleftrightarrow\quad R \ \in\ N_\Omega(\eta), \tag{7}$$

where the normal cone is equal to:

$$N_\Omega(\eta) \ =\ \Phi + \text{cone}\left(\{-e_{s,a}\}_{(s,a)\in zeros(\eta)}\right) \tag{8}$$

where Φ is the linear subspace of potential functions used for reward-shaping, and the addition is defined as the Minkowski addition.

Proof. This is a special case of theorem 4.5 of Schlaginhaufen & Kamgarpour (2023), where we consider the unconstrained- and unregularized RL problem. $\square$

From the previous lemma, we can derive the following corollary which uses the fact that Ω is a closed, and bounded convex polytope (see Proposition 1 of Karwowski et al. (2023)).

Corollary C.13. *Given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ and a corresponding occupancy measure space Ω, then for every reward function $\hat{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, and lower regret bound $L \in [0, 1]$, the following two statements are equivalent:*

a) There exists an optimal policy $\hat{\pi}$ for $\hat{R}$ such that $\hat{\pi}$ has regret at least L w.r.t. the original reward function, i.e., $\text{Reg}^R(\hat{\pi}) \geq L$.

b) $\hat{R} \in \Phi + \bigcup_{v \in V_R^L} \text{cone}\left(\{-e_{s,a}\}_{(s,a) \in zeros(v)}\right)$, where Φ is the linear subspace of potential functions used for reward-shaping, the addition is defined as the Minkowski addition.

Proof. Let $\hat{R}$ be chosen arbitrarily. Statement $a)$ can be formally expressed as:

$$\exists \hat{\pi} \in \Pi, \ \text{Reg}^{\hat{R}}(\hat{\pi}) = 0 \ \wedge \ \text{Reg}^R(\hat{\pi}) \geq L.$$

Using Theorem C.12, it follows that:

$$\begin{aligned} &\exists \hat{\pi} \in \Pi, \ \text{Reg}^{\hat{R}}(\hat{\pi}) = 0 \ \wedge \ \text{Reg}^R(\hat{\pi}) \geq L \\ &\qquad\qquad \iff \quad \exists \hat{\pi} \in \Pi, \quad \hat{R} \in N_\Omega(\eta^{\hat{\pi}}) \ \wedge \ \text{Reg}^R(\hat{\pi}) \geq L \\ &\qquad\qquad \iff \quad \hat{R} \in \bigcup_{\eta \colon \text{Reg}^R(\pi^\eta) \geq L} N_\Omega(\eta). \end{aligned}$$

It remains to be shown that the union in the previous derivation is equivalent to a union over just all V_R^L. First, note that by definition of the set of high-regret vertices V_R^L (see Definition C.9), it trivially holds that:

$$\bigcup_{v \in V_R^L} N_\Omega(v) \ \subseteq \bigcup_{\eta \colon \text{Reg}^R(\pi^\eta) \geq L} N_\Omega(\eta), \tag{9}$$

Next, because Ω is a convex polytope, it can be defined as the intersection of a set of defining half-spaces which are defined by linear inequalities:

$$\Omega \ = \ \{\eta \mid a_i^T \cdot \eta \leq b_i, \ \text{for } i = 1, ..., m\}.$$

By defining the active index set of a point $\eta \in \Omega$ as $I_\Omega(\eta) = \{a_i \mid a_i^T \cdot \eta = b_i\}$, Rockafellar & Wets (2009) then show that:

$$N_\Omega(\eta) \ = \ \Big\{y_1 \cdot a_1 + ... + y_m \cdot a_m \mid y_i \geq 0 \text{ for } i \in I_\Omega(\eta), \ y_i = 0 \text{ for } i \notin I_\Omega(\eta)\Big\}, \tag{10}$$

(see their theorem 6.46). Note that, because Ω lies in an $|\mathcal{S}| \cdot (|\mathcal{A}| - 1)$ dimensional affine subspace (see Proposition 1 of (Karwowski et al., 2023)), a subset of the linear inequalities which define Ω must always hold with equality, namely, the inequalities that correspond to half-spaces which define the affine subspace in which Ω resides. Therefore, the corresponding active index set, let's denote it by $I_{\Omega,\Phi}(\eta)$ because the subspace orthogonal to the affine subspace in which Ω lies corresponds exactly to Φ, is always non-empty and the same for every $\eta \in \Omega$.

Now, from Equation (10), it follows that for every $\eta \in \Omega$, there exists a vertex v of Ω, such that $N_\Omega(\eta) \subseteq N_\Omega(v)$. We take this one step further and show that for every η with $\text{Reg}^R(\pi^\eta) \geq L$, there must exist a vertex v with $\text{Reg}^R(\pi^v) \geq L$ such that $N_\Omega(\eta) \subseteq N_\Omega(v)$. We prove this via case distinction on η.

- η is in the interior of Ω. In this case, the index set $I_\Omega(\eta)$ reduces to $I_{\Omega,\Phi}(\eta)$ and because we have $I_{\Omega,\Phi}(\eta) \subseteq I_\Omega(\eta)$ for every $\eta \in \Omega$, the claim is trivially true.
- η itself is already a vertex in which case the claim is trivially true.
- η is on the boundary of Ω. In this case η can be expressed as the convex combination of some vertices V_η which lie on the same face of Ω as η. Note that all occupancy measures with regret $\geq L$ must lie on one side of the half-space defined by the equality $R^T \cdot \eta =$

$L \cdot \eta^{\min} + (1 - L) \cdot \eta^{\max}$, where $\eta^{\min}$ and $\eta^{\max}$ are worst-case and best-case occupancy measures. By our assumption, η also belongs to this side of the half-space. Because η lies in the interior of the convex hull of the vertices V_η, at least one $v \in V_\eta$ must therefore also lie on this side of the hyperplane and have regret $\geq L$. Because v and η both lie on the same face of Ω, we have $I_\Omega(\eta) \subset I_\Omega(v)$ and therefore also $N_\Omega(\eta) \subseteq N_\Omega(v)$.

Hence, it must also hold that:

$$\bigcup_{\eta:\ \mathrm{Reg}^R(\pi^\eta) \geq L} N_\Omega(\eta) \ \subseteq \ \bigcup_{v \in V_R^L} N_\Omega(v),$$

which, together with Equation (9) proves the claim. □

The following lemma relates the set of reward functions to the set of probability distributions D

Lemma C.14. *Given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ and a second reduced reward function $\hat{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, then the following two statements are equivalent:*

a) There exists a data distribution $D \in \Delta(\mathcal{S} \times \mathcal{A})$ such that $\mathbb{E}_{(s,a) \sim D}\left[|R(s,a) - \hat{R}(s,a)|\right] < \epsilon \cdot \text{range } R$

b) At least one component $\hat{R}_i$ of $\hat{R}$ is "close enough" to R, i.e., it holds that for some transition (s, a): $|R(s,a) - \hat{R}(s,a)| < \epsilon \cdot \text{range } R$.

Proof. We first show the direction $b) \Rightarrow a)$. Assume that $|R(s^*, a^*) - \hat{R}(s^*, a^*)| < \epsilon \cdot \text{range } R$ for a given $\hat{R}$ and transition (s^*, a^*). In that case, we can construct the data distribution D which we define as follows:

$$D(s,a) = \begin{cases} p & \text{if } (s,a) \neq (s^*, a^*) \\ 1 - (|\mathcal{S} \times \mathcal{A}| - 1) \cdot p & \text{if } (s,a) = (s^*, a^*) \end{cases}$$

where we choose $p < \min\left(\frac{\epsilon \cdot \text{range } R - |R(s^*,a^*) - \hat{R}(s^*,a^*)|}{\sum_{(s,a) \neq (s^*,a^*)} |R(s,a) - \hat{R}(s,a)|}, \frac{1}{|\mathcal{S} \times \mathcal{A}|} \right)$. From this it can be easily seen that:

$$\begin{aligned} &\mathbb{E}_{(s,a) \sim D}\left[|R(s,a) - \hat{R}(s,a)|\right] \\ &= (1 - (|\mathcal{S} \times \mathcal{A}| - 1) \cdot p) \cdot |R(s^*, a^*) - \hat{R}(s^*, a^*)| \\ &+ p \cdot \sum_{(s,a) \neq (s^*, a^*)} |R(s,a) - \hat{R}(s,a)| \\ &< \epsilon \cdot \text{range } R \end{aligned}$$

We now show the direction $a) \Rightarrow b)$ via contrapositive. Whenever it holds that $|R(s,a) - \hat{R}(s,a)| \geq \epsilon \cdot \text{range } R$ for all transitions $(s,a) \in \mathcal{S} \times \mathcal{A}$, then the expected difference under an arbitrary data distribution $D \in \Delta(\mathcal{S} \times \mathcal{A})$ can be lower bounded as follows:

$$\begin{aligned} &\mathbb{E}_{(s,a) \sim D}\left[|R(s,a) - \hat{R}(s,a)|\right] \\ &= \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} D(s,a) \cdot |R(s,a) - \hat{R}(s,a)| \\ &\geq \epsilon \cdot \text{range } R \cdot \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} D(s,a) \\ &= \epsilon \cdot \text{range } R \end{aligned}$$

Because this holds for all possible data distributions D we have $\neg b) \Rightarrow \neg a)$ which proves the result. □

Corollary C.13 describes the set of reward functions $\hat{R}$ for which there exists an optimal policy $\hat{\pi}$ that achieves worst-case regret under the true reward function R. Lemma C.14 on the other hand, describes the set of reward functions $\hat{R}$, for which there exists a data distribution D such that $\hat{R}$ is close to the true reward function R under D. We would like to take the intersection of those two sets of reward functions, and then derive the set of data distributions D corresponding to this intersection. Toward this goal we first present the following lemma:

Lemma C.15. *For all $\epsilon > 0$, $L \in [0, 1]$, MDP $M = \langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ and all data distributions $D \in \Delta(\mathcal{S} \times \mathcal{A})$, there exists a system of linear inequalities, such that $D \in \mathbf{unsafe}(R, \epsilon, L)$ if and only if the system of linear inequalities is solvable.*

More precisely, let V_R^L be the set of high-regret vertices defined as in Definition C.9. Then, there exists a matrix C, as well as a matrix $U(v)$ and a vector $b(v)$ for every $v \in V_R^L$ such that the following two statements are equivalent:

1. *$D \in \mathbf{unsafe}(R, \epsilon, L)$, i.e., there exists a reward function $\hat{R}$ and a policy $\hat{\pi}$ such that:*
   - *(a)* $\mathbb{E}_{(s,a)\sim D}\left[\frac{|\hat{R}(s,a) - R(s,a)|}{\text{range } R}\right] \leq \epsilon$;
   - *(b)* $\text{Reg}^R(\hat{\pi}) \geq L$
   - *(c)* $\text{Reg}^{\hat{R}}(\hat{\pi}) = 0$
2. *There exists a vertex $v \in V_R^L$ such that the linear system*
$$\begin{bmatrix} U(v) \\ C \cdot \text{diag}(D) \end{bmatrix} \cdot B \ \leq \ \begin{bmatrix} b(v) \\ \epsilon \cdot \text{range } R \cdot \mathbf{1} \end{bmatrix} \tag{11}$$
   has a solution B. Here, we use the vector notation of the data distribution D.

Proof. We can express any reward function $\hat{R}$ as $\hat{R} = R + B$, i.e. describing $\hat{R}$ as a deviation $B : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ from the true reward function. Note that in this case, we get $\hat{R} - R = B$. Next, note that the expression:
$$\mathbb{E}_{(s,a)\sim D}\left[|B(s,a)|\right] \ \leq \ \epsilon \cdot \text{range } R \tag{12}$$
describes a "weighted L^1 ball" around the origin in which B must lie:
$$\mathbb{E}_{(s,a)\sim D}\left[|B(s,a)|\right] \ \leq \ \epsilon \cdot \text{range } R \tag{13}$$
$$\iff \quad \sum_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a) \cdot |B(s,a)| \ \leq \ \epsilon \cdot \text{range } R \tag{14}$$
$$\iff \quad B \in \mathcal{C}(D) \ := \ \left\{ x \in \mathbb{R}^{|\mathcal{S}\times\mathcal{A}|} \ \middle| \ \sum_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a) \cdot |x_{s,a}| \ \leq \ \epsilon \cdot \text{range } R \right\}. \tag{15}$$
This "weighted L^1 ball" is a polyhedral set, which can be described by the following set of inequalities:
$$\begin{aligned} D(s_1,a_1) \cdot B(s_1,a_1) + D(s_1,a_2) \cdot B(s_1,a_2) + \ ... \ &\leq \ \epsilon \cdot \text{range } R \\ -D(s_1,a_1) \cdot B(s_1,a_1) + D(s_1,a_2) \cdot B(s_1,a_2) + \ ... \ &\leq \ \epsilon \cdot \text{range } R \\ D(s_1,a_1) \cdot B(s_1,a_1) - D(s_1,a_2) \cdot B(s_1,a_2) + \ ... \ &\leq \ \epsilon \cdot \text{range } R \\ -D(s_1,a_1) \cdot B(s_1,a_1) - D(s_1,a_2) \cdot B(s_1,a_2) + \ ... \ &\leq \ \epsilon \cdot \text{range } R \\ &\cdots . \end{aligned}$$
This can be expressed more compactly in matrix form, as:
$$C \cdot \text{diag}(D) \cdot B \leq \epsilon \cdot \text{range } R \cdot \mathbf{1}, \tag{16}$$
where $C \in \mathbb{R}^{2^{|\mathcal{S}\times\mathcal{A}|} \times |\mathcal{S}\times\mathcal{A}|}$, $\text{diag}(D) \in \mathbb{R}^{|\mathcal{S}\times\mathcal{A}| \times |\mathcal{S}\times\mathcal{A}|}$, $B \in \mathbb{R}^{|\mathcal{S}\times\mathcal{A}|}$, $\mathbf{1} \in \{1\}^{|\mathcal{S}\times\mathcal{A}|}$ and the individual matrices are defined as follows:
$$C = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ -1 & 1 & \cdots & 1 \\ 1 & -1 & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots \\ -1 & -1 & \cdots & -1 \end{bmatrix}, \qquad \text{diag}(D) = \begin{bmatrix} D(s_1,a_1) & & 0 \\ & \ddots & \\ 0 & & D(s_n,a_m) \end{bmatrix}. \tag{17}$$

Next, from Corollary C.13 we know that a reward function $\hat{R} = R + B$ has an optimal policy with regret larger or equal to L if and only if:

$$\begin{aligned} R + B \;&\in\; \Phi + \bigcup_{v \in V_R^L} \operatorname{cone}\left(\{-e_{s,a}\}_{(s,a) \in zeros(v)}\right) \\ \iff \quad B \;&\in\; -R + \Phi + \bigcup_{v \in V_R^L} \operatorname{cone}\left(\{-e_{s,a}\}_{(s,a) \in zeros(v)}\right) \end{aligned} \tag{18}$$

We can rephrase the above statement a bit. Let's focus for a moment on just a single vertex $v \in V_R^L$. First, note that because Φ and $\operatorname{cone}\left(\{-e_{s,a}\}_{(s,a) \in zeros(v)}\right)$, are polyhedral, $\Phi + \operatorname{cone}\left(\{-e_{s,a}\}_{(s,a) \in zeros(v)}\right)$ must be polyhedral as well (this follows directly from Corollary 3.53 of (Rockafellar & Wets, 2009)). Therefore, the sum on the right-hand side can be expressed by a set of linear constraints $U(v) \cdot B \leq b(v)$.

Hence, a reward function, $\hat{R} = R + B$ is close in expected L1 distance to the true reward function R, and has an optimal policy that has large regret with respect to R, if and only if there exists at least one vertex $v \in V_R^L$, such that:

$$\begin{bmatrix} U(v) \\ C \cdot \operatorname{diag}(D) \end{bmatrix} \cdot B \;\leq\; \begin{bmatrix} b(v) \\ \epsilon \cdot \operatorname{range} R \cdot \mathbf{1} \end{bmatrix} \tag{19}$$

holds. ◻

In the next few subsections, we provide a more interpretable version of the linear system of inequalities in Equation (11), and the conditions for when it is solvable and when not.

C.3.1 More interpretable statement

Ideally, we would like to have a more interpretable statement about which classes of data distributions D fulfill the condition of Equation (11). We now show that for an arbitrary MDP and data distribution D, D is a safe distribution, i.e., error-regret mismatch is not possible, if and only if D fulfills a fixed set of linear constraints (independent of D).

Theorem C.16. *For all MDPs $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ and $L \in [0, 1]$, there exists a matrix M such that for all $\epsilon > 0$ and $D \in \Delta(\mathcal{S} \times \mathcal{A})$ we have:*

$$D \in \mathbf{safe}(R, \epsilon, L) \quad \iff \quad M \cdot D > \epsilon \cdot \operatorname{range} R \cdot \mathbf{1}, \tag{20}$$

where we use the vector notation of D, and $\mathbf{1}$ is a vector containing all ones.

Proof. Remember from Lemma C.15, that a data distribution D is safe, i.e., $D \in \mathbf{safe}(R, \epsilon, L)$, if and only if for all unsafe vertices $v \in V_R^L$ the following system of linear inequalities:

$$\begin{bmatrix} U(v) \\ C \cdot \operatorname{diag}(D) \end{bmatrix} \cdot B \;\leq\; \begin{bmatrix} b(v) \\ \epsilon \cdot \operatorname{range} R \cdot \mathbf{1} \end{bmatrix} \tag{21}$$

has no solution. Let $v \in V_R^L$ be chosen arbitrarily and define $\mathcal{U}_v \coloneqq \{B \in \mathbb{R}^{|\mathcal{S} \times \mathcal{A}|} \mid U(v) \cdot B \leq b(v)\}$, i.e., $\mathcal{U}_v$ is the set of all $B \in \mathbb{R}^{|\mathcal{S} \times \mathcal{A}|}$, such that $\hat{R} \coloneqq R + B$ has an optimal policy with regret at least L. Then, Equation (21) has no solution if and only if:

$$\forall B \in \mathcal{U}_v, \quad C \cdot \operatorname{diag}(D) \cdot B \not\leq \epsilon \cdot \operatorname{range} R \cdot \mathbf{1} \tag{22}$$

$$\iff \quad \forall B \in \mathcal{U}_v, \quad \operatorname{abs}(B)^T \cdot D > \epsilon \cdot \operatorname{range} R, \tag{23}$$

where we used the definition of the matrices C, and $\operatorname{diag}(D)$ (see Equation (16)) and $\operatorname{abs}(\cdot)$ denotes the element-wise absolute value function. Now, we will finish the proof by showing that there exists a *finite* set of vectors $X \subset \mathcal{U}_v$ (which is independent of the choice of D), such that for every $x \in X$, Equation (23) holds if and only if it is true for all B, i.e., more formally:

$$\begin{aligned} &\forall B \in X, \quad \operatorname{abs}(B)^T \cdot D > \epsilon \cdot \operatorname{range} R \\ \iff \quad &\forall B \in \mathcal{U}_v, \quad \operatorname{abs}(B)^T \cdot D > \epsilon \cdot \operatorname{range} R. \end{aligned}$$

And since X is finite, we can then summarize the individual elements of X as rows of a matrix M and get the desired statement by combining the previous few statements, namely:

$$D \in \textbf{safe}(R, \epsilon, L) \iff M \cdot D > \epsilon \cdot \text{range } R \cdot \mathbf{1} \tag{24}$$

Towards this goal, we start by reformulating Equation (23) as a condition on the optimal value of a convex optimization problem:

$$\begin{aligned}
& \forall x \in \mathcal{U}_v, \quad \text{abs}(x)^T \cdot D > \epsilon \cdot \text{range } R \\
\iff & \left(\min_{x \in \mathcal{U}_v} \text{abs}(x)^T \cdot D\right) > \epsilon \cdot \text{range } R \\
\iff & \text{abs}(x^*)^T \cdot D > \epsilon \cdot \text{range } R, \quad \text{where } x^* := \quad \arg\min_{x \in \mathcal{U}_v} \quad \text{abs}(x)^T \cdot D \\
\iff & \text{abs}(x^*)^T \cdot D > \epsilon \cdot \text{range } R, \quad \text{where } x^* := \quad \arg\min_{x} \quad \text{abs}(x)^T \cdot D, \\
& \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{subject to} \quad U(v) \cdot x \leq b(v)
\end{aligned} \tag{25}$$

Note that the optimal value x^* of this convex optimization problem depends on the precise definition of the data distribution D. But importantly, the set over which we optimize (i.e., $\mathcal{U}_v$ defined as the set of all x, such that $U(v) \cdot x \leq b$) does *not* depend on D! The goal of this part of the proof is to show that for all possible D the optimal value of the optimization problem in Equation (25) is *always* going to be one of the vertices of $\mathcal{U}_v$. Therefore, we can transform the optimization problem in Equation (25) into a new optimization problem that does not depend on D anymore. It will then be possible to transform this new optimization problem into a simple set of linear inequalities which will form the matrix M in Equation (24).

Towards that goal, we continue by splitting up the convex optimization problem into a set of linear programming problems. For this, we partition $\mathbb{R}^{|\mathcal{S} \times \mathcal{A}|}$ into its different orthants O_c for $c \in \{-1, 1\}^{|\mathcal{S} \times \mathcal{A}|}$ (a high-dimensional generalization of the quadrants). More precisely, for every $x \in O_c$, we have $\text{diag}\,(c) \cdot x = \text{abs}(x)$. Using this definition, we can reformulate the constraint on the convex optimization problem as follows:

$$\min_{\substack{c \in \{-1,1\}^{|\mathcal{S} \times \mathcal{A}|} \\ x_c \neq \emptyset}} (\text{diag}\,(c) \cdot x_c)^T \cdot D \; > \; \epsilon \cdot \text{range } R, \tag{26}$$

where the individual x_c are defined as the solution of linear programming problems:

$$\begin{aligned}
x_c \; := \; \arg\min_{x} \quad & (\text{diag}\,(c) \cdot x)^T \cdot D \\
\text{subject to} \quad & U(v) \cdot x \leq b(v) \\
& \text{diag}\,(c) \cdot x \geq 0,
\end{aligned} \tag{27}$$

or $x_c := \emptyset$ in case the linear program is infeasible. Finally, by re-parametrizing each linear program using the variable transform $x' = \text{diag}\,(c) \cdot x$ we can convert these linear programs into standard form:

$$\begin{aligned}
x_c \; := \; \text{diag}\,(c) \cdot \quad \arg\min_{x'} \quad & x'^T \cdot D \\
\text{subject to} \quad & U(v) \cdot \text{diag}\,(c) \cdot x' \leq b(v) \\
& x' \geq 0,
\end{aligned} \tag{28}$$

where we used twice the fact that $\text{diag}\,(c)^{-1} = \text{diag}\,(c)$, and hence, $x = \text{diag}\,(c) \cdot x'$. Because it was possible to transform these linear programming problems described in Equation (27) into standard form using a simple variable transform, we can apply standard linear programming theory to draw the following conclusions (see Theorem 3.4 and Section 6 of Chapter 2 of (Vanderbei, 1998) for reference):

1. The set of constraints in Equations (27) and (28) are either infeasible or they form a polyhedral set of feasible solutions.
2. If the set of constraints in Equations (27) and (28) are feasible, then there exists an optimal feasible solution that corresponds to one of the vertices (also called basic feasible solutions) of the polyhedral constraint sets. This follows from the fact that the objective function is bounded from below by zero.

Let's denote the polyhedral set of feasible solutions defined by the constraints in Equation (27) by $\mathcal{F}_c(v)$. Because $\mathcal{F}_c(v)$ does not depend on the specific choice of the data distribution, this must mean that for every possible data distribution D, we have either $x_c = \emptyset$ or x_c is one of the vertices of $\mathcal{F}_c(v)$, denoted by $\text{vertices}(\mathcal{F}_c(v))$! Note that, by definition of x_c, it holds that:

$$\forall x \in \text{vertices}(\mathcal{F}_c(v)), \quad (\text{diag}\,(c) \cdot x_c)^T \cdot D \;\leq\; (\text{diag}\,(c) \cdot x)^T \cdot D. \tag{29}$$

Therefore, we can define:

$$X(v) \;:=\; \bigcup_{c \in \{-1,1\}^{|\mathcal{S}\times\mathcal{A}|}} \text{vertices}(\mathcal{F}_c(v)) \;=\; \{x_1, ..., x_k\}, \qquad \text{and} \qquad M_{X(v)} \;:=\; \begin{bmatrix} \text{abs}(x_1)^T \\ \cdots \\ \text{abs}(x_k)^T \end{bmatrix}, \tag{30}$$

where $M_X(v)$ contains the element-wise absolute value of all vectors of $X(v)$ as row vectors. Let D be an arbitrary data distribution. Then, we've shown the following equivalences:

$$\begin{aligned}
& \forall B \in \mathcal{U}_v, \quad \text{abs}(B)^T \cdot D \;>\; \epsilon \cdot \text{range}\, R && \text{(see Equation (23))} \\
\iff & \min_{\substack{c \in \{-1,1\}^{|\mathcal{S}\times\mathcal{A}|} \\ x_c \neq \emptyset}} \left(\text{diag}\,(c) \cdot x_c\right)^T \cdot D \;>\; \epsilon \cdot \text{range}\, R && \text{(see Equation (26))} \\
\iff & \min_{x \in X(v)} \text{abs}(x)^T \cdot D \;>\; \epsilon \cdot \text{range}\, R && \text{(due to Equation (29))} \\
\iff & M_X(v) \cdot D \;>\; \epsilon \cdot \text{range}\, R \cdot \mathbf{1}
\end{aligned}$$

Now, by combining the individual sets of vertices $X(v)$, as follows:

$$X \;:=\; \bigcup_{v \in V_R^L} X(v) \;=\; \{x_1, ..., x_l\}, \qquad \text{and} \qquad M = \begin{bmatrix} \text{abs}(x_1)^T \\ \cdots \\ \text{abs}(x_l)^T \end{bmatrix}, \tag{31}$$

we are now ready to finish the proof by combining all previous steps:

$$\begin{aligned}
& D \in \mathbf{safe}(R, \epsilon, L) \\
\iff & \forall v \in V_R^L, \, \forall B \in \mathcal{U}_v, && \text{abs}(B)^T \cdot D > \epsilon \cdot \text{range}\, R \\
\iff & \forall v \in V_R^L, && M_X(v) \cdot D > \epsilon \cdot \text{range}\, R \cdot \mathbf{1} \\
\iff & && M \cdot D > \epsilon \cdot \text{range}\, R \cdot \mathbf{1}.
\end{aligned}$$

That was to show. □

C.3.2 Deriving the conditions on D

In Theorem C.16 we've shown that there exists a set of linear constraints $M \cdot D > \epsilon \cdot \text{range}\, R \cdot \mathbf{1}$, such that whenever a data distribution D satisfies these constraints, it is safe. In this subsection, we derive closed-form expressions for the individual rows of M to get a general idea about the different factors determining whether an individual data distribution is safe.

In the proof of Theorem C.16, we showed that M has the form:

$$M = \begin{bmatrix} \text{abs}(x_1)^T \\ \vdots \\ \text{abs}(x_l)^T \end{bmatrix},$$

for some set $X = \{x_1, ..., x_l\}$, where each $x \in X$ belongs to a vertex of the set of linear constraints defined by the following class of system of linear inequalities:

$$\begin{bmatrix} U(v) \\ -\text{diag}\,(c) \end{bmatrix} \cdot x \leq \begin{bmatrix} b(v) \\ 0 \end{bmatrix} \qquad \begin{matrix} \text{(Corresponds to the set of unsafe reward functions)} \\ \text{(Corresponds to the orthant } O_c\text{)} \end{matrix} \tag{32}$$

for some $v \in V_R^L$ (the set of unsafe vertices of Ω), and some $c \in \{-1,1\}^{|\mathcal{S}\times\mathcal{A}|}$ (defining the orthant O_c).

To ease the notation in the following paragraphs, we will use the notation $\mathcal{U}_v$ for the polyhedral set of x such that $U(v) \cdot x \leq b(v)$, and $\mathcal{F}_c(v)$ for the set of solutions to the full set of linear inequalities in Equation (32). Furthermore, we will use $n := |\mathcal{S}|$ and $m := |\mathcal{A}|$.

We start by giving a small helper definition.

Definition C.17 (General position, (Stanley, 2024))**.** Let $\mathcal{H}$ be a set of hyperplanes in $\mathbb{R}^n$. Then $\mathcal{H}$ is in general position if:

$$\begin{aligned} \{H_1, ..., H_p\} \subseteq \mathcal{H},\ p \leq n \quad &\implies \quad \dim(H_1 \cap ... \cap H_p) = n - p \\ \{H_1, ..., H_p\} \subseteq \mathcal{H},\ p > n \quad &\implies \quad H_1 \cap ... \cap H_p = \emptyset \end{aligned}$$

We will use this definition in the next few technical lemmas. First, we claim that each of the vertices of $\mathcal{F}_c(v)$ must lie on the border of the orthant O_c.

Lemma C.18 (Vertices lie on the intersection of the two constraint sets.)**.** *All vertices of the polyhedral set, defined by the system of linear inequalities:*

$$\begin{bmatrix} U(v) \\ -\mathrm{diag}\,(c) \end{bmatrix} \cdot x \leq \begin{bmatrix} b(v) \\ 0 \end{bmatrix} \tag{33}$$

must satisfy some of the inequalities of $-\mathrm{diag}\,(c) \cdot x \ \leq\ 0$ *with equality.*

Proof. Let $\mathcal{U}_v$ be the set of solutions of the upper part of the system of linear equations in Equation (33) and O_c be the set of solutions of the lower part of the system of linear equations in Equation (33). The lemma follows from the fact that $\mathcal{U}_v$ can be expressed as follows (see Equation (18) and the subsequent paragraph):

$$\mathcal{U}_v \ = \ -R + \Phi + \mathrm{cone}\left(\{-e_{s,a}\}_{(s,a) \in zeros(v)}\right), \tag{34}$$

where Φ is a linear subspace. Hence, for every x that satisfies the constraints $U(v) \cdot x \leq b(v)$, x lies on the interior of the line segment spanned between $x' = x + \phi$, and $x'' = x - \phi$ for some $\phi \in \Phi$, $\phi \neq \mathbf{0}$. Note that every point on this line segment also satisfies the constraints $U(v) \cdot x \leq b(v)$. Therefore, x can only be a vertex if it satisfies some of the additional constraints, provided by the inequalities $-\mathrm{diag}\,(c) \cdot x \leq 0$, with equality. ☐

Consequently, every vertex of $\mathcal{F}_c(v)$ is the intersection of some k-dimensional surface of $\mathcal{U}_v$ and $k > 0$ standard hyperplanes (hyperplanes whose normal vector belongs to the standard basis).

Lemma C.19 (Basis for Φ. (Schlaginhaufen & Kamgarpour, 2023))**.** *The linear subspace* Φ *of potential shaping transformations can be defined as:*

$$\Phi \ = \ \mathrm{span}(A - \gamma \cdot P),$$

where $A, P \in \mathbb{R}^{(n \cdot m) \times n}$ *for* $n = |\mathcal{S}|, m = |\mathcal{A}|$ *are matrices defined as:*

$$A := \begin{bmatrix} \mathbf{1}^m & \mathbf{0}^m & \cdots & \mathbf{0}^m \\ \mathbf{0}^m & \mathbf{1}^m & \cdots & \mathbf{0}^m \\ \dots & \dots & \ddots & \dots \\ \mathbf{0}^m & \mathbf{0}^m & \cdots & \mathbf{1}^m \end{bmatrix}, \qquad P := \begin{bmatrix} \text{——} & \tau(\ \cdot \mid s_1, a_1) & \text{——} \\ \text{——} & \tau(\ \cdot \mid s_1, a_2) & \text{——} \\ \cdots & \cdots & \cdots \\ \text{——} & \tau(\ \cdot \mid s_n, a_m) & \text{——} \end{bmatrix},$$

where $\mathbf{0}^m, \mathbf{1}^m$ *are column vectors and* $\tau(\cdot|s_i, a_j)$ *is a row vector of the form* $[\tau(s_1 \mid s_i, a_j), \cdots, \tau(s_n \mid s_i, a_j)]$.

Furthermore, we have $\dim \Phi = n$.

Proof. This has been proven by (Schlaginhaufen & Kamgarpour, 2023) (see their paragraph "Identifiability" of Section 4). The fact that $\dim \Phi = n$ follows from the fact that Φ is the linear space orthogonal to the affine space containing the occupancy measure space Ω, i.e. $\Phi^\perp = L$ where L is the linear subspace parallel to $\mathrm{span}(\Omega)$ (see the paragraph *Convex Reformulation* of Section 3 of (Schlaginhaufen & Kamgarpour, 2023)) and the fact that $\dim \mathrm{span}(\Omega) = n \cdot (m - 1)$ (see Proposition 1 of (Karwowski et al., 2023)). ☐

Lemma C.20 (Dimension of $\mathcal{U}_v$)**.** $\dim \mathcal{U}_v = n \cdot m$.

Proof. Remember that $\mathcal{U}_v$ can be expressed as follows (see Equation (18) and the subsequent paragraph):

$$\mathcal{U}_v \ = \ -R + \Phi + \mathrm{cone}\left(\{-e_{s,a}\}_{(s,a) \in zeros(v)}\right), \tag{35}$$

From Lemma C.19 we know that $\dim \Phi = n$. We will make the argument that:

a) $\dim\left[\text{cone}\left(\{-e_{s,a}\}_{(s,a)\in zeros(v)}\right)\right] \geq n\cdot(m-1)$

b) There exist exactly $n\cdot(m-1)$ basis vectors of $\text{cone}\left(\{-e_{s,a}\}_{(s,a)\in zeros(v)}\right)$ such that the combined set of these vectors and the basis vectors of Φ is linearly independent.

From this, it must follow that:

$$\dim\left[\Phi+\text{cone}\left(\{-e_{s,a}\}_{(s,a)\in zeros(v)}\right)\right] \;=\; \dim\left[\Phi\right] +\; n\cdot(m-1) \;=\; n\cdot m$$

For a), remember that v is a vertex of the occupancy measure space Ω and that each vertex v of Ω corresponds to at least one deterministic policy π^v (see Proposition 1 of (Karwowski et al., 2023)). And since every deterministic policy is zero for exactly $n\cdot(m-1)$ transitions, it must follow that v is also zero in *at least* $n\cdot(m-1)$ transitions, since whenever $\pi^v(a|s)=0$ for some $(s,a)\in\mathcal{S}\times\mathcal{A}$, we have:

$$v(s,a) \quad=\quad \sum_{t=0}^{\infty}\gamma^t\cdot P(s_t=s,a_t=a\mid\pi^v,\tau) \quad=\quad \pi^v(a|s)\cdot\sum_{t=0}^{\infty}\gamma^t\cdot P(s_t=s\mid\pi^v,\tau) \quad=\quad 0.$$

Therefore, it follows that $\dim\left[\text{cone}\left(\{-e_{s,a}\}_{(s,a)\in zeros(v)}\right)\right] \geq n\cdot(m-1)$.

For b), (Puterman, 1994) give necessary and sufficient conditions for a point $x\in\mathbb{R}^{n\cdot m}$ to be part of Ω (see the dual linear program in section 6.9.1 and the accompanying explanation), namely:

$$x\in\Omega \quad\Longleftrightarrow\quad \left[(A-\gamma\cdot P)^T\cdot x=\mu_0 \quad\text{and}\quad I\cdot x\geq 0\right],$$

where I is the identity matrix and we use the vector notation of the initial state distribution μ_0. Because v is a vertex of Ω, it can be described as the intersection of $n\cdot m$ supporting hyperplanes of Ω that are in general position. Because $(A-\gamma\cdot P)$ has rank n (see Lemma C.19), this must mean that for v at least $n\cdot(m-1)$ inequalities of the system $I\cdot v\geq 0$ hold with equality and the combined set of the corresponding row vectors and the row vectors of $(A-\gamma\cdot P)^T$ is linearly independent (as the vectors correspond to the normal vectors of the set of $n\cdot m$ hyperplanes in general position).

Note that the set of unit vectors that are orthogonal to v is precisely defined by $\{-e_{s,a}\}_{(s,a)\in zeros(v)}$, since, by definition of $zeros(v)$ (see Definition C.10), we have

$$\forall x\in\{-e_{s,a}\}_{(s,a)\in zeros(v)},\quad x^T\cdot v=0.$$

From this, it must follow that the polyhedral set $\mathcal{U}_v$, has dimension $n\cdot m$. ☐

Lemma C.21 (Defining the faces of $\mathcal{U}_v$). *Each k-dimensional face F of $\mathcal{U}_v$ (with $k\geq n$) can be expressed as:*

$$-R+\Phi+\text{cone}\left(E_F\right), \qquad \textit{where}\;\; E_F\subset\{-e_{s,a}\}_{(s,a)\in zeros(v)}, \tag{36}$$

such that $|E_F|=k-n$ and the combined set of vectors of E_F and the columns of $A-\gamma\cdot P$ is linearly independent.

Proof. Remember that $\mathcal{U}_v$ can be expressed as follows (see Equation (18) and the subsequent paragraph):

$$\mathcal{U}_v \;=\; -R+\Phi+\text{cone}\left(\{-e_{s,a}\}_{(s,a)\in zeros(v)}\right), \tag{37}$$

This means that we can express $\mathcal{U}_v$ as a polyhedral cone, spanned by non-negative combinations of:

- The column vectors of the matrix $A-\gamma\cdot P$.
- The column vectors of the matrix $-(A-\gamma\cdot P)$. Since Φ is a linear subspace and a cone is spanned by only the positive combinations of its set of defining vectors we also have to include the negative of this matrix to allow arbitrary linear combinations.
- The set of vectors $\{-e_{s,a}\}_{(s,a)\in zeros(v)}$.

Consequently, each face of $\mathcal{U}_v$ of dimension k is spanned by a subset of the vectors that span $\mathcal{U}_v$ and is therefore also a cone of these vectors. Because the face has dimension k, we require exactly k linearly independent vectors, as it's not possible to span a face of dimension k with less than k linearly independent vectors, and every additional linearly independent vector would increase the dimension of the face. Furthermore, since Φ is a linear subspace that is unbounded by definition, it must be part of every face. Therefore, every face of $\mathcal{U}_v$ has a dimension of at least n (the dimension of Φ). □

Note that the converse of Lemma C.21 doesn't necessarily hold, i.e., not all sets of the form described in Equation (36) are necessarily surfaces of the polyhedral set $U(v) \cdot x \leq b(v)$.

We are now ready to develop closed-form expressions for the vertices of $\mathcal{F}_c(v)$. Note that it is possible for $\mathbf{0} \in \mathbb{R}^{n \cdot m}$ to be a vertex of $\mathcal{F}_c(v)$. But in this case, according to Theorem C.16, this must mean that the linear system of inequalities $M \cdot D > \epsilon \cdot \text{range } R \cdot \mathbf{1}$ is infeasible (since M would contain a zero row and all elements on the right-hand side are non-negative), which means that in this case $\mathbf{safe}(R, \epsilon, L) = \emptyset$. We will therefore restrict our analysis to all non-zero vertices of $\mathcal{F}_c(v)$.

Proposition C.22 (Vertices of $\mathcal{F}_c(v)$.)**.** *Every vertex v_{FG} of $\mathcal{F}_c(v)$, with $v_{FG} \neq \mathbf{0}$, lies on the intersection of some face F of the polyhedral set $\mathcal{U}_v$ and some face G of the orthant O_c and is defined as follows:*

$$v_{FG} \quad = \quad -R + [A - \gamma \cdot P, E_F] \cdot \Big(E_G \cdot [A - \gamma \cdot P, E_F]\Big)^{-1} \cdot E_G \cdot R,$$

where E_F, E_G are matrices whose columns contain standard unit vectors, such that:

$$\begin{aligned} F &= -R + \Phi + \operatorname{cone}(E_F), \qquad \text{for } E_F \subset \{-e_{s,a}\}_{(s,a) \in zeros(v)} \\ G &= \{x \in \mathbb{R}^{n \cdot m} \mid E_G \cdot x = \mathbf{0}\}. \end{aligned}$$

Proof. We start by defining the faces of the orthant O_c. Remember that O_c is the solution set to the system of inequalities $\operatorname{diag}(c) \cdot x \geq 0$. Therefore, each defining hyperplane of O_c is defined by one row i of $\operatorname{diag}(c)$, i.e. $\operatorname{diag}(c)_i \cdot x = 0$. Note that since $c \in \{-1, 1\}^{n \cdot m}$, this is equivalent to the equation $e_i^T \cdot x = 0$ where e_i is either the i'th standard unit vector or its negative. And because every l-dimensional face G of O_c is the intersection of l standard hyperplanes $\{e_{i_1}, ..., e_{i_l}\}$, this must mean that G is defined as the set of solutions to the system of equations $E_G \cdot x = 0$ where E_G is the matrix whose row vectors are the vectors $\{e_{i_1}, ..., e_{i_l}\}$.

Next, let v_{FG} be an arbitrary non-zero vertex of $\mathcal{F}_c(v)$. As proven in Lemma C.18, every vertex of $\mathcal{F}_c(v)$ must satisfy some of the inequalities $\operatorname{diag}(c) \cdot x \geq 0$ for $c \in \{-1, 1\}^{n \cdot m}$ with equality. This means that v_{FG} must lie on some face G of the orthant O_c. The non-zero property guarantees that not all inequalities of the system of inequalities $\operatorname{diag}(c) \cdot x \geq 0$ are satisfied with equality, i.e. that G is not a vertex. Assume that $k > 0$ inequalities are *not* satisfied with equality. Therefore, G must have dimension k, and $E_G \in \mathbb{R}^{n \cdot m \times k}$.

Since v_{FG} is a vertex of the intersection of the orthant O_c and the polyhedral set $\mathcal{U}_v$, and it only lies on a k-dimensional face of O_c, it must also lie on a $n \cdot m - k$ dimensional face F of $\mathcal{U}_v$ such that the combined set of hyperplanes defining F and G is in general position. The condition that the combined set of hyperplanes is in general position is necessary, to guarantee that v_{FG} has dimension 0 and is therefore a proper vertex.

From Lemma C.21 we know that F can be expressed as:

$$-R + \Phi + \operatorname{cone}(E_F), \qquad \text{where } \; E_F \subset \{-e_{s,a}\}_{(s,a) \in zeros(v)}, \tag{38}$$

such that $|E_F| = n \cdot (m-1) - k$ and the combined set of vectors of E_F and the columns of $A - \gamma \cdot P$ are linearly independent.

Because v_{FG} is part of both, F and G, we can combine all information that we gathered about F and G and deduce that it must hold that:

$$\underbrace{E_G \cdot v_{FG} = 0}_{\text{equivalent to } v_{FG} \in G} \qquad \text{, and} \qquad \underbrace{\exists x \in \mathbb{R}^{n \cdot m - k}, \quad v_{FG} = -R + [A - \gamma \cdot P, E_F] \cdot x}_{\text{equivalent to } v_{FG} \in F}, \tag{39}$$

where for x in Equation (39) it additionally must hold that $\forall i \in \{n+1, ..., n \cdot m - k\}$, $x_i \geq 0$. This must hold because these last entries of x should form a convex combination of the vectors in E_F (as

F is defined to lie in the cone of E_F, see Equation (38)). We briefly state the following two facts that will be used later in the proof:

a) v_{FG} is the only vector in $\mathbb{R}^{n\cdot m}$ that fulfills both conditions in Equation (39). This is because we defined F in such a way that the intersection of F and G is a single point. And only points in this intersection fulfill both conditions in Equation (39).

b) For every non-zero vertex v_{FG}, there can only exist a single x that satisfies the two conditions in Equation (39). This follows directly from the assumption that the combined set of vectors of E_F and the columns of $A - \gamma \cdot P$ are linearly independent (see Equation (38) and the paragraph below).

We can combine the two conditions in Equation (39) to get the following, unified condition that is satisfied for every non-zero vertex v_{FG}:

$$\exists x \in \mathbb{R}^{n\cdot m-k}, \quad E_G \cdot \Big(-R + [A - \gamma \cdot P, E_F] \cdot x \Big) = \mathbf{0}^{n\cdot m-k}, \tag{40}$$

From this, it is easy to compute the precise coordinates of v_{FG}:

$$x = \Big(E_G \cdot [A - \gamma \cdot P, E_F] \Big)^{-1} \cdot E_G \cdot R \tag{41}$$

$$\Longrightarrow \quad v_{FG} = -R + [A - \gamma \cdot P, E_F] \cdot \Big(E_G \cdot [A - \gamma \cdot P, E_F] \Big)^{-1} \cdot E_G \cdot R. \tag{42}$$

We finish the proof by showing that the matrix inverse in Equation (41) always exists for every non-zero vertex v_{FG}. Assume, for the sake of contradiction, that the matrix $E_G \cdot [A - \gamma \cdot P, E_F]$ is not invertible. We will show that in this case, there exists a $z \in \mathbb{R}^{n\cdot m}$ with $z \neq v_{FG}$ such that z fulfills both conditions in Equation (39). As we've shown above in fact a) this is not possible, hence this is a contradiction.

Assuming that $E_G \cdot [A - \gamma \cdot P, E_F]$ is not invertible, we know from standard linear algebra that in that case the kernel of this matrix has a dimension larger than zero. Let y_1, y_2, be two elements of this kernel with $y_1 \neq y_2$.

Earlier in this proof, we showed that for every non-zero vertex v_{FG}, Equation (40) is satisfiable. Let x be a solution to Equation (40). From our assumptions, it follows that both $x + y_1$ and $x + y_2$ must also be solutions to Equation (40) as:

$$\begin{aligned}
\forall y \in \{y_1, y_2\}, \quad & E_G \cdot \Big(-R + [A - \gamma \cdot P, E_F] \cdot (x + y) \Big) \\
&= \quad -E_G \cdot R \; + \; E_G \cdot [A - \gamma \cdot P, E_F] \cdot (x + y) \\
&= \quad -E_G \cdot R \; + \; E_G \cdot [A - \gamma \cdot P, E_F] \cdot x \\
&= \quad E_G \cdot \Big(-R + [A - \gamma \cdot P, E_F] \cdot x \Big) \\
&= \quad \mathbf{0}^{n\cdot m-k}.
\end{aligned}$$

And from this, it will follow that both, $x + y_1$ and $x + y_2$ must satisfy both conditions in Equation (39). Because $x + y_1 \neq x + y_2$, it must also hold that:

$$-R + [A - \gamma \cdot P, E_F] \cdot (x + y_1) \quad \neq \quad -R + [A - \gamma \cdot P, E_F] \cdot (x + y_2),$$

see fact b) above for a proof of this. And this would mean that there exists at least one $z \in \mathbb{R}^{n\cdot m}$ with $z \neq v_{FG}$ such that z fulfills both conditions in Equation (39). But as we have shown in fact a), this is not possible. Therefore, the matrix $E_G \cdot [A - \gamma \cdot P, E_F]$ *must* be invertible for every non-zero vertex v_{FG}. □

We are now ready to provide more specific information about the exact conditions necessary for a data distribution D to be safe.

Corollary C.23 (Vertices of $\mathcal{F}_c(v)$.)**.** *For all $\epsilon > 0$, $L \in [0, 1]$ and MDPs $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, there exists a matrix M such that:*

$$D \in \mathbf{safe}(R, \epsilon, L) \quad \Longleftrightarrow \quad M \cdot D > \epsilon \cdot \text{range}\, R \cdot \mathbf{1}, \tag{43}$$

Algorithm 1 Computes the set of conditions used to determine the safety of a data distribution.

1: **function** ComputeM($MDP = \langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, $L \in [0, 1]$)
2: $\quad I \leftarrow$ the *set* of all unit vectors of dimension $|\mathcal{S} \times \mathcal{A}|$. Create a fixed ordering of $\mathcal{S}$ and $\mathcal{A}$ and denote each vector of I by $e_{(s,a)}$ for a unique tuple $(s, a) \in \mathcal{S} \times \mathcal{A}$.

3: $\quad$ candidates $\leftarrow [\,]$
4: $\quad \Pi_d \leftarrow$ Set of deterministic policies of MDP
5: $\quad$ **for** $\pi \in \{\pi' \in \Pi_d : \text{Reg}^R(\pi') \geq L\}$ **do** $\quad \triangleright$ Create a set of potential row candidates.
6: $\quad\quad E \leftarrow \{e_{(s,a)} \in I : \pi(a|s) = 0\}$
7: $\quad\quad$ **for** $E_F \subset E$ **do**
8: $\quad\quad\quad$ **for** $subset \subseteq I \setminus E_F$, $|subset| = |\mathcal{S}|$ **do**
9: $\quad\quad\quad\quad E_G \leftarrow E_F \cup subset$
10: $\quad\quad\quad\quad E_F, E_G \leftarrow \text{ColumnMatrix}(E_F),\ \text{RowMatrix}(E_G)$
11: $\quad\quad\quad\quad$ candidates.append$((E_F, E_G))$

12: $\quad$ rows $\leftarrow [\,]$ $\quad \triangleright$ Find the valid rows amongst the candidates
13: $\quad$ **for** $(E_F, E_G) \in$ candidates **do**
14: $\quad\quad k \leftarrow$ num_columns(E_F)
15: $\quad\quad$ **if** $\text{rank}\Big(E_G \cdot [A - \gamma \cdot P, -E_F]\Big) = n + k$ **then**
16: $\quad\quad\quad x \leftarrow \Big(E_G \cdot [A - \gamma \cdot P, -E_F]\Big)^{-1} \cdot E_G \cdot R$
17: $\quad\quad\quad$ **if** $\forall i \in \{n, n+1, ..., n+k\}\ x_i \geq 0$ **then**
18: $\quad\quad\quad\quad \text{row} \leftarrow \text{abs}\Big(-R + [A - \gamma \cdot P, -E_F] \cdot x\Big)^T$
19: $\quad\quad\quad\quad$ rows.append$\big(\text{row}\big)$

20: $\quad M \leftarrow$ RowMatrix(rows)
21: $\quad$ **return** M

for all $D \in \Delta(\mathcal{S} \times \mathcal{A})$, where we use the vector notation of D, and $\mathbf{1}$ is a vector containing all ones. The matrix M is defined as:

$$M = \begin{bmatrix} \text{abs}(x_1)^T \\ \cdots \\ \text{abs}(x_l)^T \end{bmatrix},$$

where an individual row x_i of M can either be all zeros, or

$$x_i \ = \ -R + [A - \gamma \cdot P, E_{i1}] \cdot \Big(E_{i2} \cdot [A - \gamma \cdot P, E_{i1}]\Big)^{-1} \cdot E_{i2} \cdot R, \tag{44}$$

where E_{i1}, E_{i2} are special matrices whose columns contain standard unit vectors.

Proof. This is a simple combination of Theorem C.16 and Proposition C.22. □

In particular, Equation (44) shows that whether a particular data distribution D is safe or not depends on the true reward function R, as well as the transition distribution τ (encoded by the matrix P).

C.3.3 Algorithm to compute the conditions on D

The derivations of Appendix C.3.2 can be used to define a simple algorithm that constructs matrix M. An outline of such an algorithm is presented in Algorithm 1. We use the terms RowMatrix and ColumnMatrix to denote functions that take a set of vectors and arrange them as rows/columns of a matrix.

To give a brief explanation of the algorithm:

- Line 4 follows from the definitions of V_R^L, $X(v)$ and X (see Definition C.9 and eqs. (30) and (31)).

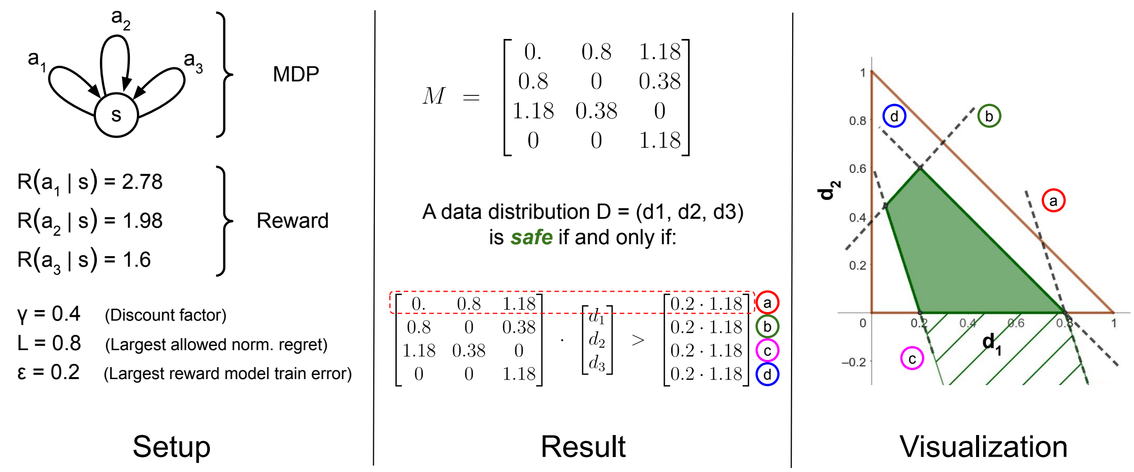

Figure 3: A working example of how to compute the matrix M on a very simple MDP with a single state and three actions. Given the information in the *Setup* column, matrix M can be computed using Algorithm 1. The constructed matrix M contains four linear constraints that a data distribution D has to fulfill in order to be in $\mathbf{safe}(R, \epsilon, L)$. The four constraints are plotted in the right-most column.

- Line 6 are taken from the definition of E_F in Proposition B.20 (except that we don't take the negative of the vectors and instead negate E_F in the final formula).
- Lines 7 and 8 are taken from the definition of E_G (see the first two paragraphs of Proposition C.22). We additionally ensure that E_F is a subset of E_G as otherwise, the matrix $E_G \cdot [A - \gamma \cdot P, -E_F]$ is not invertible (due to the multiplication of $E_G \cdot E_F$) and we know that the matrix must be invertible for every vertex.
- Lines 15 and 17 compute the row of the matrix M. The formulas are a combination of the definition of the sets $X(v), X$ (see Equations (30) and (31)), the matrix M_X (Equation (31)) and Proposition C.22.
- Line 14 checks whether the matrix $E_G \cdot [A - \gamma \cdot P, -E_F]$ is invertible. This is always the case for the rows of M (see the last few paragraphs of the proof of Proposition C.22) but might not be true for other candidates.
- To explain Line 16, remember that every row of the matrix M corresponds to the element-wise absolute value of a vector that lies on the intersection of two polyhedral sets F, and G (see Proposition C.22). The polyhedral set F is defined via a convex cone. To check that our solution candidate lies in this convex cone, we have to check whether the last entries of $x = (E_G \cdot [A - \gamma \cdot P, -E_F])^{-1} \cdot E_G \cdot R$, the entries belonging to the vectors in E_F, are non-negative.

The asymptotic runtime of this naive algorithm is exponential in $|\mathcal{S} \times \mathcal{A}|$ due to the iterations over all subsets in Lines 6 and 7. However, better algorithms might exist and we consider this an interesting direction for future work.

C.3.4 Working example of computing matrix M

Figure 3 shows a simple toy-MDP with a single state and three actions, for which we then compute matrix M using Algorithm 1. Due to the simple structure of the MDP, the auxiliary matrix A and the state-transition matrix P (both used in Algorithm 1) become trivial:

$$A = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \text{ and } \quad P = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

The resulting four constraints that a given data distribution over the state-action space of this MDP has to fulfill to be in $\mathbf{safe}(R, \epsilon, L)$ are then visualized in the right-most column of Figure 3. Note that the constraints are over three-dimensional vectors. However, because D is a probability distribution, it must live in a two-dimensional subspace of this three-dimensional space, and using the identity $d_3 = 1 - d_1 - d_2$ we can transform the constraints as follows:

$$\begin{bmatrix} | & | & | \\ m_1 & m_2 & m_3 \\ | & | & | \end{bmatrix} \cdot \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix} > \begin{bmatrix} | \\ b \\ | \end{bmatrix} \quad \iff \quad \begin{bmatrix} | & | \\ m_1 - m_3 & m_2 - m_3 \\ | & | \end{bmatrix} \cdot \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} > \begin{bmatrix} | \\ b - m_3 \\ | \end{bmatrix}$$

The brown triangle in Figure 3 depicts the 2d-probability simplex of all distributions over the three actions of the MDP.

Note that constraint ⓐ is a redundant constraint that is already covered by the constraint ⓓ and the border of the simplex. It would therefore be possible to disregard the computation of such constraints entirely, which could speed up the execution of Algorithm 1. In the next section, we discuss this possibility, as well as other potential directions in which we can extend Theorem 3.5.

C.3.5 Building up on Theorem 3.5

There are multiple ways how future work can build up on the results of Theorem 3.5:

Finding sufficient conditions for safety that require less information about the true reward function: It would be very interesting to investigate whether there exists some subset of the set of safe data distributions for which it is possible to more easily determine membership. This could be helpful in practice, as knowing that a provided data distribution is safe directly yields safety guarantees for the resulting optimal policy.

Developing faster methods to construct M: While the algorithm we provide above runs in exponential time it is unclear whether this has to be the case. The set of vectors that are computed by our algorithm is redundant in the sense that some elements can be dropped as the conditions they encode are already covered by other rows of M. Depending on what fraction of computed elements are redundant it might be possible to develop an algorithm that prevents the computation of redundant rows and can therefore drastically reduce computation time. Alternatively, it would be interesting to develop fast algorithms to compute only parts of M. This could be especially interesting to quickly prove the unsafety of a data distribution, which only requires that a single constraint is violated.

Extending Theorem 3.5 to the regularized policy optimization case: This would allow one to extend the use case we described above to an even wider variety of reward learning algorithms, such as RLHF.

A theoretical baseline (a broader view on the previous point): Most of the options above reveal the properties of the "baseline algorithm" of reinforcement learning under unknown rewards: First, a reward model is trained, and second, a policy is optimized against the trained reward model. The matrix M is valid for the simplest such baseline algorithms without any regularization in either the reward model or the policy. As we mentioned in comments to other reviewers, it would be valuable to study other training schemes (e.g., regularized reward modeling, or switching back and forth between policy optimization and reward modeling on an updated data distribution), for which the set of safe data distributions (or "safe starting conditions") is likely more favorable than for the baseline case. Then, similar to how empirical work compares new algorithms empirically against baseline algorithms, we hope our work can be a basis to theoretically study improved RL algorithms under unknown rewards, e.g. by deriving a more favorable analog of the matrix M and comparing it with our work.

C.4 Existence of negative results in the RLHF setting

C.4.1 Generalization of the error measurement

In this subsection we test the extent to which the results of the previous section generalize to different distance definitions. To ensure compatibility with the positive results of Appendix D.3, we consider MDPs with finite time horizon T. In this setting, trajectories are defined as a finite list of states and actions: $\xi = s_0, a_0, s_1, ..., a_{T-1}$. Let Ξ bet the set of all trajectories of length T. As in the previous sections, $G : \Xi \to \mathbb{R}$ denotes the trajectory return function, defined as:

$$G(\xi) = \sum_{t=0}^{T-1} \gamma^t \cdot R(s_t, a_t)$$

Proposition C.24. *Given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, a data sampling policy $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ and a second reward function $\hat{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, we can upper bound the expected difference in trajectory evaluation as follows:*

$$\mathbb{E}_{\xi \sim \pi}\left[|G_R(\xi) - G_{\hat{R}}(\xi)|\right] \;\leq\; \frac{1-\gamma^T}{1-\gamma} \cdot \mathbb{E}_{(s,a)\sim D^\pi}\left[\left|R(s,a) - \hat{R}(s,a)\right|\right] \tag{45}$$

where $D^\pi = \frac{1-\gamma}{1-\gamma^T} \cdot \eta^\pi$.

Proof. This follows from the subsequent derivation:

$$\begin{aligned}
\mathbb{E}_{\xi \sim \pi}\left[|G_R(\xi) - G_{\hat{R}}(\xi)|\right] \;&=\; \sum_{\xi \in \Xi} P(\xi \mid \pi) \cdot \left|\sum_{t=0}^{T-1} \gamma^t \cdot (R(s_t, a_t) - \hat{R}(s_t, a_t))\right| \\
&\leq\; \sum_{\xi \in \Xi} P(\xi \mid \pi) \cdot \sum_{t=0}^{T-1} \gamma^t \cdot \left|R(s_t, a_t) - \hat{R}(s_t, a_t)\right| \\
&=\; \sum_{(s,a) \in \mathcal{S}\times\mathcal{A}} \left(\sum_{t=0}^{T-1} \gamma^t \cdot P(s_t = s, a_t = a \mid \pi)\right) \cdot \left|R(s,a) - \hat{R}(s,a)\right| \\
&=\; \sum_{(s,a) \in \mathcal{S}\times\mathcal{A}} \eta^\pi(s,a) \cdot \left|R(s,a) - \hat{R}(s,a)\right| \\
&=\; \frac{1-\gamma^T}{1-\gamma} \cdot \mathbb{E}_{(s,a)\sim D^\pi}\left[\left|R(s,a) - \hat{R}(s,a)\right|\right]
\end{aligned}$$

□

Given some reward function R, define the probability of trajectory ξ_1 being preferred over trajectory ξ_2 to be:

$$p_R(\xi_1 \succ \xi_2) \;=\; \sigma(G_R(\xi_1) - G_R(\xi_2)) \;=\; \frac{\exp(G_R(\xi_1))}{\exp(G_R(\xi_1)) + \exp(G_R(\xi_2))}.$$

Then, the following statement holds:

Proposition C.25. *Given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, a data sampling policy $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ and a second reward function $\hat{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, we can upper bound the expected KL divergence over trajectory preference distributions as follows:*

$$\mathbb{E}_{\xi_1,\xi_2 \sim \pi\times\pi}\left[\mathbb{D}_{KL}\left(p_R(\cdot|\xi_1,\xi_2) || p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right)\right] \;\leq\; 2 \cdot \mathbb{E}_{\xi\sim\pi}\left[|G_R(\xi) - G_{\hat{R}}(\xi)|\right], \tag{46}$$

Proof. The right-hand-side of Equation (46) can be lower bounded as follows:

$$\begin{aligned}
2\cdot\; & \mathbb{E}_{\xi\sim\pi}\left[|G_R(\xi) - G_{\hat{R}}(\xi)|\right] && (47)\\
&= \mathbb{E}_{\xi_1,\xi_2\sim\pi\times\pi}\left[|G_R(\xi_1) - G_{\hat{R}}(\xi_1)| + |G_R(\xi_2) - G_{\hat{R}}(\xi_2)|\right] && (48)\\
&\geq \mathbb{E}_{\xi_1,\xi_2\sim\pi\times\pi}\left[\left|(G_R(\xi_1) - G_R(\xi_2)) - (G_{\hat{R}}(\xi_1) - G_{\hat{R}}(\xi_2))\right|\right] && (49)\\
&= \mathbb{E}_{\xi_1,\xi_2\sim\pi\times\pi}\left[|x_{\xi_1,\xi_2} - y_{\xi_1,\xi_2}|\right], && (50)
\end{aligned}$$

where from Equation (48) to Equation (49) we used the triangle inequality and did some rearranging of the terms, and from Equation (49) to Equation (50) we simplified the notation a bit by defining $x_{\xi_1,\xi_2} := G_R(\xi_1) - G_R(\xi_2)$ and $y_{\xi_1,\xi_2} := G_{\hat{R}}(\xi_1) - G_{\hat{R}}(\xi_2)$.

Similarly, we can reformulate the left-hand-side of Equation (46) as follows:

$$\mathbb{E}_{\xi_1,\xi_2\sim\pi\times\pi}\left[\mathbb{D}_{\text{KL}}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right)\right] \tag{51}$$

$$= \mathbb{E}_{\xi_1,\xi_2\sim\pi\times\pi}\left[\sum_{\substack{i,j\in\{1,2\}\\ i\neq j}} p_R(\xi_i\succ\xi_j|\xi_1,\xi_2)\cdot\log\left(\frac{p_R(\xi_i\succ\xi_j|\xi_1,\xi_2)}{p_{\hat{R}}(\xi_i\succ\xi_j|\xi_1,\xi_2)}\right)\right] \tag{52}$$

$$= \mathbb{E}_{\xi_1,\xi_2\sim\pi\times\pi}\left[\sum_{\substack{i,j\in\{1,2\}\\ i\neq j}} \sigma(G_R(\xi_i)-G_R(\xi_j))\cdot\log\left(\frac{\sigma(G_R(\xi_i)-G_R(\xi_j))}{\sigma(G_{\hat{R}}(\xi_i)-G_{\hat{R}}(\xi_j))}\right)\right] \tag{53}$$

$$= \mathbb{E}_{\xi_1,\xi_2\sim\pi\times\pi}\left[\sum_{\substack{i,j\in\{1,2\}\\ i\neq j}} \sigma(x_{\xi_i,\xi_j})\cdot\log\left(\frac{\sigma(x_{\xi_i,\xi_j})}{\sigma(y_{\xi_i,\xi_j})}\right)\right]. \tag{54}$$

We will now prove the lemma by showing that for all $(\xi_1,\xi_2)\in\Xi\times\Xi$ we have:

$$\sum_{\substack{i,j\in\{1,2\}\\ i\neq j}} \sigma(x_{\xi_i,\xi_j})\cdot\log\left(\frac{\sigma(x_{\xi_i,\xi_j})}{\sigma(y_{\xi_i,\xi_j})}\right) \;\leq\; |x_{\xi_1,\xi_2}-y_{\xi_1,\xi_2}|, \tag{55}$$

from which it directly follows that Equation (54) is smaller than Equation (50).

Let $(\xi_1,\xi_2)\in\Xi\times\Xi$ be chosen arbitrarily. We can then upper bound the left-hand side of Equation (55) as follows:

$$\sigma(x_{\xi_1,\xi_2})\cdot\log\left(\frac{\sigma(x_{\xi_1,\xi_2})}{\sigma(y_{\xi_1,\xi_2})}\right) \;+\; \sigma(x_{\xi_2,\xi_1})\cdot\log\left(\frac{\sigma(x_{\xi_2,\xi_1})}{\sigma(y_{\xi_2,\xi_1})}\right) \tag{56}$$

$$\leq\; \log\left(\frac{\sigma(x_{\xi_1,\xi_2})}{\sigma(y_{\xi_1,\xi_2})}\right) \;+\; \log\left(\frac{\sigma(x_{\xi_2,\xi_1})}{\sigma(y_{\xi_2,\xi_1})}\right) \tag{57}$$

$$=\; \log\left(\frac{\sigma\big(x_{\xi_1,\xi_2}\big)\cdot\sigma\big(-x_{\xi_1,\xi_2}\big)}{\sigma\big(y_{\xi_1,\xi_2}\big)\cdot\sigma\big(-y_{\xi_1,\xi_2}\big)}\right) \tag{58}$$

$$=\; \log\left(\frac{\exp(x_{\xi_1,\xi_2})\cdot(1+\exp(y_{\xi_1,\xi_2}))^2}{\exp(y_{\xi_1,\xi_2})\cdot(1+\exp(x_{\xi_1,\xi_2}))^2}\right) \tag{59}$$

$$= x_{\xi_1,\xi_2}-y_{\xi_1,\xi_2}+2\cdot\log\left(\frac{1+\exp(y_{\xi_1,\xi_2})}{1+\exp(x_{\xi_1,\xi_2})}\right), \tag{60}$$

where we used the fact that $x_{\xi_1,\xi_2}=G_R(\xi_1)-G_R(\xi_2)$ and therefore, $-x_{\xi_1,\xi_2}=x_{\xi_2,\xi_1}$ (similar for y_{ξ_1,ξ_2}). We now claim that for all $(\xi_1,\xi_2)\in\Xi\times\Xi$ it holds that:

$$x_{\xi_1,\xi_2}-y_{\xi_1,\xi_2}+2\cdot\log\left(\frac{1+\exp(y_{\xi_1,\xi_2})}{1+\exp(x_{\xi_1,\xi_2})}\right) \;\leq\; |x_{\xi_1,\xi_2}-y_{\xi_1,\xi_2}| \tag{61}$$

We prove this claim via proof by cases:

$\underline{x_{\xi_1,\xi_2}>y_{\xi_1,\xi_2}}$: In this case we have $|x_{\xi_1,\xi_2}-y_{\xi_1,\xi_2}|=x_{\xi_1,\xi_2}-y_{\xi_1,\xi_2}$ and Equation (61) becomes:

$$2\cdot\log\left(\frac{1+\exp(y_{\xi_1,\xi_2})}{1+\exp(x_{\xi_1,\xi_2})}\right) \;\leq\; 0.$$

And since $x_{\xi_1,\xi_2}>y_{\xi_1,\xi_2}$ the fraction inside the logarithm is smaller than 1, this equation must hold.

$\underline{x_{\xi_1,\xi_2}=y_{\xi_1,\xi_2}}$: In this case, Equation (61) reduces to $0\geq 0$ which is trivially true.

$\underline{x_{\xi_1,\xi_2} < y_{\xi_1,\xi_2}}$: In this case, we have $|x_{\xi_1,\xi_2} - y_{\xi_1,\xi_2}| = y_{\xi_1,\xi_2} - x_{\xi_1,\xi_2}$ and we can reformulate Equation (61) as follows:

$$\begin{aligned} x_{\xi_1,\xi_2} - y_{\xi_1,\xi_2} + 2 \cdot \log\left(\frac{1+\exp(y_{\xi_1,\xi_2})}{1+\exp(x_{\xi_1,\xi_2})}\right) &\leq y_{\xi_1,\xi_2} - x_{\xi_1,\xi_2} \\ \iff \quad \frac{1+\exp(y_{\xi_1,\xi_2})}{1+\exp(x_{\xi_1,\xi_2})} &\leq \frac{\exp(y_{\xi_1,\xi_2})}{\exp(x_{\xi_1,\xi_2})} \\ \iff \quad \exp(x_{\xi_1,\xi_2}) &\leq \exp(y_{\xi_1,\xi_2}). \end{aligned}$$

Because we assume that $x_{\xi_1,\xi_2} < y_{\xi_1,\xi_2}$, the last equation, and therefore also the first, must be true.

Combining all the previous statements concludes the proof. □

Finally, in some RLHF scenarios, one prefers to only compare trajectories with a common starting state. In the last lemma, we upper-bound the expected error in choice distributions with trajectories that share a common starting state by the expected error in choice distributions with arbitrary trajectories:

Proposition C.26. *Given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, a data sampling policy $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ and a second reward function $\hat{R} : \mathcal{S}\times\mathcal{A} \to \mathbb{R}$, we can upper bound the expected KL divergence of preference distributions over trajectories with a common starting state as follows:*

$$\mathbb{E}_{\substack{s_0\sim\mu_0,\\ \xi_1,\xi_2\sim\pi(s_0)}}\left[\mathbb{D}_{KL}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right)\right] \leq \frac{1}{\min\limits_{\substack{s'\in\mathcal{S}\\ \mu_0(s')>0}} \mu_0(s')} \mathbb{E}_{\xi_1,\xi_2\sim\pi\times\pi}\left[\mathbb{D}_{KL}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right)\right]. \tag{62}$$

Proof. Let $s_0 : \Xi \to \mathcal{S}$ define the function which outputs the starting state $s \in \mathcal{S}$ of a trajectory $\xi \in \Xi$. We can then prove the lemma by directly lower-bounding the right-hand side of Equation (62):

$$\begin{aligned} &\mathbb{E}_{\xi_1,\xi_2\sim\pi\times\pi}\left[\mathbb{D}_{\text{KL}}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right)\right] \\ &= \sum_{s_1,s_2\in\mathcal{S}\times\mathcal{S}} \mu_0(s_1)\cdot\mu_0(s_2)\cdot \sum_{\substack{\xi_1,\xi_2\in\Xi\times\Xi\\ s_0(\xi_1)=s_1\\ s_0(\xi_2)=s_2}} p_{\pi,\tau}(\xi_1|s_1)\cdot p_{\pi,\tau}(\xi_2|s_2)\cdot \mathbb{D}_{\text{KL}}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right) \\ &= \sum_{s_1=s_2} \mu_0(s_1)\cdot\mu_0(s_2)\cdot \sum_{\substack{\xi_1,\xi_2\in\Xi\times\Xi\\ s_0(\xi_1)=s_1\\ s_0(\xi_2)=s_2}} p_{\pi,\tau}(\xi_1|s_1)\cdot p_{\pi,\tau}(\xi_2|s_2)\cdot \mathbb{D}_{\text{KL}}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right) \\ &\quad + \sum_{s_1\neq s_2} \mu_0(s_1)\cdot\mu_0(s_2)\cdot \sum_{\substack{\xi_1,\xi_2\in\Xi\times\Xi\\ s_0(\xi_1)=s_1\\ s_0(\xi_2)=s_2}} p_{\pi,\tau}(\xi_1|s_1)\cdot p_{\pi,\tau}(\xi_2|s_2)\cdot \mathbb{D}_{\text{KL}}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right) \\ &\geq \sum_{s_1=s_2} \mu_0(s_1)\cdot\mu_0(s_2)\cdot \sum_{\substack{\xi_1,\xi_2\in\Xi\times\Xi\\ s_0(\xi_1)=s_1\\ s_0(\xi_2)=s_2}} p_{\pi,\tau}(\xi_1|s_1)\cdot p_{\pi,\tau}(\xi_2|s_2)\cdot \mathbb{D}_{\text{KL}}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right) \\ &\geq \min_{\substack{s'\in\mathcal{S}\\ \mu_0(s')>0}} \mu_0(s')\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot \sum_{\substack{\xi_1,\xi_2\in\Xi\times\Xi\\ s_0(\xi_1)=s\\ s_0(\xi_2)=s}} p_{\pi,\tau}(\xi_1|s)\cdot p_{\pi,\tau}(\xi_2|s)\cdot \mathbb{D}_{\text{KL}}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right) \\ &= \min_{\substack{s'\in\mathcal{S}\\ \mu_0(s')>0}} \mu_0(s')\cdot \mathbb{E}_{\substack{s_0\sim\mu_0,\\ \xi_1,\xi_2\sim\pi(s_0)}}\left[\mathbb{D}_{\text{KL}}\left(p_R(\cdot|\xi_1,\xi_2)||p_{\hat{R}}(\cdot|\xi_1,\xi_2)\right)\right], \end{aligned}$$

where we used the fact that the KL divergence is always positive. □

C.4.2 RLHF BANDIT FORMULATION

RLHF, especially in the context of large language models, is usually modeled in a *contextual bandit* setting ((Ziegler et al., 2019; Stiennon et al., 2020; Bai et al., 2022; Ouyang et al., 2022; Rafailov et al., 2023)). A *contextual bandit* $\langle \mathcal{S}, \mathcal{A}, \mu_0, R\rangle$ is defined by a set of states $\mathcal{S}$, a set of actions $\mathcal{A}$, a data distribution $\mu_0 \in \Delta(\mathcal{S})$, and a reward function $R : \mathcal{S}\times\mathcal{A} \to \mathbb{R}$. The goal is to learn a policy $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ which maximizes the expected return $J(\pi) = \mathbb{E}_{s\sim\mu_0, a\sim\pi(\cdot|s)}\left[R(s,a)\right]$. In the context of language models, $\mathcal{S}$ is usually called the set of prompts/contexts, and $\mathcal{A}$ the set of responses. We model the human preference distribution over the set of answers A using the Bradley-Terry model (Bradley & Terry, 1952). Given a prompt $s \in S$ and two answers $a_1, a_2 \in A$, then the probability that a human supervisor prefers answer a_1 to answer a_2 is modelled as:

$$p_R(a_1 \succ a_2|\ s) \ = \ \frac{\exp(R(s,a_1))}{\exp(R(s,a_1))\ +\ \exp(R(s,a_2))}, \tag{63}$$

where $R : \mathcal{S}\times\mathcal{A} \to \mathbb{R}$ is assumed to be the true, underlying reward function of the human.

RLHF is usually done with the following steps:

1. **Supervised finetuning:** Train/Fine-tune a language model π_{ref} using supervised training.
2. **Reward learning:** Given a data distribution over prompts $\mu \in \Delta(S)$, use μ and π_{ref} to sample a set of transitions $(s, a_0, a_1) \in \mathcal{S}\times\mathcal{A}\times\mathcal{A}$ where $s \sim \mu$ and $a_0, a_1 \sim \pi_{\text{ref}}(\cdot|s)$. Use this set of transitions to train a reward model $\hat{R}$ which minimizes the following loss:
$$\mathcal{L}_R(\hat{R}) \ = \ -\mathbb{E}_{(s,a_0,a_1,c)\sim\mu,\pi_{\text{ref}},p_R}\left[\log\big(\sigma(\hat{R}(s,a_c) - \hat{R}(s,a_{1-c}))\big)\right], \tag{64}$$
where $c \in \{0,1\}$ and $p(c=0|s,a_0,a_1) = p_R(a_0 \succ a_1|s)$.
3. **RL finetuning:** Use the trained reward model $\hat{R}$ to further finetune the language model π_{ref} using reinforcement learning. Make sure that the new model does not deviate too much from the original model by penalizing the KL divergence between the two models. This can be done by solving the following optimization problem for some $\lambda > 0$:
$$\pi = \arg\max_{\pi} \mathbb{E}_{s\sim\mu, a\sim\pi(\cdot|s)}\left[\hat{R}(s,a)\right] - \lambda\cdot\mathbb{D}_{\text{KL}}\left(\pi(a|s)||\pi_{\text{ref}}(a|s)\right) \tag{65}$$

C.4.3 Safe and unsafe data distributions for RLHF

Definition C.27 (Safe- and unsafe data distributions for RLHF)**.** For a given contextual bandit $\langle \mathcal{S}, \mathcal{A}, \mu_0, R\rangle$, let $\epsilon > 0$, $L \in [0,1]$, $\lambda \in [0,\infty)$, and $\pi_{\text{ref}} : \mathcal{S} \to \Delta(\mathcal{A})$ an arbitrary reference policy. Similarly to Definition 2.1, we define the set of *safe data distributions* $\mathbf{safe}^{\text{RLHF}}\big(R, \epsilon, L, \lambda, \mathbb{D}_{\text{KL}}\left(\cdot||\pi_{\text{ref}}\right)\big)$ for RLHF as all $D \in \Delta(\mathcal{S}\times\mathcal{A})$ such that for all reward functions $\hat{R} : \mathcal{S}\times\mathcal{A} \to \mathbb{R}$ and policies $\hat{\pi} : \mathcal{S} \to \Delta(\mathcal{A})$ that satisfy the following two properties:

1. **Low expected error:** $\hat{R}$ is similar to R in expected choice probabilities under D, i.e.:
$$\mathbb{E}_{(s,a_1,a_2)\sim D}\left[\mathbb{D}_{\text{KL}}\left(p_R(\cdot|s,a_1,a_2)||p_{\hat{R}}(\cdot|s,a_2,a_2)\right)\right] \le \epsilon\cdot\text{range}\, R.$$
2. **Optimality:** $\hat{\pi}$ is optimal with respect to $\hat{R}$, i.e.:
$$\hat{\pi} \ \in \ \arg\max_{\pi} J_{\hat{R}}(\pi) - \lambda\cdot\mathbb{D}_{\text{KL}}\left(\pi(a|s)||\pi_{\text{ref}}(a|s)\right).$$

we can guarantee that $\hat{\pi}$ has regret smaller than L, i.e.:

3. **Low regret:** $\hat{\pi}$ has a regret smaller than L with respect to R, i.e., $\text{Reg}^R\left(\hat{\pi}\right) < L$.

Similarly, we define the set of *unsafe data distributions* to be the complement of $\mathbf{safe}^{\text{RLHF}}\big(R, \epsilon, L, \lambda, \mathbb{D}_{\text{KL}}\left(\cdot||\pi_{\text{ref}}\right)\big)$:

$$\mathbf{unsafe}^{\text{RLHF}}\big(R, \epsilon, L, \lambda, \mathbb{D}_{\text{KL}}\left(\cdot||\pi_{\text{ref}}\right)\big) \ := \ \Big\{\ D \in \Delta(\mathcal{S}\times\mathcal{A}) \mid D \notin \mathbf{safe}^{\text{RLHF}}\big(R, \epsilon, L, \lambda, \mathbb{D}_{\text{KL}}\left(\cdot||\pi_{\text{ref}}\right)\big)\Big\}.$$

Note: Property 1 of Definition C.27 is commonly phrased as minimizing (with respect to $\hat{R}$) the loss $-\mathbb{E}_{(s,a_1,a_2)\sim D,p_R}\left[\log\big(\sigma(\hat{R}(s,a_1) - \hat{R}(s,a_2))\big)\right]$ (which includes p_R, the probability that a_1 is the preferred action over a_2, in the expectation). Our version of Property 1 is equivalent to this and can be derived from the former by adding the constant (w.r.t. $\hat{R}$) term $\mathbb{E}_{(s,a_1,a_2)\sim D,p_R}\left[\log(\sigma(R(s,a_1) - R(s,a_2)))\right]$.

C.4.4 NEGATIVE RESULTS

A more advanced result can be achieved by restricting the set of possible pre-trained policies π_{ref}. In the following proofs, we will define $\pi^{\text{rlhf}}_{R,\lambda}$ to be the optimal policy after doing RLHF on π_{ref} with some reward function R, i.e.,:

Definition C.28 (RLHF-optimal policy)**.** For any $\lambda \in \mathbb{R}_+$, reward function R and reference policy π_{ref}, we define the policy maximizing the RLHF objective by:

$$\pi^{\text{rlhf}}_{R,\lambda} = \arg\max_{\pi} \mathbb{E}_{s\sim\mu, a\sim\pi(\cdot|s)} \left[R(s,a)\right] - \lambda \cdot \mathbb{D}_{\text{KL}} \left(\pi(a|s) || \pi_{\text{ref}}(a|s)\right) \tag{66}$$

$\pi^{\text{rlhf}}_{R,\lambda}$ does have the following analytical definition (see Appendix A.1 of (Rafailov et al., 2023) for a derivation):

$$\pi^{\text{rlhf}}_{R,\lambda}(a|s) \ \coloneqq \ \frac{\pi_{\text{ref}}(a|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a)\right)}{\sum_{a' \in \mathcal{A}} \pi_{\text{ref}}(a'|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a')\right)}. \tag{67}$$

Before stating the next negative result, we prove a small helper lemma which states that doing RLHF with some reward function R on a policy π_{ref} is guaranteed to improve the policy return concerning R:

Lemma C.29. *For any $\lambda \in \mathbb{R}_+$, reward function R and reference policy π_{ref}, it holds that:*

$$J_R\left(\pi^{\text{rlhf}}_{R,\lambda}\right) \ \geq \ J_R\left(\pi_{\text{ref}}\right) \tag{68}$$

Proof. We have

$$\begin{aligned} J_R\left(\pi^{\text{rlhf}}_{R,\lambda}\right) - \lambda \mathbb{D}_{\text{KL}}\left(\pi^{\text{rlhf}}_{R,\lambda} || \pi_{\text{ref}}\right) &= J^R_{\text{KL}}(\pi^{\text{rlhf}}_{R,\lambda}, \pi_{\text{ref}}) \\ &\geq J^R_{\text{KL}}(\pi_{\text{ref}}, \pi_{\text{ref}}) \\ &= J_R(\pi_{\text{ref}}). \end{aligned}$$

The result follows from the non-negativity of the KL divergence. $\square$

We begin by proving a helper lemma that we are going to use in subsequent proofs.

Lemma C.30. *Let $\langle \mathcal{S}, \mathcal{A}, \mu_0, R \rangle$ be a contextual bandit*

Given a lower regret bound $L \in [0,1)$, we define for every state $s \in \mathcal{S}$ the reward threshold:

$$R_L(s) \coloneqq (1-L) \cdot \max_{a \in \mathcal{A}} R(s,a) + L \cdot \min_{a \in \mathcal{A}} R(s,a),$$

and define $a_s \in \mathcal{A}$ to be an action such that $R(s, a_s) < R_L(s)$.

Let $\pi_{\text{ref}} : \mathcal{S} \to \mathcal{A}$ be an arbitrary reference policy for which it holds that for every state $s \in \mathcal{S}$ we have $\pi_{\text{ref}}(a|s) > 0$.

Then, performing KL-regularized policy optimization, starting from $\pi_{\text{ref}} \in \Pi$ and using the reward function:

$$\hat{R}(s,a) \ \coloneqq \ \begin{cases} R(s,a) & \text{if } a \neq a_s \\ c_s \in \mathbb{R}_+ & \text{if } a = a_s \end{cases}, \tag{69}$$

results in an optimal policy $\hat{\pi}$ such that $\mathrm{Reg}^R(\hat{\pi}) \geq L$, whenever the constants c_s are larger than the following lower bound:

$$c_s \ \geq \ \lambda \cdot \log\left[\frac{\sum_{a \neq a_s} (R(s,a) - R_L(s)) \cdot \pi_{\text{ref}}(a|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a)\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)}\right].$$

Proof. Denote by $\pi^{\text{rlhf}}_{\hat{R},\lambda}$ the optimal policy for the following KL-regularized optimization problem:

$$\pi^{\text{rlhf}}_{\hat{R},\lambda} \in \arg\max_{\pi} J_{\hat{R}}(\pi) - \lambda \cdot \mathbb{D}_{\text{KL}}\left(\pi(a|s) || \pi_{\text{ref}}(a|s)\right).$$

The closed-form solution for this optimization problem is known (see Definition C.28). Now, we prove the statement, by assuming the specific definition of $\hat{R}$ (see Equation (69)), as well as that $\pi^{\text{rlhf}}_{\hat{R},\lambda}$

has a regret at least L, and then work backward to derive a necessary lower bound for the individual constants c_s.

We start by defining a small helper policy. Let $\pi_\top$ be a deterministic optimal policy for R and $\pi_\perp$ be a deterministic worst-case policy for R. We then define $\pi_L(a|s)$ as a convex combination of $\pi_\top$ and $\pi_\perp$:

$$\pi_L(a|s) \coloneqq (1-L)\cdot\pi_\top(a|s) + L\cdot\pi_\perp(a|s)$$
$$= \begin{cases} 1 & \text{if } R(s,a) = \min_{a'\in\mathcal{A}} R(s,a') = \max_{a'\in\mathcal{A}} R(s,a') \\ 1-L & \text{if } R(s,a) = \max_{a'\in\mathcal{A}} R(s,a') \\ L & \text{if } R(s,a) = \min_{a'\in\mathcal{A}} R(s,a') \\ 0 & \text{Otherwise} \end{cases} \tag{70}$$

Next, we show that the regret of π_L is L. Let $\eta_\top$ and $\eta_\perp$ be the corresponding occupancy measures of $\pi_\top$ and $\pi_\perp$. Then, we have:

$$J_R(\pi_L) \;=\; (1-L)\cdot R^T\cdot\eta_\top + L\cdot R^T\cdot\eta_\perp,$$

from which it directly follows that:

$$\mathrm{Reg}^R(\pi_L) \;=\; \frac{R^T\cdot\eta_\top - \left[(1-L)\cdot R^T\cdot\eta_\top + L\cdot R^T\cdot\eta_\perp\right]}{R^T\cdot\eta_\top - R^T\cdot\eta_\perp} \;=\; L.$$

Now, having defined π_L, we start the main proof. Assume that $\mathrm{Reg}^R\left(\pi^{\mathrm{rlhf}}_{\hat{R},\lambda}\right) \geq L$, which is equivalent to $J(\pi^{\mathrm{rlhf}}_{\hat{R},\lambda}) \leq J(\pi_L)$. By using the definition of the policy evaluation function, we get:

$$J(\pi^{\mathrm{rlhf}}_{\hat{R},\lambda}) \;\leq\; J(\pi_L)$$
$$\iff\quad R^T\cdot(\eta^{\pi^{\mathrm{rlhf}}_{\hat{R},\lambda}} - \eta^{\pi_L}) \;\leq\; 0$$
$$\iff\quad \sum_{(s,a)\in\mathcal{S}\times\mathcal{A}} R(s,a)\cdot\mu_0(s)\cdot(\pi^{\mathrm{rlhf}}_{\hat{R},\lambda}(a|s) - \pi_L(a|s)) \;\leq\; 0$$

We will prove the sufficient condition, that for every $s\in\mathcal{S}$, we have:

$$\sum_{a\in\mathcal{A}} R(s,a)\cdot\left(\pi^{\mathrm{rlhf}}_{\hat{R},\lambda}(a|s) - \pi_L(a|s)\right) \;\leq\; 0 \tag{71}$$

Before continuing, note that with our definition of π_L (see Equation (70)) we have:

$$\sum_{a\in\mathcal{A}} R(s,a)\cdot\pi_L(a|s) \;=\; (1-L)\cdot\max_{a\in\mathcal{A}} R(s,a) + L\cdot\min_{a\in\mathcal{A}} R(s,a) \;\eqqcolon\; R_L(s).$$

Now, using this fact as well as the definitions of π_L and $\pi^{\text{rlhf}}_{\hat{R},\lambda}$ (see Definition C.28) we prove under which conditions Equation (71) holds:

$$
\begin{aligned}
& \sum_{a\in\mathcal{A}} R(s,a)\cdot\left(\pi^{\text{rlhf}}_{\hat{R},\lambda}(a|s) - \pi_L(a|s)\right) \;\leq\; 0 \\
\iff\quad & \sum_{a\in\mathcal{A}} R(s,a)\cdot\left[\frac{\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a)\right)}{\sum_{a'\in\mathcal{A}}\pi_{\text{ref}}(a'|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a')\right)} - \pi_L(a|s)\right] \;\leq\; 0 \\
\iff\quad & \sum_{a\in\mathcal{A}} R(s,a)\cdot\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a)\right) \\
& \qquad\qquad \leq \left[\sum_{a\in\mathcal{A}} R(s,a)\cdot\pi_L(a|s)\right]\cdot\sum_{a'\in\mathcal{A}}\pi_{\text{ref}}(a'|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a')\right) \\
\iff\quad & \sum_{a\in\mathcal{A}}(R(s,a) - R_L(s))\cdot\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a)\right) \;\leq\; 0 \\
\iff\quad & \sum_{\substack{a\in\mathcal{A}\\ R(s,a)>R_L(s)}}(R(s,a) - R_L(s))\cdot\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a)\right) \\
& \qquad\qquad \leq \sum_{\substack{a\in\mathcal{A}\\ R(s,a)<R_L(s)}}(R_L(s) - R(s,a))\cdot\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a)\right)
\end{aligned}
$$

Now, according to the assumptions of the lemma, we know that there exists some action a_s for which $R(s,a_s) < R_L(s)$ and $\pi_{\text{ref}}(a_s|s) > 0$. According to our definition of $\hat{R}$ (see Equation (69)), we have $\hat{R}(s,a_s) = c_s$ and $\hat{R}(s,a) = R(s,a)$ for all other actions. We can use this definition to get a lower bound for c_s:

$$
\begin{aligned}
& \sum_{\substack{a\in\mathcal{A}\\ R(s,a)>R_L(s)}}(R(s,a) - R_L(s))\cdot\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a)\right) \\
& \qquad\qquad \leq \sum_{\substack{a\in\mathcal{A}\\ R(s,a)<R_L(s)}}(R_L(s) - R(s,a))\cdot\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a)\right) && (72) \\
\iff\quad & \sum_{a\neq a_s}(R(s,a) - R_L(s))\cdot\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot R(s,a)\right) \\
& \qquad\qquad \leq (R_L(s) - R(s,a_s))\cdot\pi_{\text{ref}}(a_s|s)\cdot\exp\left(\frac{1}{\lambda}\cdot\hat{R}(s,a_s)\right) && (73) \\
\iff\quad & \lambda\cdot\log\left[\frac{\sum_{a\neq a_s}(R(s,a) - R_L(s))\cdot\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot R(s,a)\right)}{(R_L(s) - R(s,a_s))\cdot\pi_{\text{ref}}(a_s|s)}\right] \;\leq\; \hat{R}(s,a_s). && (74)
\end{aligned}
$$

$\square$

We can now use this lemma to prove a more general result:

Proposition C.31. *Let $\langle\mathcal{S},\mathcal{A},\mu_0,R\rangle$ be a contextual bandit.*

Given a lower regret bound $L\in[0,1)$, we define for every state $s\in\mathcal{S}$ the reward threshold:

$$R_L(s) \coloneqq (1-L)\cdot\max_{a\in\mathcal{A}} R(s,a) + L\cdot\min_{a\in\mathcal{A}} R(s,a),$$

Lastly, $\pi_{\text{ref}}:\mathcal{S}\to\mathcal{A}$ be an arbitrary reference policy for which it holds that for every state $s\in\mathcal{S}$, $\pi_{\text{ref}}(a|s) > 0$ and there exists at least one action $a_s\in\mathcal{A}$ such that:

a) $\pi_{\text{ref}}(a_s|s)$ *is small enough, that the following inequality holds:*

$$\log\left[\sum_{a\neq a_s}\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot(R(s,a)-R(s,a_s))\right)\cdot\frac{R(s,a)-R_L(s)}{R_L(s)-R(s,a_s)}\right]\leq\frac{\epsilon\cdot\text{range }R}{2\cdot\lambda\cdot\pi_{\text{ref}}(a_s|s)}+\log\left(\pi_{\text{ref}}(a_s|s)\right) \tag{75}$$

b) $R(s,a_s) < R_L(s)$

Then, for all $\epsilon > 0$, $\lambda \in [0,\infty)$, *data distributions* $\mu \in \Delta(\mathcal{S})$, *and true reward functions* $R : \mathcal{S}\times\mathcal{A} \to \mathbb{R}$, *there exists a reward function* $\hat{R} : \mathcal{S}\times\mathcal{A} \to \mathbb{R}$, *and a policy* $\hat{\pi} : S \to \Delta(\mathcal{A})$ *such that:*

1. $\mathbb{E}_{s,a_1,a_2\sim\mu,\pi_{\text{ref}}}\left[\mathbb{D}_{KL}\left(p_R(\cdot|s,a_1,a_2)||p_{\hat{R}}(\cdot|s,a_1,a_2)\right)\right] \leq \epsilon\cdot\text{range }R$
2. $\hat{\pi} \in \arg\max_\pi J_{\hat{R}}(\pi) - \lambda\cdot\mathbb{D}_{KL}\left(\pi(a|s)||\pi_{\text{ref}}(a|s)\right)$
3. $\text{Reg}^R\left(\hat{\pi}\right) \geq L$,

Proof. We will prove the lemma by construction. Namely, we choose:

$$\hat{R}(s,a) \;\coloneqq\; \begin{cases} R(s,a) & \text{if } a\neq a_s \\ c_s\in\mathbb{R}_+ & \text{if } a = a_s\end{cases} \tag{76}$$

where the different c_s are some positive constants defined as follows:

$$\hat{R}(s,a_s) = c_s \;\geq\; l_s \coloneqq \max\left(R(s,a_s),\;\lambda\cdot\log\left[\frac{\sum_{a\neq a_s}(R(s,a)-R_L(s))\cdot\pi_{\text{ref}}(a|s)\cdot\exp\left(\frac{1}{\lambda}\cdot R(s,a)\right)}{(R_L(s)-R(s,a_s))\cdot\pi_{\text{ref}}(a_s|s)}\right]\right). \tag{77}$$

Furthermore, the closed-form of the optimal policy $\hat{\pi}$ of the KL-regularized optimization problem is known to be $\pi^{\text{rlhf}}_{\hat{R},\lambda}$ (see Definition C.28). We now claim that this choice of $\hat{R}$ and $\hat{\pi}$ fulfills properties (1) and (3) of the lemma (property (2) is true by assumption).

Property (3) is true because every reference policy π_{ref} and corresponding reward function R that fulfills the conditions of this proposition also fulfills the conditions of Lemma C.30. Hence, we can directly apply Lemma C.30 and get the guarantee that $\text{Reg}^R\left(\hat{\pi}\right) \geq L$.

All that remains to be shown, is that condition (1) can be satisfied by using the definition of $\hat{R}$ and the lower bounds in Equation Equation (77). First, note that we can reformulate the expected error definition in condition (1) as follows:

$$\begin{aligned}
&\mathbb{E}_{s,a_1,a_2\sim\mu,\pi_{\text{ref}}}\left[\mathbb{D}_{\text{KL}}\left(p_R(\cdot|s,a_1,a_2)||p_{\hat{R}}(\cdot|s,a_1,a_2)\right)\right]\\
&=\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\sum_{a_1,a_2\in\mathcal{A}\times\mathcal{A}}\pi_{\text{ref}}(a_1|s)\cdot\pi_{\text{ref}}(a_2|s)\cdot\sum_{i,j\in\{1,2\}}\sigma(R(s,a_i)-R(s,a_j))\cdot\log\left(\frac{\sigma(R(s,a_i)-R(s,a_j))}{\sigma(\hat{R}(s,a_i)-\hat{R}(s,a_j))}\right)\\
&=2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\sum_{a_1,a_2\in\mathcal{A}\times\mathcal{A}}\pi_{\text{ref}}(a_1|s)\cdot\pi_{\text{ref}}(a_2|s)\cdot\underbrace{\sigma(R(s,a_1)-R(s,a_2))\cdot\log\left(\frac{\sigma(R(s,a_1)-R(s,a_2))}{\sigma(\hat{R}(s,a_1)-\hat{R}(s,a_2))}\right)}_{=:\mathcal{IS}(a_1,a_2)}\\
&=2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\sum_{a_1,a_2\in\mathcal{A}\times\mathcal{A}}\pi_{\text{ref}}(a_1|s)\cdot\pi_{\text{ref}}(a_2|s)\cdot\mathcal{IS}(a_1,a_2).
\end{aligned}$$

Next, note that for every tuple $(a_1, a_2) \in \mathcal{A}$, the sum $\mathcal{IS}(a_1, a_2) + \mathcal{IS}(a_2, a_1)$ can be reformulated as follows:

$$
\begin{aligned}
&\mathcal{IS}(a_1, a_2) \; + \; \mathcal{IS}(a_2, a_1) \\
&= \; \sigma(R(s, a_1) - R(s, a_2)) \cdot \log\left(\frac{\sigma(R(s, a_1) - R(s, a_2))}{\sigma(\hat{R}(s, a_1) - \hat{R}(s, a_2))}\right) \\
&\qquad\qquad\qquad\qquad + \sigma(R(s, a_2) - R(s, a_1)) \cdot \log\left(\frac{\sigma(R(s, a_2) - R(s, a_1))}{\sigma(\hat{R}(s, a_2) - \hat{R}(s, a_1))}\right) \\
&= \; \sigma(R(s, a_1) - R(s, a_2)) \cdot \log\left(\frac{\sigma(R(s, a_1) - R(s, a_2))}{\sigma(\hat{R}(s, a_1) - \hat{R}(s, a_2))}\right) \\
&\qquad\qquad\qquad\qquad + \Big(1 - \sigma(R(s, a_1) - R(s, a_2))\Big) \cdot \log\left(\frac{\sigma(R(s, a_2) - R(s, a_1))}{\sigma(\hat{R}(s, a_2) - \hat{R}(s, a_1))}\right) \\
&= \; \sigma(R(s, a_1) - R(s, a_2)) \; \cdot \; \underbrace{\left[\log\left(\frac{\sigma(R(s, a_1) - R(s, a_2))}{\sigma(\hat{R}(s, a_1) - \hat{R}(s, a_2))}\right) \; - \; \log\left(\frac{\sigma(R(s, a_2) - R(s, a_1))}{\sigma(\hat{R}(s, a_2) - \hat{R}(s, a_1))}\right)\right]}_{(A)} \\
&\qquad\qquad\qquad\qquad + \underbrace{\log\left(\frac{\sigma(R(s, a_2) - R(s, a_1))}{\sigma(\hat{R}(s, a_2) - \hat{R}(s, a_1))}\right)}_{(B)}.
\end{aligned}
$$

The term (A) can now be simplified as follows:

$$
\begin{aligned}
&\log\left(\frac{\sigma(R(s, a_1) - R(s, a_2))}{\sigma(\hat{R}(s, a_1) - \hat{R}(s, a_2))}\right) \; - \; \log\left(\frac{\sigma(R(s, a_2) - R(s, a_1))}{\sigma(\hat{R}(s, a_2) - \hat{R}(s, a_1))}\right) \\
&= \; \log\left(\frac{\sigma(R(s, a_1) - R(s, a_2))}{1 - \sigma(R(s, a_1) - R(s, a_2))}\right) \; + \; \log\left(\frac{1 - \sigma(\hat{R}(s, a_1) - \hat{R}(s, a_2))}{\sigma(\hat{R}(s, a_1) - \hat{R}(s, a_2))}\right) \\
&= [R(s, a_1) - R(s, a_2)] - [\hat{R}(s, a_1) - \hat{R}(s, a_2)],
\end{aligned}
$$

where we used the definition of the inverse of the logistic function. Similarly, the term (B) can be simplified as follows:

$$
\begin{aligned}
&\log\left(\frac{\sigma(R(s, a_2) - R(s, a_1))}{\sigma(\hat{R}(s, a_2) - \hat{R}(s, a_1))}\right) \\
&= \; \log\left(\frac{\exp(R(s, a_2) - R(s, a_1))}{1 + \exp(R(s, a_2) - R(s, a_1)} \cdot \frac{1 + \exp(\hat{R}(s, a_2) - \hat{R}(s, a_1)}{\exp(\hat{R}(s, a_2) - \hat{R}(s, a_1)}\right) \\
&= [R(s, a_2) - R(s, a_1)] - [\hat{R}(s, a_2) - \hat{R}(s, a_1)] + \log\left(\frac{1 + \exp(\hat{R}(s, a_2) - \hat{R}(s, a_1))}{1 + \exp(R(s, a_2) - R(s, a_1))}\right)
\end{aligned}
$$

These expressions, together with the fact that $\mathcal{IS}(a, a) = 0$ for all $a \in \mathcal{A}$, allow us to choose an arbitrary ordering $\prec$ on the set of actions $\mathcal{A}$, and then re-express the sum:

$$
\sum_{a_1, a_2 \in \mathcal{A} \times \mathcal{A}} \pi_{\mathrm{ref}}(a_1|s) \cdot \pi_{\mathrm{ref}}(a_2|s) \cdot \mathcal{IS}(a_1, a_2) \; = \sum_{\substack{a_1, a_2 \in \mathcal{A} \times \mathcal{A} \\ a_1 \prec a_2}} \pi_{\mathrm{ref}}(a_1|s) \cdot \pi_{\mathrm{ref}}(a_2|s) \cdot \big(\mathcal{IS}(a_1, a_2) + \mathcal{IS}(a_2, a_1)\big). \tag{78}
$$

Summarizing all the equations above, we get:

$$\begin{aligned}
&\mathbb{E}_{s,a_1,a_2\sim\mu,\pi_{\mathrm{ref}}}\left[\mathbb{D}_{\mathrm{KL}}\left(p_R(\cdot|s,a_1,a_2)||p_{\hat{R}}(\cdot|s,a_1,a_2)\right)\right] \\
&= 2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\sum_{a_1,a_2\in\mathcal{A}\times\mathcal{A}}\pi_{\mathrm{ref}}(a_1|s)\cdot\pi_{\mathrm{ref}}(a_2|s)\cdot\mathcal{IS}(a_1,a_2) \\
&= 2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\sum_{\substack{a_1,a_2\in\mathcal{A}\times\mathcal{A}\\ a_1\prec a_2}}\pi_{\mathrm{ref}}(a_1|s)\cdot\pi_{\mathrm{ref}}(a_2|s)\cdot\Bigg[\Big(\left[R(s,a_1)-R(s,a_2)\right]-\left[\hat{R}(s,a_1)-\hat{R}(s,a_2)\right]\Big) \\
&\qquad\cdot\Big(\sigma(R(s,a_1)-R(s,a_2))\;-1\Big)+\log\left(\frac{1+\exp(\hat{R}(s,a_2)-\hat{R}(s,a_1))}{1+\exp(R(s,a_2)-R(s,a_1))}\right)\Bigg].
\end{aligned} \tag{79}$$

Now, by using our particular definition of $\hat{R}$ (see Equation (76)), we notice that whenever both $a_1 \neq a_s$, and $a_2 \neq a_s$, the inner summand of Equation (79)is zero. What remains of Equation (79) can be restated as follows:

$$\begin{aligned}
&= 2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\pi_{\mathrm{ref}}(a_s|s)\cdot\sum_{a\in\mathcal{A}}\pi_{\mathrm{ref}}(a|s)\cdot\Bigg[\Big(R(s,a_s)-c_s\Big)\;\cdot\;\Big(\sigma(R(s,a_s)-R(s,a))\;-1\Big) \\
&\qquad+\;\log\left(\frac{1+\exp(R(s,a)-c_s)}{1+\exp(R(s,a)-R(s,a_s))}\right)\Bigg]
\end{aligned} \tag{80}$$

To prove property (1), we must show that Equation (80) is smaller or equal to $\epsilon\cdot\mathrm{range}\,R$. We do this in two steps. First, note that for all states s it holds that $c_s \geq R(s,a_s)$ (this is obvious from the definition of c_s, see Equation (77)). This allows us to simplify Equation (80) by dropping the logarithm term.

$$\begin{aligned}
&\mathbb{E}_{s,a_1,a_2\sim\mu,\pi_{\mathrm{ref}}}\left[\mathbb{D}_{\mathrm{KL}}\left(p_R(\cdot|s,a_1,a_2)||p_{\hat{R}}(\cdot|s,a_1,a_2)\right)\right] \\
&= 2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\pi_{\mathrm{ref}}(a_s|s)\cdot\sum_{a\in\mathcal{A}}\pi_{\mathrm{ref}}(a|s)\cdot\Bigg[\Big(R(s,a_s)-c_s\Big)\;\cdot\;\Big(\sigma(R(s,a_s)-R(s,a))\;-1\Big) \\
&\qquad+\;\log\left(\frac{1+\exp(R(s,a)-c_s)}{1+\exp(R(s,a)-R(s,a_s))}\right)\Bigg] \\
&= 2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\pi_{\mathrm{ref}}(a_s|s)\cdot\Big(c_s-R(s,a_s)\Big)\;\cdot\sum_{a\in\mathcal{A}}\pi_{\mathrm{ref}}(a|s)\cdot\Big(1-\sigma(R(s,a_s)-R(s,a))\Big) \\
&\qquad+2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\pi_{\mathrm{ref}}(a_s|s)\cdot\sum_{a\in\mathcal{A}}\pi_{\mathrm{ref}}(a|s)\cdot\log\left(\frac{1+\exp(R(s,a)-c_s)}{1+\exp(R(s,a)-R(s,a_s))}\right).
\end{aligned} \tag{81}$$

Now, we choose to define $c_s := l_s + \delta_s$, where l_s is defined in Equation (77) and $\delta_s \geq 0$ such that:

$$\begin{aligned}
&2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\pi_{\mathrm{ref}}(a_s|s)\cdot\Big(l_s+\delta_s-R(s,a_s)\Big)\;\cdot\sum_{a\in\mathcal{A}}\pi_{\mathrm{ref}}(a|s)\cdot\underbrace{\Big(1-\sigma(R(s,a_s)-R(s,a))\Big)}_{<1} \\
&\qquad+2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\pi_{\mathrm{ref}}(a_s|s)\cdot\sum_{a\in\mathcal{A}}\pi_{\mathrm{ref}}(a|s)\cdot\underbrace{\log\left(\frac{1+\exp(R(s,a)-l_s-\delta_s)}{1+\exp(R(s,a)-R(s,a_s))}\right)}_{\leq 0\text{ (because }c_s:=l_s+\delta_s\geq R(s,a_s))} \\
&\leq\;2\cdot\sum_{s\in\mathcal{S}}\mu_0(s)\cdot\pi_{\mathrm{ref}}(a_s|s)\cdot\Big(l_s-R(s,a_s)\Big)\;\overset{!}{\leq}\;\epsilon\cdot\mathrm{range}\,R.
\end{aligned} \tag{82}$$

Note that the first inequality is always feasible, as we could just choose $\delta_s = 0$ for all $s \in \mathcal{S}$ in which case the inequality must hold due to the last term in the first line being smaller than one and the last term in the second line being negative. Now, to prove Equation (82), we prove the sufficient condition that for every state $s \in \mathcal{S}$:

$$\pi_{\text{ref}}(a_s|s) \cdot (l_s - R(s, a_s)) \overset{!}{\leq} \frac{\epsilon \cdot \text{range } R}{2}. \tag{83}$$

In case that $l_s = R(s, a_s)$, the left-hand side of Equation (83) cancels and the inequality holds trivially. We can therefore focus on the case where $l_s > R(s, a_s)$. In this case, we get:

$$\begin{aligned} &\pi_{\text{ref}}(a_s|s) \cdot \lambda \cdot \log \left[\frac{\sum_{a \neq a_s} (R(s,a) - R_L(s)) \cdot \pi_{\text{ref}}(a|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a)\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a_s)\right)} \right] \overset{!}{\leq} \frac{\epsilon \cdot \text{range } R}{2} \\ \iff \quad &\log \left[\sum_{a \neq a_s} \pi_{\text{ref}}(a|s) \cdot \exp\left(\frac{1}{\lambda} \cdot (R(s,a) - R(s,a_s))\right) \cdot \frac{R(s,a) - R_L(s)}{R_L(s) - R(s,a_s)} \right] \\ &\overset{!}{\leq} \frac{\epsilon \cdot \text{range } R}{2 \cdot \lambda \cdot \pi_{\text{ref}}(a_s|s)} + \log(\pi_{\text{ref}}(a_s|s)) \end{aligned}$$

which holds by assumption (a) of the lemma. Therefore, property (1) of the lemma must hold as well which concludes the proof. $\square$

Proposition C.32. *Let $\langle \mathcal{S}, \mathcal{A}, \mu_0, R \rangle$ be a contextual bandit.*

Given a lower regret bound $L \in [0, 1)$, we define for every state $s \in \mathcal{S}$ the reward threshold:

$$R_L(s) := (1 - L) \cdot \max_{a \in \mathcal{A}} R(s, a) + L \cdot \min_{a \in \mathcal{A}} R(s, a),$$

Lastly, let $\pi_{\text{ref}} : \mathcal{S} \to \mathcal{A}$ be an arbitrary reference policy for which it holds that for every state $s \in \mathcal{S}$, $\pi_{\text{ref}}(a|s) > 0$, and there exists at least one action $a_s \in \mathcal{A}$ such that:

a) $\pi_{\text{ref}}(a_s|s) > 0$, but $\pi_{\text{ref}}(a_s|s)$ is also small enough, that the following inequality holds:

$$\pi_{\text{ref}}(a_s|s) \leq \frac{(R_L(s) - R(s, a_s))}{L} \cdot \frac{\text{range } R}{\exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)} \cdot \frac{\epsilon^2}{4 \cdot \lambda^2} \tag{84}$$

b) $R(s, a_s) < R_L(s)$

Then Π is a subset of the set of policies in Proposition C.31.

Proof. We show this via a direct derivation:

$$\begin{aligned} &\pi_{\text{ref}}(a_s|s) \leq \frac{R_L(s) - R(s,a_s)}{L} \cdot \frac{\text{range } R}{\exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)} \cdot \frac{\epsilon^2}{4 \cdot \lambda^2} \\ \implies \quad &\frac{1}{\sqrt{\text{range } R}} \cdot \lambda \cdot \sqrt{\frac{\pi_{\text{ref}}(a_s|s) \cdot L \cdot \exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)}{R_L(s) - R(s,a_s)}} \leq \frac{\epsilon}{2} \\ \implies \quad &\pi_{\text{ref}}(a_s|s) \cdot \lambda \cdot \sqrt{\frac{L \cdot \text{range } R \cdot \exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)}} \leq \frac{\epsilon \cdot \text{range } R}{2} \end{aligned}$$

We continue by lower-bounding the square-root term as follows:

$$
\begin{aligned}
&\lambda \cdot \sqrt{\frac{L \cdot \text{range } R \cdot \exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)}} \\
\geq \quad &\lambda \cdot \log \left[\frac{L \cdot \text{range } R \cdot \exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)}\right] \\
\geq \quad &\lambda \cdot \log \left[\frac{L \cdot \text{range } R \cdot \exp\left(\frac{1}{\lambda} \cdot \left[\max_{a \in \mathcal{A}} R(s,a) - R(s,a_s)\right]\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)}\right] \\
\geq \quad &\lambda \cdot \log \left[\frac{(\max_{a \in \mathcal{A}} R(s,a) - R_L(s)) \cdot \exp\left(\frac{1}{\lambda} \cdot \max_{a \in \mathcal{A}} R(s,a)\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a_s)\right)}\right] \\
\geq \quad &\lambda \cdot \log \left[\frac{\sum_{a \neq a_s} (R(s,a) - R_L(s)) \cdot \pi_{\text{ref}}(a|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a)\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a_s)\right)}\right]
\end{aligned}
$$

By applying this lower bound, we can finish the proof:

$$
\begin{aligned}
&\pi_{\text{ref}}(a_s|s) \quad \leq \quad \frac{R_L(s) - R(s,a_s)}{L} \cdot \frac{\text{range } R}{\exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)} \cdot \frac{\epsilon^2}{4 \cdot \lambda^2} \\
\implies \quad &\pi_{\text{ref}}(a_s|s) \cdot \lambda \cdot \sqrt{\frac{L \cdot \text{range } R \cdot \exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s) \cdot}} \quad \leq \quad \frac{\epsilon \cdot \text{range } R}{2} \\
\implies \quad &\pi_{\text{ref}}(a_s|s) \cdot \lambda \cdot \log \left[\frac{\sum_{a \neq a_s} (R(s,a) - R_L(s)) \cdot \pi_{\text{ref}}(a|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a)\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a_s)\right)}\right] \quad \leq \quad \frac{\epsilon \cdot \text{range } R}{2} \\
\implies \quad &\log \left[\sum_{a \neq a_s} \pi_{\text{ref}}(a|s) \cdot \exp\left(\frac{1}{\lambda} \cdot (R(s,a) - R(s,a_s))\right) \cdot \frac{R(s,a) - R_L(s)}{R_L(s) - R(s,a_s)}\right] \\
&\qquad\qquad \leq \quad \frac{\epsilon \cdot \text{range } R}{2 \cdot \lambda \cdot \pi_{\text{ref}}(a_s|s)} + \log(\pi_{\text{ref}}(a_s|s))
\end{aligned}
$$

That was to show. ☐

C.4.5 Another negative result with regularization

Proposition C.33. *Let $\langle \mathcal{S}, \mathcal{A}, \mu_0, R \rangle$ be a contextual bandit.*
Given a lower regret bound $L \in [0, 1)$, we define for every state $s \in \mathcal{S}$ the reward threshold:

$$
R_L(s) \coloneqq (1 - L) \cdot \max_{a \in \mathcal{A}} R(s,a) + L \cdot \min_{a \in \mathcal{A}} R(s,a),
$$

Lastly, let $\pi_{\text{ref}} : \mathcal{S} \to \mathcal{A}$ be an arbitrary reference policy for which it holds that for every state $s \in \mathcal{S}$, $\pi_{\text{ref}}(a|s) > 0$ and there exists at least one action $a_s \in \mathcal{A}$ such that:

a) $\pi_{\text{ref}}(a_s|s)$ *is small enough, that the following inequality holds:*

$$
\pi_{\text{ref}}(a_s|s) \;\leq\; \frac{(R_L(s) - R(s,a_s))}{L} \cdot \frac{\text{range } R}{\exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)} \cdot \frac{\epsilon^2}{\lambda^2} \tag{85}
$$

b) $R(s,a_s) < R_L(s)$

Let $D^{\text{ref}}(s,a) \coloneqq \mu_0(s) \cdot \pi_{\text{ref}}(a \mid s)$. Then $D^{\text{ref}} \in \textbf{unsafe}(R, \epsilon, L, \lambda, \omega)$.

Proof. To prove the proposition we show that there exists some reward function $\hat{R}$, as well as a policy $\hat{\pi}$ such that the following properties hold:

1. $\mathbb{E}_{(s,a)\sim D^{\text{ref}}}\left[\frac{|R(s,a)-\hat{R}(s,a)|}{\text{range } R}\right] \leq \epsilon$.

2. $\hat{\pi} \in \arg\max_\pi J_{\hat{R}}(\pi) - \lambda\omega(\pi)$

3. $\text{Reg}^R(\hat{\pi}) \geq L$.

In particular, we choose:

$$\hat{R}(s,a) \;\coloneqq\; \begin{cases} R(s,a) & \text{if } a \neq a_s \\ c_s \in \mathbb{R}_+ & \text{if } a = a_s \end{cases}, \tag{86}$$

where the different c_s are some positive constants defined as follows:

$$\hat{R}(s,a_s) = c_s \;\coloneqq \max\left(R(s,a_s),\; \lambda \cdot \log\left[\frac{\sum_{a\neq a_s}(R(s,a) - R_L(s)) \cdot \pi_{\text{ref}}(a|s) \cdot \exp\left(\frac{1}{\lambda}\cdot R(s,a)\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)}\right]\right). \tag{87}$$

Furthermore, the closed-form of the optimal policy $\hat{\pi}$ of the KL-regularized optimization problem is known to be $\pi^{\text{rlhf}}_{\hat{R},\lambda}$ (see Definition C.28). We now claim that this choice of $\hat{R}$ and $\hat{\pi}$ fulfills properties (1) and (3) of the lemma (property (2) is true by assumption).

Property (3) is true because every reference policy π_{ref} and corresponding reward function R that fulfills the conditions of this proposition also fulfills the conditions of Lemma C.30. Hence, we can directly apply Lemma C.30 and get the guarantee that $\text{Reg}^R(\hat{\pi}) \geq L$.

All that remains to be shown, is that condition (1) can be satisfied by using the definition of $\hat{R}$ and in particular, the definition of the individual c_s (see Equation (87)). The expected error expression in condition (1) can be expanded as follows:

$$\mathbb{E}_{(s,a)\sim D^{\text{ref}}}\left[\frac{|R(s,a)-\hat{R}(s,a)|}{\text{range } R}\right] = \sum_{(s,a)\in\mathcal{S}\times\mathcal{A}} \mu_0(s)\cdot\pi_{\text{ref}}(a|s)\cdot\frac{|R(s,a)-\hat{R}(s,a)|}{\text{range } R} \overset{!}{\leq} \epsilon.$$

We show the sufficient condition that for each state $s \in \mathcal{S}$ it holds:

$$\sum_{a\in\mathcal{A}} \pi_{\text{ref}}(a|s)\cdot\frac{|R(s,a)-\hat{R}(s,a)|}{\text{range } R} \quad \overset{!}{\leq} \quad \epsilon.$$

By using our definition of $\hat{R}$ (see Equation (86)), this further simplifies as follows:

$$\sum_{a\in\mathcal{A}} \pi_{\text{ref}}(a|s)\cdot\frac{|R(s,a)-\hat{R}(s,a)|}{\text{range } R} \;=\; \pi_{\text{ref}}(a_s|s)\cdot\frac{\hat{R}(s,a_s)-R(s,a_s)}{\text{range } R} \overset{!}{\leq} \quad \epsilon. \tag{88}$$

In the last equation, we were able to drop the absolute value sign because our definition of the constants c_s (see Equation (87)) guarantees that $\hat{R}(s,a_s) \geq R(s,a_s)$.

Next, note that whenever $\hat{R}(s,a_s) = R(s,a_s)$ the left-hand side of Equation (88) cancels out and so the inequality holds trivially. In the following, we will therefore only focus on states where $\hat{R}(s,a_s) > R(s,a_s)$. Note that this allows us to drop the max statement in the definition of the c_s constants (see Equation (87)).

We continue by upper-bounding the difference $\hat{R}(s,a_s) - R(s,a_s)$. By making use of the following identity:

$$R(s,a_s) \quad = \quad \lambda\cdot\log\left[\exp\left(\frac{1}{\lambda}\cdot R(s,a_s)\right)\right],$$

we can move the $R(s, a_s)$ term into the logarithm term of the c_s constants, and thereby upper-bounding the difference $\hat{R}(s, a_s) - R(s, a_s)$ as follows:

$$
\begin{aligned}
& \hat{R}(s, a_s) - R(s, a_s) \\
= \quad & \lambda \cdot \log \left[\frac{\sum_{a \neq a_s} (R(s,a) - R_L(s)) \cdot \pi_{\text{ref}}(a|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a)\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a_s)\right)} \right] \\
\leq \quad & \lambda \cdot \log \left[\frac{(\max_{a \in \mathcal{A}} R(s,a) - R_L(s)) \cdot \exp\left(\frac{1}{\lambda} \cdot \max_{a \in \mathcal{A}} R(s,a)\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s) \cdot \exp\left(\frac{1}{\lambda} \cdot R(s,a_s)\right)} \right] \\
\leq \quad & \lambda \cdot \log \left[\frac{L \cdot \text{range } R \cdot \exp\left(\frac{1}{\lambda} \cdot \left[\max_{a \in \mathcal{A}} R(s,a) - R(s,a_s)\right]\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)} \right] \\
\leq \quad & \lambda \cdot \log \left[\frac{L \cdot \text{range } R \cdot \exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)} \right] \\
\leq \quad & \lambda \cdot \sqrt{\frac{L \cdot \text{range } R \cdot \exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)}}
\end{aligned}
$$

We can now put this upper bound back into Equation (88) and convert the inequality into an upper bound for $\pi_{\text{ref}}(a_s|s)$ as follows:

$$
\begin{aligned}
& \pi_{\text{ref}}(a_s|s) \cdot \frac{\hat{R}(s,a_s) - R(s,a_s)}{\text{range } R} \\
\leq \quad & \frac{\pi_{\text{ref}}(a_s|s)}{\text{range } R} \cdot \lambda \cdot \sqrt{\frac{L \cdot \text{range } R \cdot \exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)}{(R_L(s) - R(s,a_s)) \cdot \pi_{\text{ref}}(a_s|s)}} \\
= \quad & \frac{1}{\sqrt{\text{range } R}} \cdot \lambda \cdot \sqrt{\frac{\pi_{\text{ref}}(a_s|s) \cdot L \cdot \exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)}{R_L(s) - R(s,a_s)}} \quad \overset{!}{\leq} \quad \epsilon \\
\implies \quad & \pi_{\text{ref}}(a_s|s) \quad \leq \quad \frac{R_L(s) - R(s,a_s)}{L} \cdot \frac{\text{range } R}{\exp\left(\frac{1}{\lambda} \cdot \text{range } R\right)} \cdot \frac{\epsilon^2}{\lambda^2}.
\end{aligned}
$$

The last line in the previous derivation holds by assumption of the proposal. That was to show. $\square$

C.5 A REGULARIZED NEGATIVE RESULT FOR GENERAL MDPS

Throughout, let $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be an MDP. Additionally, assume there to be a data distribution $D \in \Delta(\mathcal{S} \times \mathcal{A})$ used for learning the reward function. We do a priori *not assume* that D is induced by a reference policy, but we will specialize to that case later on.

We also throughout fix $\epsilon > 0, \lambda > 0, L \in (0, 1)$, which will represent, respectively, an approximation-error for the reward function, the regularization strength, and a lower regret bound. Furthermore, let $\omega : \Pi \to \mathbb{R}$ be any continuous regularization function of policies with $\omega(\pi) \geq 0$ for all $\pi \in \Pi$. For example, if there is a nowhere-zero reference policy π_{ref}, then ω could be given by $\omega(\pi) = \mathbb{D}_{\text{KL}}(\pi || \pi_{\text{ref}})$. For any reward function $\hat{R}$, a policy $\hat{\pi}$ exists that is optimal with respect to regularized maximization of reward:

$$\hat{\pi} \in \arg\max_{\pi} J_{\hat{R}}(\pi) - \lambda \omega(\pi).$$

We will try to answer the following question: Do there exist realistic conditions on ω and D for which there exists $\hat{R}$ together with $\hat{\pi}$ such that the following properties hold?

- $\mathbb{E}_{(s,a) \sim D} \left[\frac{|\hat{R}(s,a) - R(s,a)|}{\text{range } R} \right] \leq \epsilon.$
- $\text{Reg}^R(\hat{\pi}) \geq L.$

Furthermore, we now fix π_*, a worst-case policy for R, meaning that $\mathrm{Reg}^R(\pi_*) = 1$. We assume π_* to be deterministic.

Lemma C.34. *Define $C(L,R) := \frac{(1-L)\cdot \mathrm{range}\ J_R}{\|R\|}$. Then the following implication holds:*

$$\|D^\pi - D^{\pi_*}\| \leq C(L,R) \quad \Longrightarrow \quad \mathrm{Reg}^R(\pi) \geq L.$$

Proof. Using the Cauchy-Schwarz inequality, the left side of the implication implies:

$$\begin{aligned} J_R(\pi) - \min J_R &= J_R(\pi) - J_R(\pi_*) \\ &= \big(D^\pi - D^{\pi_*}\big)\cdot R \\ &\leq \|D^\pi - D^{\pi_*}\| \cdot \|R\| \\ &\leq (1-L)\cdot \mathrm{range}\ J_R. \end{aligned}$$

By subtracting $\mathrm{range}\ J_R = \max J_R - \min J_R$ from both sides, then multiplying by -1, and then dividing by $\mathrm{range}\ R$, we obtain the result. □

Lemma C.35. *For any (s,a), we have*

$$\frac{D^\pi(s,a)}{1-\gamma} = \sum_{t=0}^{\infty}\gamma^t \sum_{s_0,a_0,\dots,s_{t-1},a_{t-1}} \tau(s_0,a_0,\dots,s_{t-1},a_{t-1},s)\cdot \pi(s_0,a_0,\dots,s_{t-1},a_{t-1},s,a),$$

where

$$\tau(s_0,a_0,\dots,s) := \mu_0(s_0)\cdot \left[\prod_{i=1}^{t-1}\tau(s_i \mid s_{i-1},a_{i-1})\right]\cdot \tau(s \mid s_{t-1},a_{t-1}),$$

which is the part in the probability of a trajectory that does not depend on the policy, and

$$\pi(s_0,a_0,\dots,s,a) := \pi(a\mid s)\cdot \prod_{i=0}^{t-1}\pi(a_i \mid s_i).$$

Proof. We have

$$\begin{aligned} \frac{D^\pi(s,a)}{1-\gamma} &= \sum_{t=0}^{\infty}\gamma^t P(s_t = s, a_t = a \mid \xi \sim \pi) \\ &= \sum_{t=0}^{\infty}\gamma^t \sum_{s_0,a_0,\dots,s_{t-1},a_{t-1}} P(s_0,a_0,\dots,s_{t-1},a_{t-1},s,a \mid \pi) \\ &= \sum_{t=0}^{\infty}\gamma^t \sum_{s_0,a_0,\dots,s_{t-1},a_{t-1}} \mu_0(s_0)\pi(a_0\mid s_0)\left[\prod_{i=1}^{t-1}\tau(s_i\mid s_{i-1},a_{i-1})\pi(a_i\mid s_i)\right]\tau(s\mid s_{t-1},a_{t-1})\pi(a\mid s) \\ &= \sum_{t=0}^{\infty}\gamma^t \sum_{s_0,a_0,\dots,s_{t-1},a_{t-1}} \tau(s_0,a_0,\dots,s_{t-1},a_{t-1},s)\cdot \pi(s_0,a_0,\dots,s_{t-1},a_{t-1},s,a). \end{aligned}$$

□

Lemma C.36. *Let $1 \geq \delta > 0$. Assume that $\pi(a\mid s) \geq 1-\delta$ for all $(s,a) \in \mathrm{supp}\ D^{\pi_*}$ and that π_* is a deterministic policy.*[2] *Then for all $(s,a) \in \mathcal{S}\times\mathcal{A}$, one has*

$$D^{\pi_*}(s,a) - \delta\cdot(1-\gamma)\cdot\frac{\partial}{\partial\gamma}\left(\frac{\gamma}{1-\gamma}D^{\pi_*}(s,a)\right) \leq D^\pi(s,a) \leq D^{\pi_*}(s,a) + \frac{\delta}{1-\gamma}. \tag{89}$$

This also results in the following two inequalities:

$$D^\pi(\mathrm{supp}\ D^{\pi_*}) \geq 1 - \frac{\delta}{1-\gamma}, \quad \|D^\pi - D^{\pi_*}\| \leq \sqrt{|\mathcal{S}\times\mathcal{A}|}\cdot\frac{\delta}{1-\gamma}. \tag{90}$$

[2] In this lemma, one does not need the assumption that π_* is a worst-case policy, but this case will be the only application later on.

Proof. Let $(s, a) \in \text{supp } D^{\pi_*}$. We want to apply the summation formula in Lemma C.35, which we recommend to recall. For simplicity, in the following we will write $s_0, a_0, \ldots$ when we implicitly mean trajectories up until s_{t-1}, a_{t-1}. Now, we will write "π_*-comp" into a sum to indicate that we only sum over states and actions that make the whole trajectory-segment *compatible* with policy π_*, meaning all transitions have positive probability and the actions are deterministically selected by π_*. Note that if we restrict to such summands, then each consecutive pair $(s_i, a_i) \in \text{supp } D^{\pi_*}$ is in the support of D^{π_*}, and thus we can use our assumption $\pi(a_i \mid s_i) \geq 1 - \delta$ on those. We can use this strategy for a lower-bound:

$$\begin{aligned}
\frac{D^{\pi}(s,a)}{1-\gamma} &\geq \sum_{t=0}^{\infty} \gamma^t \sum_{\substack{s_0, a_0, \ldots \\ \pi_* - \text{comp}}} \tau(s_0, a_0, \ldots, s) \cdot \pi(s_0, a_0, \ldots, s, a) \\
&\geq \sum_{t=0}^{\infty} \gamma^t \sum_{\substack{s_0, a_0, \ldots \\ \pi_* - \text{comp}}} \tau(s_0, a_0, \ldots, s) \cdot (1-\delta)^{t+1} \\
&\geq \sum_{t=0}^{\infty} \gamma^t \sum_{\substack{s_0, a_0, \ldots \\ \pi_* - \text{comp}}} \tau(s_0, a_0, \ldots, s) \cdot \big(1 - \delta \cdot (t+1)\big).
\end{aligned} \tag{91}$$

In the last step, we used the classical formula $(1-\delta)^t \geq 1 - \delta \cdot t$, which can easily be proved by induction over t. Now, we split the sum up into two parts. For the first part, we note:

$$\begin{aligned}
\sum_{t=0}^{\infty} \gamma^t \sum_{\substack{s_0, a_0, \ldots \\ \pi_* - \text{comp}}} \tau(s_0, a_0, \ldots, s) \cdot 1 &= \sum_{t=0}^{\infty} \gamma^t \sum_{\substack{s_0, a_0, \ldots \\ \pi_* - \text{comp}}} \tau(s_0, a_0, \ldots, s) \cdot \pi_*(s_0, a_0, \ldots, s, a) \\
&= \sum_{t=0}^{\infty} \gamma^t \sum_{s_0, a_0, \ldots} \tau(s_0, a_0, \ldots, s) \cdot \pi_*(s_0, a_0, \ldots, s, a) \\
&= \frac{D^{\pi_*}(s,a)}{1-\gamma}.
\end{aligned} \tag{92}$$

For the second part, we similarly compute:

$$\begin{aligned}
\sum_{t=0}^{\infty} (t+1)\gamma^t \sum_{\substack{s_0, a_0, \ldots \\ \pi_* - \text{comp}}} \tau(s_0, a_0, \ldots, s) &= \sum_{t=0}^{\infty} \frac{\partial}{\partial \gamma} \gamma^{t+1} P(s_t = s, a_t = a \mid \pi_*) \\
&= \frac{\partial}{\partial \gamma} \left(\frac{\gamma}{1-\gamma} \cdot D^{\pi_*}(s,a) \right).
\end{aligned} \tag{93}$$

Putting Equations (92) and (93) into Equation (91) gives the first equation of Equation (89) for the case that $(s,a) \in \text{supp } D^{\pi_*}$. For the case that $(s,a) \notin \text{supp } D^{\pi_*}(s,a)$, the inequality is trivial since then $D^{\pi_*}(s,a) = 0$ and since the stated derivative is easily shown to be non-negative by writing out the occupancy explicitly (i.e., by reversing the previous computation).

This then implies

$$\begin{aligned}
D^{\pi}(\text{supp } D^{\pi_*}) &= \sum_{(s,a) \in \text{supp } D^{\pi_*}} D^{\pi}(s,a) \\
&\geq \sum_{(s,a) \in \text{supp } D^{\pi_*}} \left(D^{\pi_*}(s,a) - \delta \cdot (1-\gamma) \cdot \frac{\partial}{\partial \gamma} \left(\frac{\gamma}{1-\gamma} D^{\pi_*}(s,a) \right) \right) \\
&= 1 - \delta \cdot (1-\gamma) \cdot \frac{\partial}{\partial \gamma} \left(\frac{\gamma}{1-\gamma} \sum_{(s,a) \in \text{supp } D^{\pi_*}} D^{\pi_*}(s,a) \right) \\
&= 1 - \delta \cdot (1-\gamma) \cdot \frac{1}{(1-\gamma)^2} \\
&= 1 - \frac{\delta}{1-\gamma}.
\end{aligned}$$

This shows the first inequality in Equation (90). To show the second inequality in Equation (89), we use the first one and compute:

$$
\begin{aligned}
D^{\pi}(s,a) &= 1 - \sum_{(s',a') \neq (s,a)} D^{\pi}(s',a') \\
&\leq 1 - \sum_{(s',a') \in \operatorname{supp} D^{\pi_*} \setminus \{(s,a)\}} D^{\pi}(s',a') \\
&\leq 1 - \sum_{(s',a') \in \operatorname{supp} D^{\pi_*} \setminus \{(s,a)\}} D^{\pi_*}(s',a') \\
&\quad + \sum_{(s',a') \in \operatorname{supp} D^{\pi_*} \setminus \{(s,a)\}} \delta \cdot (1-\gamma) \cdot \frac{\partial}{\partial \gamma} \left(\frac{\gamma}{1-\gamma} D^{\pi_*}(s',a') \right) \\
&\leq D^{\pi_*}(s,a) + \frac{\delta}{1-\gamma},
\end{aligned}
$$

where in the last step we again used the trick of the previous computation of pulling the sum through the derivative. Finally, we prove the second inequality in Equation (90), using what we know so far. First, note that

$$
\delta \cdot (1-\gamma) \cdot \frac{\partial}{\partial \gamma} \left(\frac{\gamma}{1-\gamma} D^{\pi_*}(s,a) \right) \leq \frac{\delta}{1-\gamma}
$$

since we showed that the left-hand-side is non-negative and sums to the right-hand-side over all (s,a). Consequently, we obtain:

$$
\begin{aligned}
\|D^{\pi} - D^{\pi_*}\| &= \sqrt{\sum_{(s,a)} \left(D^{\pi}(s,a) - D^{\pi_*}(s,a) \right)^2} \\
&\leq \sqrt{\sum_{(s,a)} \left| \frac{\delta}{1-\gamma} \right|^2} \\
&= \sqrt{|\mathcal{S} \times \mathcal{A}|} \cdot \frac{\delta}{1-\gamma}.
\end{aligned}
$$

This finishes the proof. $\square$

We now fix more constants and notation. Define $\mathcal{S}_0 \coloneqq \operatorname{supp} \mu_0$ as the support of μ_0, and more generally $\mathcal{S}_t$ as the states reachable within t timesteps using the fixed worst-case policy π_*:

$$
\mathcal{S}_t \coloneqq \Big\{ s \;\Big|\; \exists \pi_* - \text{compatible sequence } s_0, a_0, \ldots, s_{k-1}, a_{k-1}, s \text{ for } k \leq t \Big\}.
$$

Since there are only finitely many states and $\mathcal{S}_t \subseteq \mathcal{S}_{t+1}$, there is a t_0 such that $\mathcal{S}_{t_0}$ is maximal. Set $D^{\pi_*}(s) \coloneqq \sum_a D^{\pi_*}(s,a)$. Recall the notation τ from Lemma C.35. Define the following constant which, given the MDP, only depends on $\delta > 0$ and π_*:

$$
C(\delta, \pi_*, \mu_0, \tau, \gamma) \coloneqq \min_{\substack{t \in [0:t_0] \\ s_0, a_0, \ldots, s_{t-1}, a_{t-1}, s:\ \pi_* - \text{comp}}} \gamma^t \tau(s_0, a_0 \ldots, s) \cdot (1-\delta)^t \cdot \delta > 0. \tag{94}
$$

We get the following result:

Lemma C.37. *Define the reward function $\hat{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ as follows:*

$$
\hat{R}(s,a) \coloneqq \begin{cases} R(s,a), & (s,a) \notin \operatorname{supp} D^{\pi_*}, \\ \max R + \frac{\lambda}{C(\delta, \pi_*, \mu_0, \tau, \gamma)} \cdot \omega(\pi_*), & \textit{else}. \end{cases} \tag{95}
$$

Assume that $\hat{\pi}$ is (λ, ω)-RLHF optimal with respect to $\hat{R}$. Then for all $(s,a) \in \operatorname{supp} D^{\pi_*}$, we have $\hat{\pi}(a \mid s) \geq 1 - \delta$.

Proof. We show this statement by induction over the number of timesteps that π_* needs to reach a given state. Thus, first assume $s \in \mathcal{S}_0$ and $a = \pi_*(s)$. We do a proof by contradiction. Thus, assume that $\hat{\pi}(a \mid s) < 1 - \delta$. This means that $\sum_{a' \neq a} \hat{\pi}(a' \mid s) \geq \delta$, and consequently

$$\sum_{a' \neq a} D^{\hat{\pi}}(s, a') \geq \mu_0(s) \cdot \delta \geq C(\delta, \pi_*, \mu_0, \tau, \gamma). \tag{96}$$

We now claim that from this it follows that π_* is more optimal than $\hat{\pi}$ with respect to RLHF, a contradiction to the optimality of $\hat{\pi}$. Indeed:

$$\begin{aligned}
J_{\hat{R}}(\hat{\pi}) - \lambda\omega(\hat{\pi}) &\overset{(1)}{\leq} J_{\hat{R}}(\hat{\pi}) \\
&\overset{(2)}{=} \sum_{a' \neq a} D^{\hat{\pi}}(s, a') \cdot R(s, a') + \sum_{(s', a') \notin \{s\} \times \mathcal{A} \setminus \{a\}} D^{\hat{\pi}}(s', a') \cdot \hat{R}(s', a') \\
&\overset{(3)}{\leq} \sum_{a' \neq a} D^{\hat{\pi}}(s, a') \cdot \max R + \hat{R}(s, a) \cdot \sum_{(s', a') \notin \{s\} \times \mathcal{A} \setminus \{a\}} D^{\hat{\pi}}(s', a'') \\
&= \sum_{a' \neq a} D^{\hat{\pi}}(s, a') \cdot \max R + \left(1 - \sum_{a' \neq a} D^{\hat{\pi}}(s, a')\right) \cdot \hat{R}(s, a) \qquad (97) \\
&\overset{(4)}{\leq} C(\delta, \pi_*, \mu_0, \tau, \gamma) \cdot \max R + \big(1 - C(\delta, \pi_*, \mu_0, \tau, \gamma)\big) \cdot \hat{R}(s, a) \\
&\overset{(5)}{=} J_{\hat{R}}(\pi_*) + C(\delta, \pi_*, \mu_0, \tau, \gamma) \cdot \Big(\max R - \hat{R}(s, a)\Big) \\
&\overset{(6)}{=} J_{\hat{R}}(\pi_*) - C(\delta, \pi_*, \mu_0, \tau, \gamma) \cdot \frac{\lambda}{C(\delta, \pi_*, \mu_0, \tau, \gamma)} \cdot \omega(\pi_*) \\
&= J_{\hat{R}}(\pi_*) - \lambda\omega(\pi_*).
\end{aligned}$$

In step (1), we use the non-negativity of ω. In step (2), we use that $(s, a') \notin \operatorname{supp} D^{\pi_*}$, and so $\hat{R}(s, a') = R(s, a')$. In the right term in step (3), we use that $(s, a) \in \operatorname{supp} D^{\pi_*}$, and thus $\hat{R}(s, a) \geq \hat{R}(s', a')$, by definition of $\hat{R}$. In step (4), we use that $\hat{R}(s, a) \geq \max R$ and Equation (96). Step (5) uses that $J_{\hat{R}}(\pi_*) = \hat{R}(s, a)$, following from the fact that $\hat{R}$ is constant for policy π_*. Step (6) uses the concrete definition of $\hat{R}$. Thus, we have showed a contradiction to the RLHF-optimality of $\hat{\pi}$, from which it follows that $\hat{\pi}(a \mid s) \geq 1 - \delta$.

Now assume the statement is already proven for $t - 1$ and let $s \in \mathcal{S}_t \setminus \mathcal{S}_{t-1}$. Then there exists a π_*-compatible sequence $s_0, a_0, \ldots, s_{t-1}, a_{t-1}$ leading to s. We necessarily have $s_i \in \mathcal{S}_i$ for all $i = 0, \ldots, t-1$, and so we obtain $\hat{\pi}(a_i \mid s_i) \geq 1 - \delta$ by the induction hypothesis. Now, let $a := \pi_*(s)$ and assume we had $\hat{\pi}(a \mid s) < 1 - \delta$. As before, we then have $\sum_{a' \neq a} \hat{\pi}(a' \mid s) \geq \delta$. Consequently, we get

$$\begin{aligned}
\sum_{a' \neq a} D^{\hat{\pi}}(s, a') &\geq \gamma^t \cdot \sum_{a' \neq a} \tau(s_0, a_0, \ldots, s) \cdot \hat{\pi}(s_0, a_0, \ldots, s, a') \\
&\geq \gamma^t \cdot \tau(s_0, a_0, \ldots, s) \cdot (1 - \delta)^t \cdot \delta \\
&\geq C(\delta, \pi_*, \mu_0, \tau, \gamma)
\end{aligned}$$

Then the same computation as in Equation (97) leads to the same contradiction again, and we are done. ☐

Theorem C.38. *Define*

$$\delta := \frac{(1 - \gamma) \cdot (1 - L) \cdot \operatorname{range} J_R}{\sqrt{|\mathcal{S} \times \mathcal{A}|} \cdot \|R\|} > 0.$$

Let $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be our MDP. Set

$$C := C(\mathcal{M}, \pi_*, L, \lambda, \omega) := \frac{\lambda \cdot \omega(\pi_*)}{\operatorname{range} R \cdot C(\delta, \pi_*, \mu_0, \tau, \gamma)} < \infty, \tag{98}$$

with the "inner" $C(\delta, \pi_*, \mu_0, \tau, \gamma)$ defined in Equation (94)*. Assume that*

$$D(\text{supp } D^{\pi_*}) \leq \frac{\epsilon}{1+C}. \tag{99}$$

Then $D \in \mathbf{unsafe}(R, \epsilon, L, \lambda, \omega)$.

Proof. We prove the theorem by showing that for every data distribution $D \in \Delta(\mathcal{S}\times\mathcal{A})$ that fulfills the conditions of Theorem C.38, there exists a reward function $\hat{R}$ together with a (λ, ω)-RLHF optimal policy $\hat{\pi}$ with respect to $\hat{R}$ such that

- $\mathbb{E}_{(s,a)\sim D}\left[\frac{|\hat{R}(s,a)-R(s,a)|}{\text{range } R}\right] \leq \epsilon$,
- $\text{Reg}^R(\hat{\pi}) \geq L$.

Towards that goal, define $\hat{R}$ as in Equation (95) and $\hat{\pi}$ as a (λ, ω)-RLHF optimal policy for $\hat{R}$. Then Lemma C.37 shows that $\hat{\pi}(s \mid a) \geq 1-\delta$ for all $(s,a) \in \text{supp } D^{\pi_*}$. Consequently, Lemma C.36 implies that

$$\|D^{\hat{\pi}} - D^{\pi_*}\| \leq \sqrt{|\mathcal{S}\times\mathcal{A}|}\cdot\frac{\delta}{1-\gamma} = \frac{(1-L)\cdot\text{range } J_R}{\|R\|}.$$

Consequently, Lemma C.34 shows that $\text{Reg}^R(\hat{\pi}) \geq L$, and thus the second claim. For the first claim, note that

$$\begin{aligned}\mathbb{E}_{(s,a)\sim D}\left[|\hat{R}(s,a) - R(s,a)|\right] &= \sum_{(s,a)\in\text{supp } D^{\pi_*}} D(s,a)\cdot\left(\max R + \frac{\lambda}{C(\delta,\pi_*,\mu_0,\tau,\gamma)}\omega(\pi_*) - R(s,a)\right)\\ &\leq D(\text{supp } D^{\pi_*})\cdot\left(\text{range } R + \frac{\lambda}{C(\delta,\pi_*,\mu_0,\tau,\gamma)}\omega(\pi_*)\right)\\ &\leq \epsilon\cdot\text{range } R,\end{aligned}$$

where the last claim follows from the assumed inequality in $D(\text{supp } D^{\pi_*})$. □

We obtain the following corollary, which is very similar to Proposition C.5. The main difference is that the earlier result only assumed a poliy of regret L and not regret 1:

Corollary C.39. *Theorem C.38 specializes as follows for the case $\lambda = 0$: Assume $D(\text{supp } D^{\pi_*}) \leq \epsilon$. Then there exists a reward function $\hat{R}$ together with an optimal policy $\hat{\pi}$ that satisfies the two inequalities from the previous result.*

Proof. This directly follows from $\lambda = 0$. For completeness, we note that the definition of $\hat{R}$ also simplifies, namely to

$$\hat{R}(s,a) = \begin{cases} R(s,a), & (s,a) \notin \text{supp } D^{\pi_*} \\ \max R, & \text{else.}\end{cases}$$

□

We now present another specialization of Theorem C.38. Namely, from now on, assume that $D = D^{\pi_{\text{ref}}}$ and $\omega(\pi) = \mathbb{D}_{\text{KL}}(\pi||\pi_{\text{ref}})$. In other words, the dataset used to evaluate the reward function is sampled from the same (safe) policy used in KL-regularization. This leads to the following condition specializing the one from Equation (99):

$$D^{\pi_{\text{ref}}}(\text{supp } D^{\pi_*}) \leq \frac{\epsilon}{1 + \frac{\lambda\cdot\mathbb{D}_{\text{KL}}(\pi_*||\pi_{\text{ref}})}{\text{range } R\cdot C(\delta,\pi_*,\mu_0,\tau,\gamma)}}. \tag{100}$$

π_{ref} now appears on both the left and right side of the equation, and so one can wonder whether it is ever possible that the inequality holds. After all, if $D^{\pi_{\text{ref}}}(\text{supp } D^{\pi_*})$ "gets smaller", then $\mathbb{D}_{\text{KL}}(\pi_*||\pi_{\text{ref}})$ should usually get "larger". However, halfing each of the probabilities $D^{\pi_{\text{ref}}}(s,a)$ for $(s,a) \in \text{supp } D^{\pi_*}$ leads to only an increase by the addition of $\log 2$ of $\mathbb{D}_{\text{KL}}(\pi_*||\pi_{\text{ref}})$. Thus, intuitively, we expect the inequality to hold when the left-hand-side is very small. An issue is that the

KL divergence can disproportionately blow up in size if some *individual* probabilities $D^{\pi_{\text{ref}}}(s,a)$ for $(s,a) \in \text{supp } D^{\pi_*}$ are very small compared to other such probabilities. This can be avoided by a bound in the proportional difference of these probabilities. We thus obtain the following sufficient condition for a "negative result":[3]

Corollary C.40. *Let the notation be as in Theorem C.38 and assume $D = D^{\pi_{\text{ref}}}$ and $\omega(\pi) = \mathbb{D}_{KL}(\pi||\pi_{\text{ref}})$. Let $K \geq 0$ be a constant such that*

$$\max_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s,a) \leq K \cdot \min_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s,a).$$

Assume that

$$\min_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s,a) \leq \left(\frac{\epsilon}{K \cdot |\mathcal{S}| \cdot \left(1 + \frac{\lambda}{\text{range } R \cdot C(\delta,\pi_*,\mu_0,\tau,\gamma)}\right)} \right)^2. \tag{101}$$

Then Equation (99) *holds, and the conclusion of the theorem thus follows.*

Proof. As argued before, the equation to show can be written as Equation (100). We can upper-bound the left-hand-side as follows:

$$\begin{aligned}
D^{\pi_{\text{ref}}}(\text{supp } D^{\pi_*}) &= \sum_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s,a) \\
&\leq |\text{supp } D^{\pi_*}| \cdot \max_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s,a) \qquad (102) \\
&\leq |\mathcal{S}| \cdot K \cdot \min_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s,a).
\end{aligned}$$

In one step, we used that π_* is assumed to be deterministic, which leads to a bound in the size of the support. Now, we lower-bound the other side by noting that

$$\begin{aligned}
\mathbb{D}_{\text{KL}}(\pi_*||\pi_{\text{ref}}) &= \sum_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_*}(s,a) \cdot \log \frac{D^{\pi_*}(s,a)}{D^{\pi_{\text{ref}}}(s,a)} \\
&\leq \sum_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_*}(s,a) \cdot \log \frac{1}{\min_{(s',a')\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s',a')} \\
&= \log \frac{1}{\min_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s,a)}.
\end{aligned}$$

Thus, for the right-hand-side, we obtain

$$\frac{\epsilon}{1 + \frac{\lambda \cdot \mathbb{D}_{\text{KL}}(\pi_*||\pi_{\text{ref}})}{\text{range } R \cdot C(\delta,\pi_*,\mu_0,\tau,\gamma)}} \geq \frac{\epsilon}{1 + \frac{\lambda}{\text{range } R \cdot C(\delta,\pi_*,\mu_0,\tau,\gamma)} \cdot \log \frac{1}{\min_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s,a)}} \tag{103}$$

Now, set $A := |\mathcal{S}| \cdot K$, $B := \frac{\lambda}{\text{range } R \cdot C(\delta,\pi_*,\mu_0,\tau,\gamma)}$ and $x := \min_{(s,a)\in\text{supp } D^{\pi_*}} D^{\pi_{\text{ref}}}(s,a)$. Then comparing with Equations (102) and (103), we are left with showing the following, which we also equivalently rewrite:

$$\begin{aligned}
A \cdot x &\leq \frac{\epsilon}{1 + B \cdot \log \frac{1}{x}} \\
\iff A \cdot \left(x + Bx \log \frac{1}{x}\right) &\leq \epsilon.
\end{aligned}$$

Now, together with the assumed condition on x from Equation (101), and upper-bounding the logarithm with a square-root, and x by $\sqrt{x}$ since $x \leq 1$, we obtain:

$$\begin{aligned}
A \cdot \left(x + Bx \log \frac{1}{x}\right) &\leq A \cdot \left(x + B\sqrt{x}\right) \\
&\leq A \cdot \left((1+B) \cdot \sqrt{x}\right) \\
&\leq A \cdot (1+B) \cdot \frac{\epsilon}{A \cdot (1+B)} \\
&= \epsilon.
\end{aligned}$$

[3]The condition is quite strong and we would welcome attempts to weaken it.

That was to show. □

D REQUIREMENTS FOR SAFE OPTIMIZATION

In this section, we answer the question under which circumstances we can guarantee a safe optimization of a given reward function. Wherever applicable, we make the same assumptions as stated in Appendix C.1.

D.1 APPLYING BERGE'S MAXIMUM THEOREM

Definition D.1 (Correspondence)**.** Let X, Y be two sets. A *correspondence* $C : X \rightrightarrows Y$ is a function $X \to \mathcal{P}(Y)$ from X to the power set of Y.

Definition D.2 (Upper Hemicontinuous, Lower Hemicontinuous, Continuous, Compact-Valued)**.** Let $C : X \rightrightarrows Y$ be a correspondence where X and Y are topological spaces. Then:

- C is called *upper hemicontinuous* if for every $x \in X$ and every open set $V \subseteq Y$ with $C(x) \subseteq V$, there exists an open set $U \subseteq X$ with $x \in U$ and such that for all $x' \in U$ one has $C(x') \subseteq V$.
- C is called *lower hemicontinuous* if for every $x \in X$ and every open set $V \subseteq Y$ with $C(x) \cap V \neq \emptyset$, there exists an open set $U \subseteq X$ with $x \in U$ and such that for all $x' \in U$ one has $C(x') \cap V \neq \emptyset$.
- C is called *continuous* if it is both upper and lower hemicontinuous.
- C is called *compact-valued* if $C(x)$ is a compact subset of Y for all $x \in X$.

Theorem D.3 (Maximum Theorem, (Berge, 1963))**.** *Let Θ and X be topological spaces, $f : \Theta \times X \to \mathbb{R}$ a continuous function, and $C : \Theta \rightrightarrows X$ be a continuous, compact-valued correspondence such that $C(\theta) \neq \emptyset$ for all $\theta \in \Theta$. Define the* optimal value function *$f^* : \Theta \to \mathbb{R}$ by*

$$f^*(\theta) := \max_{x \in C(\theta)} f(\theta, x)$$

and the maximizer function *$C^* : \Theta \rightrightarrows X$ by*

$$C^*(\theta) := \arg\max_{x \in C(\theta)} f(\theta, x) = \big\{x \in C(\theta) \mid f(\theta, x) = f^*(\theta)\big\}.$$

Then f^* is continuous and C^* is a compact-valued, upper hemicontinuous correspondence with nonempty values, i.e. $C^*(\theta) \neq \emptyset$ for all $\theta \in \Theta$.

We now show that this theorem corresponds to our setting. Namely, replace X be by Π, the set of all policies. Every policy $\pi \in \Pi$ can be viewed as a vector $\vec{\pi} = \big(\pi(a \mid s)\big)_{s \in \mathcal{S}, a \in \mathcal{A}} \in \mathbb{R}^{\mathcal{S} \times \mathcal{A}}$, and so we view Π as a subset of $\mathbb{R}^{\mathcal{S} \times \mathcal{A}}$. Π inherits the standard Euclidean metric and thus topology from $\mathbb{R}^{\mathcal{S} \times \mathcal{A}}$. Replace Θ by $\mathcal{R}$, the set of all reward functions. We can view each reward function $R \in \mathcal{R}$ as a vector $\vec{R} = \big(R(s,a)\big)_{(s,a) \in \mathcal{S} \times \mathcal{A}} \in \mathbb{R}^{\mathcal{S} \times \mathcal{A}}$. So we view $\mathcal{R}$ as a subset of $\mathbb{R}^{\mathcal{S} \times \mathcal{A}}$ and thus a topological space. Replace f by the function $J : \mathcal{R} \times \Pi \to \mathbb{R}$ given by

$$J(R, \pi) := J^R(\pi) = \eta^\pi \cdot \vec{R}.$$

Take as the correspondence $C : \mathcal{R} \rightrightarrows \Pi$ the trivial function $C(R) := \Pi$ that maps every reward function to the full set of policies.

Proposition D.4. *These definitions satisfy the conditions of Theorem D.3, that is:*

1. *$J : \mathcal{R} \times \Pi \to \mathbb{R}$ is continuous.*
2. *$C : \mathcal{R} \rightrightarrows \Pi$ is continuous and compact-valued with non-empty values.*

Proof. Let us prove 1. Since the scalar product is continuous, it is enough to show that $\eta : \Pi \to \mathbb{R}^{\mathcal{S} \times \mathcal{A}}$ is continuous. Let $(s,a) \in \mathcal{S} \times \mathcal{A}$ be arbitrary. Then it is enough to show that each componentfunction $\eta(s,a) : \Pi \to \mathbb{R}$ given by

$$\big[\eta(s,a)\big](\pi) := \eta^\pi(s,a)$$

is continuous.

Now, for any $t \geq 0$, define the function $P_t(s, a) : \Pi \to \mathbb{R}$ by

$$\big[P_t(s, a)\big](\pi) \coloneqq P(s_t = s, a_t = a \mid \xi \sim \pi).$$

We obtain

$$\eta(s, a) = \sum_{t=0}^{\infty} \gamma^t P_t(s, a).$$

Furthermore, this convergence is uniform since $\big[P_t(s, a)\big](\pi) \leq 1$ for all π and since $\sum_{t=0}^{\infty} \gamma^t$ is a convergent series. Thus, by the uniform limit theorem, it is enough to show that each $P_t(s, a)$ is a continuous function.

Concretely, we have

$$\big[P_t(s, a)\big](\pi) = \sum_{s_0, a_0, \dots, s_{t-1}, a_{t-1}} P\big(s_0, a_0, \dots, s_{t-1}, a_{t-1}, s, a \mid \xi \sim \pi\big)$$

$$= \sum_{s_0, a_0, \dots, s_{t-1}, a_{t-1}} \mu_0(s_0) \cdot \pi(a_0 \mid s_0) \cdot \left[\prod_{l=1}^{t-1} \tau(s_l \mid s_{l-1}, a_{l-1}) \cdot \pi(a_l \mid s_l)\right] \cdot \tau(s \mid s_{t-1}, a_{t-1}) \cdot \pi(a \mid s).$$

Since $\mathcal{S}$ and $\mathcal{A}$ are finite, this whole expression can be considered as a polynomial with variables given by all $\pi(a \mid s)$ for all $(s, a) \in \mathcal{S} \times \mathcal{A}$ and coefficients specified by μ_0 and τ. Since polynomials are continuous, this shows the result.

Let us prove 2. Since $\Pi \neq \emptyset$, C has non-empty values. Furthermore, Π is compact because it is a finite cartesian product of compact simplices. And finally, since C is constant, it is easily seen to be continuous. That was to show. □

Define the optimal value function $J^* : \mathcal{R} \to \mathbb{R}$ by

$$J^*(R) \coloneqq \max_{\pi \in \Pi} J^R(\pi)$$

and the maximizer function $\Pi^* : \mathcal{R} \rightrightarrows \Pi$ by

$$\Pi^*(R) \coloneqq \arg\max_{\pi \in \Pi} J^R(\pi) = \big\{\pi \in \Pi \mid J^R(\pi) = J^*(R)\big\}.$$

Corollary D.5. *J^* is continuous and Π^* is upper hemicontinuous and compact-valued with non-empty values.*

Proof. This follows from Theorem D.3 and Proposition D.4. □

In particular, every reward function has a compact and non-empty set of optimal policies, and their value changes continuously with the reward function. The most important part of the corollary is the upper hemicontinuity, which has the following consequence:

Corollary D.6. *Let R be a fixed, non-trivial reward function, meaning that $\max J^R \neq \min J^R$. Let $U \in (0, 1]$ be arbitrary. Then there exists $\epsilon > 0$ such that for all $\hat{R} \in \mathcal{B}_\epsilon(R)$ and all $\hat{\pi} \in \Pi^*(\hat{R})$, we have $\mathrm{Reg}^R(\hat{\pi}) < U$.*

Proof. The condition $\max J^R \neq \min J^R$ ensures that the regret function $\mathrm{Reg}^R : \Pi \to [0, 1]$ is well-defined. Recall its definition:

$$\mathrm{Reg}^R(\pi) = \frac{\max J^R - J^R(\pi)}{\max J^R - \min J^R}.$$

Since J^R is continuous by Proposition D.4, the regret function Reg^R is continuous as well. Consequently, the set $V \coloneqq \big(\mathrm{Reg}^R\big)^{-1}\big([0, U)\big)$ is open in Π.

Notice that $\Pi^*(R) \subseteq V$ (optimal policies have no regret). Thus, by Corollary D.5, there exists an open set $W \subseteq \mathcal{R}$ with $R \in W$ such that for all $\hat{R} \in W$ we have $\Pi^*(\hat{R}) \subseteq V$. Consequently, for all $\hat{\pi} \in \Pi^*(\hat{R})$, we get $\mathrm{Reg}^R(\hat{\pi}) < U$. Since W is open, it contains a whole epsilon ball around R, showing the result. □

Now we translate the results to the distance defined by D, a data distribution. Namely, let $D \in \Delta(\mathcal{S}\times\mathcal{A})$ a distribution that assigns a positive probability to each transition. Then define the D-norm by

$$d^D(R) := \mathbb{E}_{(s,a)\sim D}\left[\left|R(s,a)\right|\right].$$

This is indeed a norm, i.e.: for all $\alpha \in \mathbb{R}$ and all $R, R' \in \mathcal{R}$, we have

- $d^D(R+R') \leq d^D(R) + d^D(R')$;
- $d^D(\alpha \cdot R) = |\alpha| \cdot d^D(R)$;
- $d^D(R) = 0$ if and only if $R = 0$.

For the third property, one needs the assumption that $D(s,a) > 0$ for all $(s,a) \in \mathcal{S}\times\mathcal{A}$.

This norm then induces a metric that we denote the same way:

$$d^D(R, R') := d^D(R - R').$$

We obtain:

Corollary D.7. *Let $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ be an arbitrary non-trivial MDP, meaning that $\max J^R \neq \min J^R$. Furthermore, let $L \in (0,1]$ be arbitrary, and $D \in \Delta(\mathcal{S}\times\mathcal{A})$ a positive data distribution, i.e., a distribution D such that $\forall (s,a) \in \mathcal{S}\times\mathcal{A}$, $D(s,a) > 0$. Then there exists $\epsilon > 0$ such that $D \in \mathbf{safe}(R, \epsilon, L)$*

Proof. To prove the corollary, we will show that there exists $\epsilon > 0$ such that for all $\hat{R} \in \mathcal{R}$ with

$$\frac{d^D(R, \hat{R})}{\text{range } R} < \epsilon$$

and all $\hat{\pi} \in \Pi^*(\hat{R})$ we have $\text{Reg}^R(\hat{\pi}) < L$. We know from Corollary D.6 that there is $\epsilon' > 0$ such that for all $\hat{R} \in \mathcal{B}_{\epsilon'}(R)$ and all $\hat{\pi} \in \Pi^*(\hat{R})$, we have $\text{Reg}^R(\hat{\pi}) < L$. Now, let $c > 0$ be a constant such that

$$c \cdot \|R' - R''\| \leq d^D(R', R'')$$

for all $R', R'' \in \mathcal{R}$, where $\|\cdot\|$ is the standard Euclidean norm. This exists since all norms in $\mathbb{R}^{\mathcal{S}\times\mathcal{A}}$ are equivalent, but one can also directly argue that

$$c := \min_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a)$$

is a valid choice. Then, set

$$\epsilon := \epsilon' \cdot \frac{c}{\text{range } R}.$$

Then for all $\hat{R} \in \mathcal{R}$ with

$$\frac{d^D(R, \hat{R})}{\text{range } R} < \epsilon$$

we obtain

$$\begin{aligned}
\|R - \hat{R}\| &\leq \frac{d^D(R, \hat{R})}{c} \\
&= \frac{d^D(R, R')}{\text{range } R} \cdot \frac{\text{range } R}{c} \\
&\leq \epsilon \cdot \frac{\text{range } R}{c} \\
&= \epsilon'.
\end{aligned}$$

Thus, for all $\hat{\pi} \in \Pi^*(\hat{R})$, we obtain $\text{Reg}^R(\hat{\pi}) < L$, showing the result. □

Remark D.8. If $c := \min_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a)$ is very small, then the proof of the preceding corollary shows that $d^D(R, \hat{R})$ must be correspondingly smaller to guarantee a low regret of $\hat{\pi} \in \Pi^*(\hat{R})$. This makes sense since a large effective distance between R and $\hat{R}$ can "hide" in the regions where D is small when distance is measured via d^D.

D.2 Elementary proof of a regret bound

In this section, we provide another elementary proof of a regret bound, but without reference to Berge's theorem. This will also lead to a better quantification of the bound. In an example, we will show that the bound we obtain is tight.

Define the cosine of an angle between two vectors ad hoc as usual:

$$\cos\Big(\operatorname{ang}\big(v, w\big)\Big) \coloneqq \frac{v \cdot w}{\|v\| \cdot \|w\|},$$

where $v \cdot w$ is the dot product.

Lemma D.9. *Let R, $\hat{R}$ be two reward functions. Then for any policy π, we have*

$$J^R(\pi) - J^{\hat{R}}(\pi) = \frac{1}{1-\gamma} \cdot \|D^\pi\| \cdot \big\|R - \hat{R}\big\| \cdot \cos\Big(\operatorname{ang}\big(\eta^\pi, \vec{R} - \vec{\hat{R}}\big)\Big).$$

Proof. We have

$$J^R(\pi) - J^{\hat{R}}(\pi) = \eta^\pi \cdot \big(\vec{R} - \vec{\hat{R}}\big) = \|\eta^\pi\| \cdot \big\|\vec{R} - \vec{\hat{R}}\big\| \cdot \cos\Big(\operatorname{ang}\big(\eta^\pi, \vec{R} - \vec{\hat{R}}\big)\Big).$$

The result follows from $\eta^\pi = \frac{1}{1-\gamma} \cdot D^\pi$. □

we will make use of another lemma:

Lemma D.10. *Let $a, \hat{a}$, and r be three vectors. Assume $a \cdot \hat{a} \geq 0$, where $\cdot$ is the dot product. Then*

$$\cos\big(\operatorname{ang}(a, r)\big) - \cos\big(\operatorname{ang}(\hat{a}, r)\big) \leq \sqrt{2}.$$

Proof. None of the angles change by replacing any of the vectors with a normed version. We can thus assume $\|a\| = \|\hat{a}\| = \|r\| = 1$. We obtain

$$\begin{aligned}
\Big|\cos\big(\operatorname{ang}(a, r)\big) - \cos\big(\operatorname{ang}(\hat{a}, r)\big)\Big|^2 &= \big|a \cdot r - \hat{a} \cdot r\big|^2 \\
&= \big|(a - \hat{a}) \cdot r\big|^2 \\
&\leq \|a - \hat{a}\|^2 \cdot \|r\|^2 \\
&= \|a - \hat{a}\|^2 \\
&= \|a\|^2 + \|\hat{a}\|^2 - 2a \cdot \hat{a} \\
&\leq 2.
\end{aligned}$$

In the first, fourth, and sixth step, we used that all vectors are normed. In the third step, we used the Cauchy-Schwarz inequality. Finally, we used that $a \cdot \hat{a} \geq 0$. The result follows. □

Recall that for two vectors v, w, the projection of v onto w is defined by

$$\operatorname{proj}_w v \coloneqq \frac{v \cdot w}{\|w\|^2} w.$$

This projection is a multiple of w, and it minimizes the distance to v:

$$\big\|v - \operatorname{proj}_w v\big\| = \min_{\alpha \in \mathbb{R}} \big\|v - \alpha w\big\|.$$

We can now formulate and prove our main regret bound:

Theorem D.11. *Let R be a fixed, non-trivial reward function, meaning that $\max J^R \neq \min J^R$. Then for all $\hat{R} \in \mathcal{R}$ and all $\hat{\pi} \in \Pi^*(\hat{R})$, we have*

$$\operatorname{Reg}^R(\hat{\pi}) \leq \frac{\sqrt{2}}{(1-\gamma) \cdot (\max J^R - \min J^R)} \cdot \big\|\vec{R} - \vec{\hat{R}}\big\|.$$

Furthermore, if $\vec{R} \cdot \vec{\hat{R}} \geq 0$, then we also obtain the following stronger bound:

$$\operatorname{Reg}^R(\hat{\pi}) \leq \frac{\sqrt{2}}{(1-\gamma) \cdot (\max J^R - \min J^R)} \cdot \Big\|\vec{R} - \operatorname{proj}_{\vec{\hat{R}}} \vec{R}\Big\|.$$

Now, let $D \in \Delta(\mathcal{S}\times\mathcal{A})$ be a data distribution. Then we obtain the following consequence:

$$\mathrm{Reg}^R\left(\hat{\pi}\right) \leq \frac{\sqrt{2}}{(1-\gamma)\cdot\left(\max J^R - \min J^R\right)\cdot \min_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a)} \cdot d^D\big(R, \hat{R}\big).$$

Proof. We start with the first claim. First, notice that the inequality we want to show is equivalent to the following:

$$J^R(\hat{\pi}) \geq \max J^R - \frac{\sqrt{2}}{1-\gamma}\cdot \big\|\vec{R} - \vec{\hat{R}}\big\|. \tag{104}$$

From Lemma D.9, we obtain

$$J^R(\hat{\pi}) = J^{\hat{R}}(\hat{\pi}) + \frac{1}{1-\gamma}\cdot \|D^{\hat{\pi}}\|\cdot\big\|\vec{R}-\vec{\hat{R}}\big\|\cdot\cos\Big(\operatorname{ang}\big(\eta^{\hat{\pi}}, R-\hat{R}\big)\Big).$$

Now, let $\pi \in \Pi^*(R)$ be an optimal policy for R. Then also from Lemma D.9, we obtain

$$\begin{aligned}\max J^R = J^R(\pi) &= J^{\hat{R}}(\pi) + \frac{1}{1-\gamma}\cdot\|D^{\pi}\|\cdot\big\|\vec{R}-\vec{\hat{R}}\big\|\cdot\cos\Big(\operatorname{ang}\big(\eta^{\pi}, R-\hat{R}\big)\Big)\\ &\leq J^{\hat{R}}(\hat{\pi}) + \frac{1}{1-\gamma}\cdot\|D^{\pi}\|\cdot\big\|\vec{R}-\vec{\hat{R}}\big\|\cdot\cos\Big(\operatorname{ang}\big(\eta^{\pi}, R-\hat{R}\big)\Big).\end{aligned}$$

In the last step, we used that $\hat{\pi}\in\Pi^*(\vec{R})$ and so $J^{\hat{R}}(\pi) \leq J^{\hat{R}}(\hat{\pi})$. Combining both computations, we obtain:

$$J^R(\hat{\pi}) \geq \max J^R - \frac{1}{1-\gamma}\cdot\big\|\vec{R}-\vec{\hat{R}}\big\|\cdot\Big[\|D^{\pi}\|\cdot\cos\Big(\operatorname{ang}\big(\eta^{\pi}, R-\hat{R}\big)\Big) - \|D^{\hat{\pi}}\|\cdot\cos\Big(\operatorname{ang}\big(\eta^{\hat{\pi}}, R-\hat{R}\big)\Big)\Big]$$

Since we want to show Equation (104), we are done if we can bound the big bracket by $\sqrt{2}$. By the Cauchy-Schwarz inequality, $\cos\Big(\operatorname{ang}\big(v,w\big)\Big)\in[-1,1]$ for all vectors v, w. Thus, if the first cosine term is negative or the second cosine term is positive, then since $\|D^{\pi}\| \leq \|D^{\pi}\|_1 = 1$, the bound by $\sqrt{2}$ is trivial. Thus, assume that the first cosine term is positive and the second is negative. We obtain

$$\begin{aligned}&\|D^{\pi}\|\cdot\cos\Big(\operatorname{ang}\big(\eta^{\pi}, R-\hat{R}\big)\Big) - \|D^{\hat{\pi}}\|\cdot\cos\Big(\operatorname{ang}\big(\eta^{\hat{\pi}}, R-\hat{R}\big)\Big)\\ &\leq \cos\Big(\operatorname{ang}\big(\eta^{\pi}, R-\hat{R}\big)\Big) - \cos\Big(\operatorname{ang}\big(\eta^{\hat{\pi}}, R-\hat{R}\big)\Big)\\ &\leq \sqrt{2}\end{aligned}$$

by Lemma D.10. Here, we used that η^{π} and $\eta^{\hat{\pi}}$ have only non-negative entries and thus also nonnegative dot product $\eta^{\pi}\cdot\eta^{\hat{\pi}}\geq 0$.

For the second claim, notice the following: if $\vec{R}\cdot\vec{\hat{R}}\geq 0$, then $\operatorname{proj}_{\vec{\hat{R}}}\vec{R} = \alpha\cdot\vec{\hat{R}}$ for some constant $\alpha \geq 0$. Consequently, we have $\hat{\pi}\in\Pi^*\Big(\operatorname{proj}_{\vec{\hat{R}}}\vec{R}\Big)$. The claim thus follows from the first result.

For the third claim, notice that

$$\begin{aligned}\min_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a)\cdot\big\|\vec{R}-\vec{\hat{R}}\big\| &\leq \min_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a)\cdot\big\|\vec{R}-\vec{\hat{R}}\big\|_1\\ &= \min_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a)\cdot\sum_{(s,a)\in\mathcal{S}\times\mathcal{A}}\big|R(s,a)-\hat{R}(s,a)\big|\\ &\leq \sum_{(s,a)\in\mathcal{S}\times\mathcal{A}} D(s,a)\cdot\big|R(s,a)-\hat{R}(s,a)\big|\\ &= d^D(R,\hat{R}).\end{aligned}$$

So the first result implies the third. $\square$

Remark D.12. As one can easily see geometrically, but also prove directly, there is the following equality of sets for a reward function R

$$\Big\{\operatorname{proj}_{\vec{\hat{R}}}\vec{R}\ \Big|\ \hat{R}\in\mathcal{R}\Big\} = \Big\{\frac{1}{2}\vec{R} + \frac{1}{2}\|\vec{R}\|v\ \Big|\ v\in\mathbb{R}^{\mathcal{S}\times\mathcal{A}},\ \|v\| = 1\Big\}.$$

In other words, the projections form a sphere of radius $\frac{1}{2}\|\vec{R}\|$ around the midpoint $\frac{1}{2}\vec{R}$.

We now show that the regret bound is tight:

Example D.13. *Let $U \in [0,1]$ and $\gamma \in [0,1)$ be arbitrary. Then there exists an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$ together with a reward function $\hat{R}$ with $\vec{R} \cdot \vec{\hat{R}} \geq 0$ and a policy $\hat{\pi} \in \Pi^*(\hat{R})$ such that*

$$U = \mathrm{Reg}^R(\hat{\pi}) = \frac{\sqrt{2}}{(1-\gamma) \cdot \big(\max J^R - \min J^R\big)} \cdot \Big\| \vec{R} - \mathrm{proj}_{\vec{\hat{R}}} \vec{R} \Big\|.$$

Furthermore, there exists a data distribution $D \in \Delta(\mathcal{S} \times \mathcal{A})$ such that

$$\mathrm{Reg}^R(\hat{\pi}) = \frac{1}{(1-\gamma) \cdot \big(\max J^R - \min J^R\big) \cdot \min_{(s,a) \in \mathcal{S} \times \mathcal{A}} D(s,a)} \cdot d^D\big(R, \hat{R}\big).$$

Proof. If $U = 0$ then $\hat{R} = R$ always works. If $U > 0$, then set $\mathcal{S} = \{\star\}$ and $\mathcal{A} = \{a, b, c\}$. This determines τ and μ_0. Define $R(x) \coloneqq R(\star, x, \star)$ for any action $x \in \mathcal{A}$. Let $R(a) > R(b)$ be arbitrary and set

$$R(c) \coloneqq R(a) - \frac{R(a) - R(b)}{U} \leq R(b).$$

Define

$$\hat{R}(a) \coloneqq \hat{R}(b) \coloneqq \frac{R(a) + R(b)}{2}, \quad \hat{R}(c) \coloneqq R(c).$$

For a policy π, define $\pi(x) \coloneqq \pi(x \mid \star)$ for any action $x \in \mathcal{A}$ and set the policy $\hat{\pi}$ by $\hat{\pi}(b) = 1$.

We obtain:

$$\begin{aligned}
\|\vec{R} - \vec{\hat{R}}\| &= \sqrt{\big(R(a) - \hat{R}(a)\big)^2 + \big(R(b) - \hat{R}(b)\big)^2 + \big(R(c) - \hat{R}(c)\big)^2} \\
&= \frac{1}{2} \cdot \sqrt{\big(R(a) - R(b)\big)^2 + \big(R(b) - R(a)\big)^2} \\
&= \frac{1}{\sqrt{2}} \cdot \big(R(a) - R(b)\big) \\
&= U \cdot \frac{R(a) - R(c)}{\sqrt{2}} \\
&= U \cdot \frac{\max R - \min R}{\sqrt{2}} \\
&= U \cdot \frac{(1-\gamma) \cdot \big(\max J^R - \min J^R\big)}{\sqrt{2}}.
\end{aligned}$$

Furthermore, we have

$$\begin{aligned}
\mathrm{Reg}^R(\hat{\pi}) &= \frac{\frac{1}{1-\gamma} \cdot R(a) - \frac{1}{1-\gamma} \cdot R(b)}{\frac{1}{1-\gamma} \cdot R(a) - \frac{1}{1-\gamma} \cdot R(c)} \\
&= U.
\end{aligned}$$

This shows

$$U = \mathrm{Reg}^R(\hat{\pi}) = \frac{\sqrt{2}}{(1-\gamma) \cdot \big(\max J^R - \min J^R\big)} \cdot \|\vec{R} - \vec{\hat{R}}\|.$$

We are done if we can show that $\mathrm{proj}_{\vec{\hat{R}}} \vec{R} = \vec{\hat{R}}$. This is equivalent to

$$\vec{\hat{R}} \cdot \vec{R} = \|\vec{\hat{R}}\|^2,$$

which is in turn equivalent to

$$\vec{\hat{R}} \cdot \Big[\vec{R} - \vec{\hat{R}}\Big] = 0.$$

This can easily be verified.

Finally, for the claim about the data distribution, simply set $D(a) = D(b) = D(c) = \frac{1}{3}$. Then one can easily show that

$$\sqrt{2} \cdot \|\vec{R} - \vec{\hat{R}}\| = R(a) - R(b) = \frac{d^D(R, \hat{R})}{\min_{(s,a) \in \mathcal{S} \times \mathcal{A}} D(s,a)}.$$

That shows the result. $\square$

D.3 SAFE OPTIMIZATION VIA APPROXIMATED CHOICE PROBABILITIES

In this section, we will show that for any chosen upper regret bound U, there is an $\epsilon > 0$ s.t. if the choice probabilities of $\hat{R}$ are ϵ-close to those of R, the regret of an optimal policy for $\hat{R}$ is bounded by U.

Assume a finite time horizon T. Trajectories are then given by $\xi = s_0, a_0, s_1, \dots, a_{T-1}, s_T$. Let Ξ be the set of all trajectories of length T. Let $D \in \Delta(\Xi)$ be a distribution. Assume that the human has a true reward function R and makes choices in trajectory comparisons given by

$$P_R\big(1 \mid \xi_1, \xi_2\big) = \frac{\exp\big(G(\xi_1)\big)}{\exp\big(G(\xi_1)\big) + \exp\big(G(\xi_2)\big)}. \tag{105}$$

Here, the return function G is given by

$$G(\xi) = \sum_{t=0}^{T-1} \gamma^t R(s_t, a_t, s_{t+1}).$$

We can then define the choice distance of proxy reward $\hat{R}$ to true reward R as

$$d^D_{\mathrm{KL}}(R, \hat{R}) \coloneqq \mathbb{E}_{\xi_1,\xi_2 \sim D \times D}\left[D_{\mathrm{KL}}\Big(P_R\big(\cdot \mid \xi_1, \xi_2\big) \;\|\; P_{\hat{R}}\big(\cdot \mid \xi_1, \xi_2\big)\Big)\right]$$

Here, $D_{\mathrm{KL}}\Big(P_R\big(\cdot \mid \xi_1, \xi_2\big) \;\|\; P_{\hat{R}}\big(\cdot \mid \xi_1, \xi_2\big)\Big)$ is the Kullback-Leibler divergence of two binary distributions over values $1, 2$. Explicitly, for $P \coloneqq P_R\big(\cdot \mid \xi_1, \xi_2\big)$ and similarly $\hat{P}$, we have

$$\begin{aligned} D_{\mathrm{KL}}\big(P \,\|\, \hat{P}\big) &= P(1) \log \frac{P(1)}{\hat{P}(1)} + \big(1 - P(1)\big) \log \frac{1 - P(1)}{1 - \hat{P}(1)} \\ &= -\Big[P(1) \log \hat{P}(1) + \big(1 - P(1)\big) \log\big(1 - \hat{P}(1)\big)\Big] - H\big(P(1)\big). \end{aligned} \tag{106}$$

Here, $H(p) \coloneqq -\big[p \log p + (1-p) \log(1-p)\big]$ is the binary entropy function.

Fix in this whole section the true reward function R with $\max J^R \neq \min J^R$ in a fixed MDP.

The goal of this section is to prove the following proposition:

Proposition D.14. *Let $U \in (0, 1]$. Then there exists an $\epsilon > 0$ such that for all $\hat{R}$ with*

$$d^D_{\mathrm{KL}}(R, \hat{R}) < \epsilon$$

and all $\hat{\pi} \in \Pi^*(\hat{R})$ we have $\mathrm{Reg}^R(\hat{\pi}) < U$.

We prove this by chaining together four lemmas. The first of the four lemmas needs its own lemma, so we end up with five lemmas overall:

Lemma D.15. *Assume $R, \hat{R}$ are two reward functions and π a policy. Then*

$$\big|J^R(\pi) - J^{\hat{R}}(\pi)\big| \leq \max_{\xi \in \Xi} \big|G(\xi) - \hat{G}(\xi)\big|.$$

Proof. We have

$$\begin{aligned} \big|J^R(\pi) - J^{\hat{R}}(\pi)\big| &= \big|\widetilde{D}^\pi \cdot \big(G - \hat{G}\big)\big| \\ &= \left|\sum_{\xi \in \Xi} \widetilde{D}^\pi(\xi) \cdot \big(G(\xi) - \hat{G}(\xi)\big)\right| \\ &\leq \sum_{\xi \in \Xi} \widetilde{D}^\pi(\xi) \cdot \big|G(\xi) - \hat{G}(\xi)\big| \\ &\leq \max_{\xi \in \Xi} \big|G(\xi) - \hat{G}(\xi)\big| \cdot \sum_{\xi \in \Xi} \widetilde{D}^\pi(\xi) \\ &= \max_{\xi \in \Xi} \big|G(\xi) - \hat{G}(\xi)\big| \end{aligned}$$

In the last step, we used that distributions sum to one. □

Lemma D.16. *Let $U \in (0,1]$. Then there exists $\sigma(U) > 0$ such that for all $\hat{R}$ and $\hat{\pi} \in \Pi^*(\hat{R})$ for which there exists $c \in \mathbb{R}$ such that $\max_{\xi \in \Xi} \left|\hat{G}(\xi) - G(\xi) - c\right| < \sigma(U)$, we have $\mathrm{Reg}^R(\hat{\pi}) < U$.*

Concretely, we can set $\sigma(U) := \frac{\max J^R - \min J^R}{2} \cdot U$.

Proof. Set $\sigma(U)$ as stated and let $\hat{R}$, $\hat{\pi}$ and c have the stated properties. The regret bound we want to show is equivalent to the following statement:

$$J^R(\hat{\pi}) > \max J^R - \big(\max J^R - \min J^R\big) \cdot U = \max J^R - 2\sigma(U). \tag{107}$$

Let $\tilde{c}$ be the constant such that $\hat{G} - c$ is the return function of $\hat{R} - \tilde{c}$. Concretely, one can set $\tilde{c} = \frac{1-\gamma}{1-\gamma^{T+1}} \cdot c$. Lemma D.15 ensures that

$$J^R(\hat{\pi}) > J^{\hat{R}-\tilde{c}}(\hat{\pi}) - \sigma(U). \tag{108}$$

Now, let π be an optimal policy for R. Again, Lemma D.15 ensures

$$\max J^R = J^R(\pi) < J^{\hat{R}-\tilde{c}}(\pi) + \sigma(U) \leq J^{\hat{R}-\tilde{c}}(\hat{\pi}) + \sigma(U). \tag{109}$$

In the last step, we used that $\hat{\pi}$ is optimal for $\hat{R}$ and thus also $\hat{R} - \tilde{c}$. Combining Equations (108) and (109), we obtain the result, Equation (107). $\square$

Lemma D.17. *For $q \in (0,1)$, define $g_q : (-q, 1-q) \to \mathbb{R}$ by*

$$g_q(x) := \log \frac{q+x}{1-(q+x)}.$$

Then for all $\sigma > 0$ there exists $\delta(q,\sigma) > 0$ such that for all $x \in (-q, 1-q)$ with $|x| < \delta(q,\sigma)$, we have $|g_q(x) - g_q(0)| < \sigma$.

Concretely, one can choose

$$\delta(q,\sigma) := \big(\exp(\sigma) - 1\big) \cdot \min\left\{ \frac{1}{\frac{1}{q} + \frac{\exp(\sigma)}{1-q}}, \ \frac{1}{\frac{1}{1-q} + \frac{\exp(\sigma)}{q}} \right\}$$

Proof. If one does not care about the precise quantification, then the result is simply a reformulation of the continuity of g_q at the point $x_0 = 0$.

Now we show more specifically that $\delta(q,\sigma)$, as defined above, has the desired property. Namely, notice the following sequence of equivalences (followed by a one-sided implication) that holds whenever $x \geq 0$:

$$\begin{aligned}
\big|g_q(x) - g_q(0)\big| < \sigma \quad &\Longleftrightarrow \quad \log \frac{(q+x)\cdot(1-q)}{\big(1-(q+x)\big)\cdot q} < \sigma \\
&\Longleftrightarrow \quad \frac{(q+x)\cdot(1-q)}{\big(1-(q+x)\big)\cdot q} < \exp(\sigma) \\
&\Longleftrightarrow \quad (q+x) < (1-q-x) \cdot \frac{q}{1-q} \cdot \exp(\sigma) \\
&\Longleftrightarrow \quad \left(1 + \frac{q}{1-q} \cdot \exp(\sigma)\right) \cdot x < q \cdot \big(\exp(\sigma) - 1\big) \\
&\Longleftrightarrow \quad x < \frac{\exp(\sigma) - 1}{\frac{1}{q} + \frac{\exp(\sigma)}{1-q}} \\
&\Longleftarrow \quad |x| < \delta(q,\sigma).
\end{aligned}$$

In the first step, we used the monotonicity of g_q to get rid of the absolute value. Similarly, whenever $x \leq 0$, we have

$$\begin{aligned}
\big|g_q(x) - g_q(0)\big| < \sigma \quad &\Longleftrightarrow \quad x > \frac{1 - \exp(\sigma)}{\frac{1}{1-q} + \frac{\exp(\sigma)}{q}} \\
&\Longleftarrow \quad |x| < \delta(q,\sigma).
\end{aligned}$$

This shows the result. $\square$

Lemma D.18. *For $q \in (0,1)$, define $f_q : (0,1) \to \mathbb{R}$ by*

$$f_q(p) \coloneqq -\big[q \log p + (1-q)\log(1-p)\big].$$

Then for all $\delta > 0$ there exists $\mu(\delta) > 0$ such that for all $p \in (0,1)$ with $f_q(p) < H(q) + \mu(\delta)$, we have $|p-q| < \delta$. Concretely, one can choose $\mu(\delta) \coloneqq 2\delta^2$.

Proof. Let $\delta > 0$ and define $\mu(\delta) \coloneqq 2\delta^2$. Assume that $f_q(p) < H(q) + \mu(\delta)$. By Pinker's inequality, we have

$$\begin{aligned}
2(p-q)^2 &\leq q \log \frac{q}{p} + (1-q) \cdot \log \frac{1-q}{1-p} \\
&= -H(q) + f_q(p) \\
&< \mu(\delta) \\
&= 2\delta^2.
\end{aligned}$$

Consequently, we have $|p-q| < \delta$. □

Lemma D.19. *Define $f_q(p)$ as in Lemma D.18. Then for all $\mu > 0$ there exists $\epsilon(\mu) > 0$ such that for all $\hat{R}$ with $d^D_{\mathrm{KL}}(R, \hat{R}) < \epsilon(\mu)$, we have the following for all $\xi_1, \xi_2 \in \Xi$:*

$$f_{P_R(1 \mid \xi_1, \xi_2)}\big(P_{\hat{R}}(1 \mid \xi_1, \xi_2)\big) < H\big(P_R(1 \mid \xi_1, \xi_2)\big) + \mu.$$

Concretely, we can set $\epsilon(\mu) \coloneqq \mu \cdot \min_{\xi_1, \xi_2 \in \Xi} D(\xi_1) \cdot D(\xi_2)$

Proof. We have the following for all $\xi_1, \xi_2 \in \Xi$:

$$\begin{aligned}
\mu \cdot \min_{\xi, \xi'} D(\xi) \cdot D(\xi) &= \epsilon(\mu) \\
&> d^D_{\mathrm{KL}}(R, \hat{R}) \\
&= \mathbb{E}_{\xi, \xi' \sim D \times D}\Big[D_{\mathrm{KL}}\Big(P_R(\cdot \mid \xi, \xi') \,\big\|\, P_{\hat{R}}(\cdot \mid \xi, \xi')\Big)\Big] \\
&\geq \Big(\min_{\xi, \xi'} D(\xi) \cdot D(\xi')\Big) \cdot D_{\mathrm{KL}}\Big(P_R(\cdot \mid \xi_1, \xi_2) \,\big\|\, P_{\hat{R}}(\cdot \mid \xi_1, \xi_2)\Big)
\end{aligned}$$

Now, Equation (106) shows that

$$D_{\mathrm{KL}}\Big(P_R(\cdot \mid \xi_1, \xi_2) \,\big\|\, P_{\hat{R}}(\cdot \mid \xi_1, \xi_2)\Big) = f_{P_R(1 \mid \xi_1, \xi_2)}\big(P_{\hat{R}}(1 \mid \xi_1, \xi_2)\big) - H\big(P_R(1 \mid \xi_1, \xi_2)\big).$$

The result follows. □

Corollary D.20. *Let $\sigma > 0$. Then there exists $\epsilon \coloneqq \epsilon(\sigma) > 0$ such that $d^D_{\mathrm{KL}}(R, \hat{R}) < \epsilon$ implies that there exists $c \in \mathbb{R}$ such that $\big\|G - (\hat{G} - c)\big\|_\infty < \sigma$.*

Proof. Set

$$\delta \coloneqq \min_{\xi_1, \xi_2 \in \Xi \times \Xi} \delta\Big(P_R(1 \mid \xi_1, \xi_2), \sigma\Big),\ \mu \coloneqq \mu(\delta),\ \epsilon \coloneqq \epsilon(\mu),$$

with the constants satisfying the properties from Lemmas D.17, D.18, and D.19. Now, let $\hat{R}$ be such that $d^D_{\mathrm{KL}}(R, \hat{R}) < \epsilon$.

First of all, Lemma D.19 ensures that

$$f_{P_R(1 \mid \xi_1, \xi_2)}\big(P_{\hat{R}}(1 \mid \xi_1, \xi_2)\big) < H\big(P_R(1 \mid \xi_1, \xi_2)\big) + \mu$$

for all $\xi_1, \xi_2 \in \Xi$. Then Lemma D.18 shows that

$$\big|P_{\hat{R}}(1 \mid \xi_1, \xi_2) - P_R(1 \mid \xi_1, \xi_2)\big| < \delta$$

for all $\xi_1, \xi_2 \in \Xi$. From Lemma D.17, we obtain that

$$\left| g_{P_R(1 \mid \xi_1, \xi_2)}\Big(P_{\hat{R}}\big(1 \mid \xi_1, \xi_2\big) - P_R\big(1 \mid \xi_1, \xi_2\big)\Big) - g_{P_R(1 \mid \xi_1, \xi_2)}(0) \right| < \sigma \tag{110}$$

for all $\xi_1, \xi_2 \in \Xi$. Now, note that

$$g_{P_R(1|\xi_1,\xi_2)}\Big(P_{\hat{R}}\big(1 \mid \xi_1, \xi_2\big) - P_R\big(1 \mid \xi_1, \xi_2\big)\Big) = g_{P_{\hat{R}}(1|\xi_1,\xi_2)}(0).$$

Furthermore, for $R' \in \{R, \hat{R}\}$, Equation (105) leads to the following computation:

$$\begin{aligned} g_{P_{R'}(1|\xi_1,\xi_2)}(0) &= \log \frac{P_{R'}(1 \mid \xi_1, \xi_2)}{P_{R'}(2 \mid \xi_1, \xi_2)} \\ &= \log \frac{\exp\big(G'(\xi_1)\big)}{\exp\big(G'(\xi_2)\big)} \\ &= G'(\xi_1) - G'(\xi_2). \end{aligned}$$

Therefore, Equation (110) results in

$$\Big|\big(\hat{G}(\xi_1) - G(\xi_1)\big) - \big(\hat{G}(\xi_2) - G(\xi_2)\big)\Big| = \Big|\big(\hat{G}(\xi_1) - \hat{G}(\xi_2)\big) - \big(G(\xi_1) - G(\xi_2)\big)\Big| < \sigma$$

for all $\xi_1, \xi_2 \in \Xi$. Now, let $\xi^* \in \Xi$ be any reference trajectory. Define $c := \hat{G}(\xi^*) - G(\xi^*)$. Then the preceding equation shows that

$$\big|\hat{G}(\xi) - G(\xi) - c\big| < \sigma$$

for all $\xi \in \Xi$. That shows the claim. □

Proof of Proposition D.14. We prove Proposition D.14 by chaining together the constants from the preceding results. We have $U \in (0, 1]$ given. Then, set $\sigma := \sigma(U)$ and $\epsilon := \epsilon(\sigma)$ as in Lemma D.16 and Corollary D.20. Now, let $\hat{R}$ be such that $d^D_{\mathrm{KL}}(R, \hat{R}) < \epsilon$ and let $\hat{\pi} \in \Pi^*(\hat{R})$. Our goal is to show that $\mathrm{Reg}^R(\hat{\pi}) < U$.

By Corollary D.20, there is $c > 0$ such that $\max_{\xi \in \Xi} \big|\hat{G}(\xi) - G(\xi) - c\big| < \sigma$. Consequently, Lemma D.16 ensures that $\mathrm{Reg}^R(\hat{\pi}) < U$. This was to show. □

D.4 POSITIVE RESULT FOR REGULARIZED RLHF

Here, we present simple positive results for regularized RLHF, both in a version with the expected reward distance, and in a version using the distance in choice probabilities. Some of it will directly draw from the positive results proved before.

Theorem D.21. *Let $\lambda \in (0, \infty)$ be given and fixed. Assume we are given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, and a data distribution $D \in \mathcal{S} \times \mathcal{A}$ which assigns positive probability to all transitions, i.e., $\forall (s, a) \in \mathcal{S} \times \mathcal{A},\ D(s, a) > 0$. Let $\omega : \Pi \to \mathbb{R}$ be a continuous regularization function that has a reference policy π_{ref} as one of its minima.*[4] *Assume that π_{ref} is* not *(λ, ω)-optimal for R and let $L = \mathrm{Reg}^R(\pi_{\mathrm{ref}})$. Then there exists $\epsilon > 0$ such that $D \in \mathbf{safe}(R, \epsilon, L, \lambda, \omega)$.*

Proof. We prove the theorem by showing that for every $D \in \Delta(\mathcal{S} \times \mathcal{A})$ such that $D(s, a) > 0$ for all $(s, a) \in \mathcal{S} \times \mathcal{A}$, there exists $\epsilon > 0$ such that for all $\hat{R}$ with $\mathbb{E}_{(s,a)\sim D}\left[\frac{|\hat{R}(s,a) - R(s,a)|}{\mathrm{range}\ R}\right] < \epsilon$ and all policies $\hat{\pi}$ that are (λ, ω)-RLHF optimal wrt. $\hat{R}$, we have $\mathrm{Reg}^R(\hat{\pi}) < \mathrm{Reg}^R(\pi_{\mathrm{ref}})$. Because $L = \mathrm{Reg}^R(\hat{\pi}) < \mathrm{Reg}^R(\pi_{\mathrm{ref}})$ this proves that then $D \in \mathbf{safe}(R, \epsilon, L, \lambda, \omega)$.

The proof is an application of Berge's maximum Theorem, Theorem D.3. Namely, define the function

$$f : \mathcal{R} \times \Pi \to \mathbb{R}, \quad f(R, \pi) := J_R(\pi) - \lambda\omega(\pi).$$

Furthermore, define the correspondence $C : \mathcal{R} \rightrightarrows \Pi$ as the trivial map $C(R) = \Pi$. Let $f^* : \mathcal{R} \to \mathbb{R}$ map a reward function to the value of a (λ, ω)-RLHF optimal policy, i.e., $f^*(R) := \max_{\pi \in \Pi} f(R, \pi)$. Define C^* as the corresponding argmax, i.e., $C^*(R) := \big\{\pi \mid f(R, \pi) = f^*(R)\big\}$. Assume on $\mathcal{R}$ we have the standard Euclidean topology. Since ω is assumed continuous and by Proposition D.4

[4] E.g., if $\pi_{\mathrm{ref}}(a \mid s) > 0$ for all $(s, a) \in \mathcal{S} \times \mathcal{A}$ and $\omega(\pi) := \mathbb{D}_{\mathrm{KL}}(\pi || \pi_{\mathrm{ref}})$, then the minimum is given by π_{ref}.

also J is continuous, it follows that f is continuous. Thus, Theorem D.3 implies that C^* is upper hemicontinuous, see Definition D.2. The rest of the proof is simply an elaboration of why upper hemicontinuity of C^* gives the result.

Now, define the set

$$\mathcal{V} := \left\{ \pi' \in \Pi \mid \mathrm{Reg}^R(\pi') < \mathrm{Reg}^R(\pi_{\mathrm{ref}}) \right\}.$$

Since the regret is a continuous function, this set is open. Now, let $\pi \in C^*(R)$ be (λ, ω)-RLHF optimal with respect to R. It follows

$$\begin{aligned} J_R(\pi) &= f(R, \pi) + \lambda\omega(\pi) \\ &> f(R, \pi_{\mathrm{ref}}) + \lambda\omega(\pi_{\mathrm{ref}}) \\ &= J_R(\pi_{\mathrm{ref}}), \end{aligned}$$

where we used the optimality of π for f, that π_{ref} is not optimal for it, and that π_{ref} is the minimum of ω. So overall, this shows $C^*(R) \subseteq \mathcal{V}$.

Since C^* is upper hemicontinuous, this means there exists an open set $\mathcal{U} \subseteq \mathcal{R}$ with $R \in \mathcal{U}$ and such that for all $\hat{R} \in \mathcal{U}$, we have $C^*(\hat{R}) \subseteq \mathcal{V}$. Let $\epsilon > 0$ be so small that all reward functions $\hat{R}$ with $\mathbb{E}_{(s,a)\sim D}\left[\frac{|\hat{R}(s,a) - R(s,a)|}{\mathrm{range}\ R}\right] < \epsilon$ satisfy $\hat{R} \in \mathcal{U}$ — which exists since $\mathcal{U}$ is open in the Euclidean topology. Then for all such $\hat{R}$ and any policy $\hat{\pi}$ that is (λ, ω)-RLHF optimal wrt. $\hat{R}$, we by definition have

$$\hat{\pi} \in C^*(\hat{R}) \subseteq \mathcal{V},$$

and thus, by definition of $\mathcal{V}$, the desired regret property. This was to show. $\square$

Now, we show the same result, but with the choice distance instead of expected reward distance:

Theorem D.22. *Let $\lambda \in (0, \infty)$ be given and fixed. Assume we are given an MDP $\langle \mathcal{S}, \mathcal{A}, \tau, \mu_0, R, \gamma \rangle$, and a data distribution $D \in \mathcal{S}\times\mathcal{A}$ which assigns positive probability to all transitions, i.e., $\forall (s,a) \in \mathcal{S}\times\mathcal{A},\ D(s,a) > 0$. Let $\omega : \Pi \to \mathbb{R}$ be a continuous regularization function that has a reference policy π_{ref} as one of its minima. Assume that π_{ref} is* not *(λ, ω)-optimal for R and let $L = \mathrm{Reg}^R(\pi_{\mathrm{ref}})$. Then there exists $\epsilon > 0$ such that $D \in \mathbf{safe}^{\mathbb{D}_{KL}}(R, \epsilon, L, \lambda, \omega)$.*

Proof. Let $\mathcal{G} := \mathbb{R}^{\Xi}$ be the vector space of return functions, which becomes a topological space when equipped with the infinity norm. Define the function

$$f : \mathcal{G} \times \Pi \to \mathbb{R}, \quad f(G, \pi) := J^G(\pi) - \lambda\omega(\pi),$$

where $J^G(\pi) := \mathbb{E}_{\xi\sim\pi}[G(\xi)]$ is the policy evaluation function of the return function G. f is continuous. Define the correspondence $C : \mathcal{G} \rightrightarrows \Pi$ as the trivial map $C(G) = \Pi$. Let $f^* : \mathcal{G} \to \mathbb{R}$ map a return function to the value of a (λ, ω)-optimal policy, i.e., $f^*(G) := \max_{\pi\in\Pi} f(G, \pi)$. Define C^* as the corresponding argmax. Then Theorem D.3 implies that C^* is upper hemicontinuous, see Definition D.2. As in the previous proof, the rest is an elaboration of why this gives the desired result.

Set G as the return function corresponding to R. Define

$$\mathcal{V} := \left\{ \pi' \in \Pi \mid \mathrm{Reg}^R(\pi') < L \right\}.$$

We now claim that $C^*(G) \subseteq \mathcal{V}$. Indeed, let $\pi \in C^*(G)$. Then

$$\begin{aligned} J^R(\pi) &= f(G, \pi) + \lambda\omega(\pi) \\ &> f(G, \pi_{\mathrm{ref}}) + \lambda\omega(\pi_{\mathrm{ref}}) \\ &= J^R(\pi_{\mathrm{ref}}). \end{aligned}$$

Note that we used the optimality of π for f, that π_{ref} is not optimal for it, and also that π_{ref} minimizes ω by assumption. This shows $\mathrm{Reg}^R(\pi) < \mathrm{Reg}^R(\pi_{\mathrm{ref}}) = L$, and thus the claim.

Since C^* is upper hemicontinuous and $\mathcal{V}$ an open set, this implies that there exists $\sigma > 0$ such that for all $\hat{G} \in \mathcal{G}$ with $\left\|G - \hat{G}\right\|_\infty < \sigma$, we have $C^*(\hat{G}) \subseteq \mathcal{V}$.

Now, define $\epsilon := \epsilon(\sigma)$ as in Corollary D.20 and let $\hat{R}$ be any reward function with $d^D_{\mathrm{KL}}(R, \hat{R}) < \epsilon$. Then by that corollary, there exists $c \in \mathbb{R}$ such that $\left\|G - \left(\hat{G} - c\right)\right\|_\infty < \sigma$. Consequently, we have $C^*(\hat{G}) = C^*(\hat{G} - c) \subseteq \mathcal{V}$ by what we showed before, which shows the result. $\square$