Regret Bounds for Information-Directed Reinforcement Learning

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Abstract

Information-directed sampling (IDS) has revealed its potential as a data-efficient algorithm [Lu et al., 2021] for reinforcement learning (RL). However, theoretical understanding of IDS for Markov Decision Processes (MDPs) is still limited. We develop novel information-theoretic tools to bound the information ratio and cumulative information gain about the learning target. Our theoretical results shed light on the importance of choosing the learning target such that the practitioners can balance the computation and regret bounds. As a consequence, we derive prior-free Bayesian regret bounds for `vanilla-IDS` which learns the whole environment under tabular finite-horizon MDPs. In addition, we propose a computationally-efficient `regularized-IDS` that maximizes an additive form rather than the ratio form and show that it enjoys the same regret bound as `vanilla-IDS`. With the aid of rate-distortion theory, we improve the regret bound by learning a surrogate, less informative environment. Furthermore, we extend our analysis to linear MDPs and prove similar regret bounds for Thompson sampling as a by-product.

1 Introduction

Information-directed sampling (IDS) is a *design principle* proposed by [Russo and Van Roy, 2014, 2018] that optimizes the trade-off between *information* and *regret*. Comparing with other design principles such as UCB and Thompson sampling (TS), IDS can automatically adapt to different information-regret structures. As a result, IDS demonstrates impressive empirical performance [Russo and Van Roy, 2018] and outperforms UCB and TS in terms of asymptotic optimality [Kirschner et al., 2021] and minimax optimality in heteroscedastic bandits [Kirschner and Krause, 2018] and sparse linear bandits [Hao et al., 2021].

In the context of full RL, mutiple works have examined the empirical performance of IDS [Nikolov et al., 2018, Lu et al., 2021]. However, formal regret guarantee for IDS is still lacking. IDS minimizes a notion of *information ratio* that is the ratio of per-episode regret and information gain about the learning target. While different choices of the learning target could lead to different regret bounds and computational methods, the most natural choice is the whole environment and we name the corresponding IDS as `vanilla-IDS`.

In this work, we prove the first prior-free $\widetilde{O}(\sqrt{S^3A^2H^4L})$ Bayesian regret bound for `vanilla-IDS`, where S is the size of state space, A is the size of action space, H is the length of episodes and L is the number of episodes. Computationally, `vanilla-IDS` needs to optimize over the full policy space, which is not efficient in general. To facilitate the computation, we consider its regularized form,

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named `regularized-IDS`, that can be solved by any dynamic programming solver. By carefully choosing the tunable parameter, we prove that `regularized-IDS` enjoys the same regret bound as `vanilla-IDS`.

Although learning the whole environment offers certain computational advantages, the agent could take too much information to learn the whole environment exactly. A key observation is that different states may correspond to the same value function which eventually determines the behavior of the optimal policy. Through the rate-distortion theory, we construct a surrogate environment that is less informative to learn but enough to identify the optimal policy. As a result, we propose `surrogate-IDS` that takes the surrogate environment as the learning target and prove a sharper $\widetilde{O}(\sqrt{S^2A^2H^4L})$ bound for tabular MDPs.

In the end, we extend our analysis to linear MDPs where we *must* learn a surrogate environment due to potentially infinitely many states and derive a $\widetilde{O}(dH^2\sqrt{T})$ Bayesian regret bound that matches the existing minimax lower bound up to a factor of H. As a by-product of our analysis, we also prove prior-free Bayesian regret bounds for TS under tabular and linear MDPs.

Related work. In general, there are two ways to prove Bayesian regret bounds. The first is to introduce confidence sets such that the Bayesian regret bounds of TS can match the best possible frequentist regret bounds by UCB [Russo and Van Roy, 2014] and has been extended to RL by Osband et al. [2013], Osband and Van Roy [2014], Osband et al. [2019]. However, when the best possible bound for UCB is sub-optimal (for instance, sparse linear bandits [Hao et al., 2021]), this technique yields a sub-optimal Bayesian regret bound. In addition, this technique can only be used to analyze TS but not IDS.

The second is to decompose the Bayesian regret into an *information ratio* term and a *cumulative information gain* term and bound them by tools from information theory [Russo and Van Roy, 2016]. This technique can be used to analyze both TS [Dong and Roy, 2018, Bubeck and Sellke, 2020] and IDS in bandits setting [Russo and Van Roy, 2014, Liu et al., 2018, Kirschner et al., 2020b, Hao et al., 2021, 2022], partial monitoring [Lattimore and Szepesvári, 2019, Kirschner et al., 2020a, Lattimore and Gyorgy, 2021] but not in RL as far as we know. One exception is Lu and Van Roy [2019], Lu [2020] who bounded the information ratio for a specific Dirichlet prior with additional assumptions.

Frequentist regret bounds in episodic RL have received considerable attention recently. For tabular MDPs, several representative works include UCBVI [Azar et al., 2017], optimistic Q-learning [Jin et al., 2018], RLSVI [Russo, 2019], UCB-Advantage [Zhang et al., 2020], UCB-MQ [Ménard et al., 2021]. While our regret bounds are not state of the art, the primary goal of this paper is to broaden the set of efficient RL design principles known to satisfy $\sqrt{T}$ regret bounds.

For linear or linear mixture MDPs, several representative works include LSVI-UCB [Jin et al., 2020], OPPO [Cai et al., 2020], UCRL-VTR [Ayoub et al., 2020, Zhou et al., 2021], RLSVI [Zanette et al., 2020]. Notably, Zhang [2021], Dann et al. [2021] derived minimax regret bounds for a variant of TS. Beyond linear cases, several works consider general function approximation based on Bellman rank [Jiang et al., 2017], eluder dimension [Wang et al., 2020], Bellman-eluder dimension [Jin et al., 2021] and bilinear class [Du et al., 2021].

It is worth mentioning the recent impressive work by Foster et al. [2021] who proposed a general Estimation-to-Decisions (E2D) design principle. Although motivated by different design principles, E2D shares the similar form as `regularized-IDS`. On one hand, Foster et al. [2021] mainly focuses on statistical complexity, while we offer a specific computationally-efficient algorithm thanks to the chain rule of mutual information and independent priors. On the other hand, while E2D tends to learn the whole environment, our theory in Section 4 suggests learning a surrogate environment could yield better regret bounds.

2 Preliminary

Finite-horizon MDPs The environment is characterized by a finite-horizon time-inhomogeneous MDP, which is a tuple $\mathcal{E} = (\mathcal{S}, \mathcal{A}, H, \{P_h\}_{h=1}^H, \{r_h\}_{h=1}^H)$, where $\mathcal{S}$ is the countable state space with $|\mathcal{S}| = S$, $\mathcal{A}$ is the finite action space with $|\mathcal{A}| = A$, H is the episode length, $P_h : \mathcal{S} \times \mathcal{A} \to \Delta_{\mathcal{S}}$ is the transition probability kernel and $r_h : \mathcal{S} \times \mathcal{A} \to [0, 1]$ is the reward function. For a finite set $\mathcal{S}$, let $\Delta_{\mathcal{S}}$ be the set of probability distributions over $\mathcal{S}$. We assume $\mathcal{S}$, $\mathcal{A}$, r_h are known and deterministic while the transition probability kernel is unknown and random. Throughout the paper, we may write P_h and r_h explicitly depend on $\mathcal{E}$ when necessary.

Let $\Theta_h = [0, 1]^{S \times A \times S}$ be the parameter space of P_h and $\Theta = \Theta_1 \times \cdots \times \Theta_H$ be the full parameter space. We assume ρ_h is the prior probability measure for P_h on Θ_h with Borel σ-algebra and $\rho = \rho_1 \otimes \cdots \otimes \rho_H$ as the product prior probability measure for the whole environment on Θ with Borel σ-algebra. This ensures the priors over different layers are independent and the prior is assumed to be known to the learner.

Interaction protocol An agent interacts with a finite-horizon MDP as follows. The initial state s_1^ℓ is assumed to be fixed over episodes. In each episode $\ell \in [L]$ and each layer $h \in [H]$, the agent observes a state s_h^ℓ, takes an action a_h^ℓ, and receives a reward r_h^ℓ. Then, the environment evolves to a random next state s_{h+1}^ℓ according to distribution $P_h(\cdot|s_h^\ell, a_h^\ell)$. The episode terminates when s_{H+1} is reached and is reset to the initial state.

Denote $\mathcal{H}_{\ell,h}$ as the history of episode ℓ up to layer h, e.g., $\mathcal{H}_{\ell,h} = (s_1^\ell, a_1^\ell, r_1^\ell, \ldots, s_h^\ell, a_h^\ell, r_h^\ell)$ and the set of such possible history is $\Omega_h = \prod_{i=1}^h (\mathcal{S} \times \mathcal{A} \times [0, 1])$. Let $\mathcal{D}_\ell = (\mathcal{H}_{1,H}, \ldots, \mathcal{H}_{\ell-1,H})$ as the entire history up to episode ℓ with $\mathcal{D}_1 = \emptyset$. A policy π is a collection of (possibly randomised) mappings $(\pi_1, \ldots, \pi_H)$ where each π_h maps an element from $\Omega_{h-1} \times \mathcal{S}$ to $\Delta(\mathcal{A})$ and Π is the whole policy class. A *stationary policy* chooses actions based on only the current state and current layer. The set of such policies is denoted by Π_{S} where we denote $\pi_h(a|s)$ as the probability that the agent chooses action a at state s and layer h.

Value function For each $h \in [H]$ and a policy π, the value function $V_{h,\pi}^{\mathcal{E}} : \mathcal{S} \to \mathbb{R}$ is defined as the expected value of cumulative rewards received under policy π when starting from an arbitrary state at hth layer; that is,

$$V_{h,\pi}^{\mathcal{E}}(s) := \mathbb{E}_\pi^{\mathcal{E}} \left[\sum_{h'=h}^{H} r_{h'}(s_{h'}, a_{h'}) \middle| s_h = s \right] ,$$

where $\mathbb{E}_\pi^{\mathcal{E}}$ denotes the expectation over the sample path generated under policy π and environment $\mathcal{E}$. We adapt the convention that $V_{H+1,\pi}^{\mathcal{E}}(\cdot) = 0$. There always exists an optimal policy π^* which gives the optimal value $V_{h,\pi^*}^{\mathcal{E}}(s) = \max_{\pi \in \Pi_{\mathrm{S}}} V_{h,\pi}^{\mathcal{E}}(s)$ for all $s \in \mathcal{S}$ and $h \in [H]$. Note that in the Bayesian setting, π^* is a function of $\mathcal{E}$ so it is also a random variable. In addition, we define the action-value function as follows:

$$Q_{h,\pi}^{\mathcal{E}}(s, a) := \mathbb{E}_\pi^{\mathcal{E}} \left[\sum_{h'=h}^{H} r_{h'}(s_{h'}, a_{h'}) \middle| s_h = s, a_h = a \right] ,$$

which satisfies the Bellman equation: $Q_{h,\pi}^{\mathcal{E}}(s, a) = r_h(s, a) + \mathbb{E}_{s' \sim P_h(\cdot|s,a)}[V_{h+1,\pi}^{\mathcal{E}}(s')]$. Furthermore, we denote the *state-action occupancy measure* as

$$d_{h,\pi}^{\mathcal{E}}(s, a) = \mathbb{P}_\pi^{\mathcal{E}}(s_h = s, a_h = a) ,$$

where we denote $\mathbb{P}_\pi^{\mathcal{E}}$ as the law of the sample path generated under policy π and environment $\mathcal{E}$.

Bayesian regret The agent interacts with the environment for L episodes and the total number of steps is $T = LH$. The expected cumulative regret of an algorithm $\pi = \{\pi^\ell\}_{\ell=1}^L$ with respect to an environment $\mathcal{E}$ is defined as

$$\mathfrak{R}_L(\mathcal{E}, \pi) = \mathbb{E} \left[\sum_{\ell=1}^{L} \left(V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell) - V_{1,\pi^\ell}^{\mathcal{E}}(s_1^\ell) \right) \right] ,$$

where the expectation is taken with respect to the randomness of π^ℓ. The Bayesian regret then is defined as

$$\mathfrak{BR}_L(\pi) = \mathbb{E}[\mathfrak{R}_L(\mathcal{E}, \pi)]\,,$$

where the expectation is taken with respect to the prior distribution of $\mathcal{E}$. At each episode, TS finds

$$\pi^\ell_{\text{TS}} = \operatorname*{argmax}_{\pi\in\Pi} V^{\mathcal{E}_\ell}_{1,\pi}(s^\ell_1)\,,$$

where $\mathcal{E}_\ell$ is a sample from the posterior distribution of $\mathcal{E}$, e.g., $\mathcal{E}_\ell \sim \mathbb{P}(\mathcal{E} \in \cdot|\mathcal{D}_\ell)$.

Notations We write $\mathbb{P}_\ell(\cdot) = \mathbb{P}(\cdot|\mathcal{D}_\ell)$, $\mathbb{E}_\ell[\cdot] = \mathbb{E}[\cdot|\mathcal{D}_\ell]$ and also define the conditional mutual information $\mathbb{I}_\ell(X;Y) = D_{\text{KL}}(\mathbb{P}((X,Y) \in \cdot|\mathcal{D}_\ell)||\mathbb{P}(X \in \cdot|\mathcal{D}_\ell) \otimes \mathbb{P}(Y \in \cdot|\mathcal{D}_\ell))$. For a random variable χ we define:

$$\mathbb{I}^\pi_\ell(\chi; \mathcal{H}_{\ell,h}) = D_{\text{KL}}(\mathbb{P}_{\ell,\pi}((\chi, \mathcal{H}_{\ell,h}) \in \cdot)||\mathbb{P}_{\ell,\pi}(\chi \in \cdot) \otimes \mathbb{P}_{\ell,\pi}(\mathcal{H}_{\ell,h} \in \cdot))\,,$$

where $\mathbb{P}_{\ell,\pi}$ is the law of χ and the history induced by policy π interacting with a sample from the posterior distribution of $\mathcal{E}$ given $\mathcal{D}_\ell$. We define $\bar{\mathcal{E}}_\ell$ as the mean MDP where for each state-action pair (s,a), $P^{\bar{\mathcal{E}}_\ell}_h(\cdot|s,a) = \mathbb{E}_\ell[P^{\mathcal{E}}_h(\cdot|s,a)]$ is the mean of posterior measure.

3 Learning the whole environment

The core design of IDS for RL relies on a notion of *information ratio*. The information ratio for a policy π at episode ℓ is defined as

$$\Gamma_\ell(\pi, \chi) := \frac{(\mathbb{E}_\ell[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi}(s^\ell_1)])^2}{\mathbb{I}^\pi_\ell(\chi; \mathcal{H}_{\ell,H})}\,, \tag{3.1}$$

where χ is the learning target to prioritize information sought by the agent. The choice of χ plays a crucial role in designing the IDS and could lead to different regret bounds and computational methods. We first consider the most natural choice of χ which is the whole environment $\mathcal{E}$.

3.1 Vanilla IDS

`Vanilla-IDS` takes the whole environment $\mathcal{E}$ as the learning target and at the beginning of each episode, the agent computes a stochastic policy:

$$\pi^\ell_{\text{IDS}} = \operatorname*{argmin}_{\pi\in\Pi} \left[\Gamma_\ell(\pi) := \frac{(\mathbb{E}_\ell[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi}(s^\ell_1)])^2}{\mathbb{I}^\pi_\ell(\mathcal{E}; \mathcal{H}_{\ell,H})}\right]\,. \tag{3.2}$$

Define the worst-case information ratio Γ^* such that $\Gamma_\ell(\pi^\ell_{\text{IDS}}) \le \Gamma^*$ for any $\ell \in [L]$ almost surely. The next theorem derives a generic regret bound for `vanilla-IDS` in terms of Γ^* and the mutual information between $\mathcal{E}$ and the history.

Theorem 3.1. *A generic regret bound for `vanilla-IDS` is*

$$\mathfrak{BR}_L(\pi_{IDS}) \le \sqrt{\mathbb{E}[\Gamma^*]\mathbb{I}(\mathcal{E}; \mathcal{D}_{L+1})\,L}\,.$$

The proof is deferred to Appendix B.1 and follows standard information-theoretical regret decomposition and the chain rule of mutual information that originally was exploited by Russo and Van Roy [2014]. For tabular MDPs, it remains to bound the $\mathbb{E}[\Gamma^*]$ and $\mathbb{I}(\mathcal{E}; \mathcal{D}_{L+1})$ separately.

Lemma 3.2. *The worst-case information ratio for tabular MDPs is upper bounded by*

$$\mathbb{E}[\Gamma^*] \le 2SAH^3\,.$$

We sketch the main steps of the proof and defer the full proof to Appendix B.2.

Proof sketch. Since `vanilla-IDS` minimizes the information ratio over all the policies, we can bound the information ratio of `vanilla-IDS` by the information ratio of TS.

- *Step one.* Our regret decomposition uses the value function based on $\bar{\mathcal{E}}_\ell$ as a bridge:

$$\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1)\right] = \underbrace{\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\bar{\mathcal{E}}_\ell}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1)\right]}_{I_1} + \underbrace{\mathbb{E}_\ell\left[V^{\bar{\mathcal{E}}_\ell}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1)\right]}_{I_2} .$$

  Note that conditional on $\mathcal{D}_\ell$, the law of π^ℓ_{TS} is the same as the law of π^* and both π^* and π^ℓ_{TS} are independent of $\bar{\mathcal{E}}_\ell$. This implies $\mathbb{E}_\ell[V^{\bar{\mathcal{E}}_\ell}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1)] = \mathbb{E}_\ell[V^{\bar{\mathcal{E}}_\ell}_{1,\pi^*}(s^\ell_1)]$.

- *Step two.* Denote $\Delta^{\mathcal{E}}_h(s,a) = \mathbb{E}_{s'\sim P^{\mathcal{E}}_h(\cdot|s,a)}[V^{\mathcal{E}}_{h+1,\pi^*}(s')] - \mathbb{E}_{s'\sim P^{\bar{\mathcal{E}}}_h(\cdot|s,a)}[V^{\mathcal{E}}_{h+1,\pi^*}(s')]$ as the value function difference. With the use of *state-action occupancy measure* and Lemma E.3, we can derive

$$I_1 = \sum_{h=1}^{H}\mathbb{E}_\ell\left[\sum_{(s,a)}\frac{d^{\bar{\mathcal{E}}}_{h,\pi^*}(s,a)}{(\mathbb{E}_\ell[d^{\bar{\mathcal{E}}}_{h,\pi^*}(s,a)])^{1/2}}(\mathbb{E}_\ell[d^{\bar{\mathcal{E}}}_{h,\pi^*}(s,a)])^{1/2}\Delta^{\mathcal{E}}_h(s,a)\right] .$$

  Applying the Cauchy–Schwarz inequality and Pinsker's inequality (see Eqs. (B.2)-(B.4) in the appendix for details), we can obtain

$$I_1 \le \sqrt{SAH^3}\left(\sum_{h=1}^{H}\mathbb{E}_\ell\left[\mathbb{E}^{\bar{\mathcal{E}}_\ell}_{\pi^\ell_{\text{TS}}}\left[\frac{1}{2}D_{\text{KL}}\left(P^{\mathcal{E}}_h(\cdot|s^\ell_h,a^\ell_h)||P^{\bar{\mathcal{E}}_\ell}_h(\cdot|s^\ell_h,a^\ell_h)\right)\right]\right]\right)^{1/2} ,$$

  where we interchange π^ℓ_{TS} and π^* again and $\mathbb{E}^{\bar{\mathcal{E}}_\ell}_{\pi^\ell_{\text{TS}}}$ is taken with respect to s^ℓ_h, a^ℓ_h and $\mathbb{E}_\ell$ is taken with respect to π^ℓ_{TS} and $\mathcal{E}$.

- *Step three.* It remains to establish the following equivalence of above KL-divergence and the information gain (Lemma B.1):

$$\sum_{h=1}^{H}\mathbb{E}_\ell\left[\mathbb{E}^{\bar{\mathcal{E}}_\ell}_{\pi^\ell_{\text{TS}}}\left[D_{\text{KL}}\left(P^{\mathcal{E}}_h(\cdot|s_h,a_h)||P^{\bar{\mathcal{E}}_\ell}_h(\cdot|s_h,a_h)\right)\right]\right] = \mathbb{I}^{\pi^\ell_{\text{TS}}}_\ell(\mathcal{E};\mathcal{H}_{\ell,H}) .$$

  A crucial step is to use the linearity of the expectation and the independence of priors over different layers (from the product prior as we assumed in Section 2) to show

$$\mathbb{P}_{\ell,\pi^\ell_{\text{TS}}}(s_{h-1}=s,a_{h-1}=a) = \mathbb{P}^{\bar{\mathcal{E}}_\ell}_{\pi^\ell_{\text{TS}}}(s_{h-1}=s,a_{h-1}=a) .$$

Combining Steps 1-3, we can reach the conclusion and the bound for I_2 is similar. □

The next lemma directly bounds the mutual information for tabular MDPs.

Lemma 3.3. *The mutual information can be bounded by*

$$\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1}) \le 2S^2AH\log(SLH) .$$

The proof relies on the construction of Bayes mixture density and a covering set for KL-divergence and is deferred to Appendix B.3. Combining Theorem 3.1, Lemmas 3.2 and 3.3 yields the following:

Theorem 3.4 (Regret bound for tabular MDPs)**.** *Suppose $\pi_{IDS} = \{\pi^\ell_{IDS}\}_{\ell=1}^L$ is the vanilla IDS policy. The following Bayesian regret bound holds for tabular MDPs*

$$\mathfrak{BR}_L(\pi_{IDS}) \le \sqrt{8S^3A^2H^4L\log(SLH)} .$$

Although this regret bound is sub-optimal, this is the first sub-linear prior-free Bayesian regret bound for `vanilla-IDS`.

Remark 3.5. *It is worth mentioning that Lu and Van Roy [2019], Lu [2020] also derived Bayesian regret bound using information-theoretical tools but only hold for a specific Dirichlet prior as well other distribution-specific assumptions. Their proof heavily exploits the property of Dirichlet distribution and can not easily be extended to prior-free regret bounds.*

In the context of finite-horizon MDPs, Lu et al. [2021] considered a `conditional-IDS` such that at each time step, conditional on s_h^ℓ, `conditional-IDS` takes the action according to

$$\pi_h(\cdot|s_h^\ell) = \operatorname*{argmin}_{\nu\in\Delta_{\mathcal{A}}} \frac{\left(\mathbb{E}_\ell\left[V_{h,\pi^*}^{\mathcal{E}}(s_h^\ell) - Q_{h,\pi^*}^{\mathcal{E}}(s_h^\ell, A_h)\right]\right)^2}{\mathbb{I}_\ell\left(\chi; (A_h, Q_{h,\pi^*}^{\mathcal{E}}(s_h^\ell, A_h))\right)},$$

where A_h is sampled from ν. `Conditional-IDS` defined the information ratio *per-step* rather than *per-episode* such that it only needs to optimize over action space rather than the policy space. This offers great computational benefits but there is no regret guarantee for `conditional-IDS`. Recently, Hao et al. [2022] has demonstrated the theoretical limitation of `conditional-IDS` in contextual bandits.

3.2 Regularized IDS

Computing an IDS policy practically usually involves two steps: 1. *approximating the information ratio*; 2. *optimizing the information ratio*. In bandits where the optimal policy is only a function of action space, optimizing Eq. (3.2) is a convex optimization problem and has an optimal solution with at most two non-zero components (Russo and Van Roy [2018, Proposition 6]). However in MDPs where the optimal policy is a mapping from the state space to the action space, `vanilla-IDS` needs to traverse two non-zero components over the full policy space which suggests the computational time might grow exponentially in S and H.

To overcome this obstacle, we propose `regularized-IDS` that can be efficiently computed by any dynamic programming solver and enjoy the same regret bound as `vanilla-IDS`. At each episode ℓ, `regularized-IDS` finds the policy:

$$\pi_{\text{r-IDS}}^\ell = \operatorname*{argmax}_{\pi\in\Pi} \mathbb{E}_\ell[V_{1,\pi}^{\mathcal{E}}(s_1^\ell)] + \lambda \mathbb{I}_\ell^\pi\left(\mathcal{E}; \mathcal{H}_{\ell,H}^\pi\right), \tag{3.3}$$

where $\lambda > 0$ is a tunable parameter.

To approximate the objective function in Eq. (3.3), we assume the access to a *posterior sampling oracle*.

Definition 3.6 (Posterior sampling oracle)**.** *Given a prior over $\mathcal{E}$ and history $\mathcal{D}_\ell$, the* posterior sampling oracle*, SAMP, is a subroutine which returns a sample from the posterior distribution $\mathbb{P}_\ell(\mathcal{E})$. Multiple calls to the procedure result in independent samples.*

Remark 3.7. *SAMP can be exactly obtained when the conjugate prior such as Dirichlet distribution is put on the transition kernel. When one uses neural nets to estimate the model, SAMP can be approximated by epistemic neural networks [Osband et al., 2021a], a general framework to quantify uncertainty for neural nets. The effectiveness of different epistemic neural networks such as deep ensemble, dropout and stochastic gradient MCMC has been examined empirically by Osband et al. [2021b].*

We compute $\pi_{\text{r-IDS}}^\ell$ in two steps:

- Firstly, we prove an equivalent form of the objective function in Eq. (3.3) using the chain rule of mutual information. Define $r_h'(s,a)$ as an *augmented* reward function:

$$r_h'(s,a) = r_h(s,a) + \lambda \int D_{\text{KL}}\left(P_h^{\mathcal{E}}(\cdot|s,a) || P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s,a)\right) \mathrm{d}\mathbb{P}_\ell(\mathcal{E}).$$

  Proposition 3.8. *The following equivalence holds*

$$\mathbb{E}_\ell[V_{1,\pi}^{\mathcal{E}}(s_1^\ell)] + \lambda \mathbb{I}_\ell^\pi\left(\mathcal{E}; \mathcal{H}_{\ell,H}\right) = \mathbb{E}_\pi^{\bar{\mathcal{E}}_\ell}\left[\sum_{h=1}^H r_h'(s_h, a_h)\right].$$

  The proof is deferred to Appendix B.4.

- Given *SAMP*, the augmented reward r'_h and the MDP $\bar{\mathcal{E}}_\ell$ can be well approximated by Monte Carlo sampling. Therefore, at each episode ℓ, finding $\pi^\ell_{\text{r-IDS}}$ is equivalent to find an optimal policy based on a computable and augmented MDP $\{P_h^{\bar{\mathcal{E}}_\ell}, r'_h\}_{h=1}^H$. This can be solved efficiently by any dynamic programming solver such as value iteration or policy iteration.

In the end, we show that $\pi^\ell_{\text{r-IDS}}$ enjoys the same regret bound as `vanilla-IDS` when the tunable parameter is carefully chosen.

Theorem 3.9. *By choosing* $\lambda = \sqrt{L\mathbb{E}[\Gamma^*]/\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1})}$*, we have*

$$\mathfrak{BR}_L(\pi^{\text{r-IDS}}) \le \sqrt{\frac{3}{2}L\mathbb{E}[\Gamma^*]\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1})}\,.$$

The proof is deferred to Appendix B.5. Let M_1, M_2 be upper bounds of $\mathbb{E}[\Gamma^*]$ and $\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1})$ respectively. In practice, we could conservatively choose $\lambda = \sqrt{LM_1/M_2}$ such that $\mathfrak{BR}_L(\pi^{\text{r-IDS}}) \le \sqrt{3/2M_1M_2L}$. From Lemmas 3.2 and 3.3 for tabular MDPs, we could choose $M_1 = 2SAH^3$ and $M_2 = 2S^2AH\log(SLH)$.

Remark 3.10. *Russo and Van Roy [2018, Section 9.3] also considered a tunable version of IDS (for bandits) but took a square form of* $\mathbb{E}_\ell[V^{\mathcal{E}}_{1,\pi}(s_1^\ell)]$*. While this makes no difference in bandits setting, this prevented us to use dynamic programming solver in RL setting. We are also inspired by Foster et al. [2021, Section 9.3] who studied the relationship between information ratio and Decision-Estimation Coefficient.*

4 Learning a surrogate environment

When the state space is large, the agent could take too much information to learn exactly the whole environment $\mathcal{E}$ which is reflected through $\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1})$. A key observation is that different states may correspond to the same value function who eventually determines the behavior of the optimal policy. Based on the rate-distortion theory developed in Dong and Roy [2018], we reduce this redundancy and construct a surrogate environment that needs less information to learn.

4.1 A rate distortion approach

The rate-distortion theory [Cover and Thomas, 1991] addresses the problem of determining the minimal number of bits per symbol that should be communicated over a channel, so that the source (input signal) can be approximately reconstructed at the receiver (output signal) without exceeding an expected distortion. It was recently introduced to bandits community to develop sharper bounds for linear bandits [Dong and Roy, 2018] and time-sensitive bandits [Russo and Van Roy, 2022]. We take a similar approach to construct a surrogate environment.

Surrogate environment Suppose there exists a partition $\{\Theta_k^\varepsilon\}_{k=1}^K$ over Θ such that for any $\mathcal{E}, \mathcal{E}' \in \Theta_k^\varepsilon$ and any $k \in [K]$, we have

$$V^{\mathcal{E}}_{1,\pi^*_{\mathcal{E}}}(s_1^\ell) - V^{\mathcal{E}'}_{1,\pi^*_{\mathcal{E}}}(s_1^\ell) \le \varepsilon\,, \tag{4.1}$$

where $\varepsilon > 0$ is the distortion tolerance and we write the optimal policy explicitly depending on the environment. Let ζ be a discrete random variable taking values in $\{1,\dots,K\}$ that indicates the region $\mathcal{E}$ lies such that $\zeta = k$ if and only if $\mathcal{E} \in \Theta_k^\varepsilon$. Therefore, ζ can be viewed as a statistic of $\mathcal{E}$ and less informative than $\mathcal{E}$ if K is small.

The next lemma shows the existence of the surrogate environment based on the partition.

Lemma 4.1. *For any partition* $\{\Theta_k^\varepsilon\}_{k=1}^K$ *and any* $\ell \in [L]$*, we can construct a surrogate environment* $\widetilde{\mathcal{E}}_\ell^* \in \Theta$ *which is a random MDP such that the law of* $\widetilde{\mathcal{E}}_\ell^*$ *only depends on* ζ *and*

$$\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^*_{\mathcal{E}}}(s_1^\ell) - V^{\mathcal{E}}_{1,\pi^\ell_{TS}}(s_1^\ell)\right] - \mathbb{E}_\ell\left[V^{\widetilde{\mathcal{E}}_\ell^*}_{1,\pi^*_{\mathcal{E}}}(s_1^\ell) - V^{\widetilde{\mathcal{E}}_\ell^*}_{1,\pi^\ell_{TS}}(s_1^\ell)\right] \le \varepsilon\,. \tag{4.2}$$

The concrete form of $\widetilde{\mathcal{E}}_\ell^*$ is deferred to Eq. (C.1) in the appendix.

Surrogate IDS We refer the IDS based on the surrogate environment $\widetilde{\mathcal{E}}_\ell^*$ as `surrogate-IDS` that minimizes

$$\pi_{\text{s-IDS}}^\ell = \operatorname*{argmin}_{\pi\in\Pi} \frac{(\mathbb{E}_\ell[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell) - V_{1,\pi}^{\mathcal{E}}(s_1^\ell)] - \varepsilon)^2}{\mathbb{I}_\ell^\pi(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})}\,, \tag{4.3}$$

for some parameters $\varepsilon > 0$ the will be chosen later. Denote the surrogate information ratio of TS as

$$\widetilde{\Gamma} = \max_{\ell\in[L]} \frac{\left(\mathbb{E}_\ell\left[V_{1,\pi^*}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell)\right]\right)^2}{\mathbb{I}_\ell^{\pi_{\text{TS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})}\,.$$

We first derive a generic regret bound for surrogate IDS in the following theorem.

Theorem 4.2. *A generic regret bound for surrogate IDS is*

$$\mathfrak{BR}_L(\pi_{\textit{s-IDS}}) \le \sqrt{\mathbb{E}[\widetilde{\Gamma}]\mathbb{I}(\zeta; \mathcal{D}_{L+1})L} + L\varepsilon\,.$$

We defer the proof to Appendix C.2. Given ζ, we have $\widetilde{\mathcal{E}}_\ell^*$ and $\mathcal{H}_{\ell,H}$ are independent under the law of $\mathbb{P}_{\ell,\pi_{\text{s-IDS}}^\ell}$. By the data processing inequality, the proof uses the fact that

$$\mathbb{I}_\ell^{\pi_{\text{s-IDS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H}) \le \mathbb{I}_\ell^{\pi_{\text{s-IDS}}^\ell}(\zeta; \mathcal{H}_{\ell,H})\,.$$

Comparing with regret bound of `vanilla-IDS` in Lemma 3.1, the regret bound of `surrogate-IDS` depends on the information gain about ζ rather than the whole environment $\mathcal{E}$. If there exists a partition with small covering number K, the agent could pay less information to learn. The second term $L\varepsilon$ is the price of distortions. In the following, we will bound the $\mathbb{E}[\widetilde{\Gamma}]$ and $\mathbb{I}(\zeta; \mathcal{D}_{L+1})$ for tabular and linear MDPs separately.

4.2 Tabular MDPs

We first show the existence of the partition required in Lemma 4.1 for tabular MDPs and an upper bound of the covering number K.

Lemma 4.3. *There exists a partition $\{\Theta_k^\varepsilon\}_{k=1}^K$ over Θ such that for any $k \in [K]$ and $\mathcal{E}_1, \mathcal{E}_2 \in \Theta_k$,*

$$V_{1,\pi_{\mathcal{E}_1}^*}^{\mathcal{E}_1}(s_1) - V_{1,\pi_{\mathcal{E}_1}^*}^{\mathcal{E}_2}(s_1) \le \varepsilon\,,$$

and the log covering number satisfies $\log(K) \le SAH\log(4H^2/\varepsilon)$.

The proof is deferred to Lemma C.3. For tabular MDPs, the mutual information between ζ and the history can be bounded by

$$\mathbb{I}(\zeta; \mathcal{D}_{L+1}) \le \mathbb{H}(\zeta) \le \log(K) \le SAH\log(4H^2/\varepsilon)\,,$$

where $\mathbb{H}(\cdot)$ is the Shannon entropy. Comparing with Lemma 3.3 when learning the whole environment, learning the surrogate environment saves a factor of S through the bound of mutual information.

Lemma 4.4. *The surrogate information ratio for tabular MDPs is upper bounded by $\mathbb{E}[\widetilde{\Gamma}] \le 2SAH^3$.*

The proof is the same as Lemma 3.2 and thus is omitted. Putting Lemmas 4.3-4.4 yields an improved bound for tabular MDPs using `surrogate-IDS`.

Theorem 4.5 (Improved regret bound for tabular MDPs)**.** *By choosing $\varepsilon = 1/L$, the regret bound of `surrogate-IDS` for tabular MDPs satisfies*

$$\mathfrak{BR}_L(\pi_{\textit{s-IDS}}) \le \sqrt{2S^2A^2H^4L\log(4HL)}\,.$$

For tabular MDPs, `surrogate-IDS` improves the regret bound of `vanilla-IDS` by a factor of S. However, it is still away from the minimax lower bound by a factor of $\sqrt{SAH}$. We conjecture `surrogate-IDS` can achieve the optimal bound with a price of lower order term but leave it as a future work.

Remark 4.6. *Although the existence of $\widetilde{\mathcal{E}}_\ell^*$ is established using a constructive argument, finding $\widetilde{\mathcal{E}}_\ell^*$ needs a grid search and is not computationally efficient.*

4.3 Linear MDPs

We extend our analysis to linear MDPs that is a fundamental model to study the theoretical properties of linear function approximations in RL. All the proofs are deferred to Appendix C.4-C.5.

Definition 4.7 (Linear MDPs [Yang and Wang, 2019, Jin et al., 2020])**.** *Let $\phi : \mathcal{S} \times \mathcal{A} \to \mathbb{R}^d$ be a feature map which assigns to each state-action pair a d-dimensional feature vector and assume $\|\phi(s,a)\|_2 \le 1$. An MDP is called a linear MDP if for any $h \in [H]$, there exist d unknown (signed) measures $\psi_h^1, \dots, \psi_h^d$ over $\mathcal{S}$, such that for any $(s,a) \in \mathcal{S} \times \mathcal{A}$, we have*

$$P_h(\cdot|s,a) = \langle \phi(s,a), \psi_h(\cdot) \rangle \,,$$

where $\psi_h = (\psi_h^1, \dots, \psi_h^d)$. Let us denote Θ^{Lin} be the parameter space of linear MDPs and assume $\left\|\sum_{s'} \psi_h(s')\right\|_2 \le C_\psi$.

Note that the degree of freedom of linear MDPs still depends on S which implies that $\mathbb{I}(\mathcal{E}; \mathcal{D}_{L+1})$ may still scale with S. Therefore, we *must* learn a surrogate environment rather than the whole environment for linear MDPs based on the current regret decomposition in Theorem 3.4. We first show the existence of a partition over linear MDPs with the log covering number only depending on the feature dimension d.

Lemma 4.8. *There exists a partition $\{\Theta_k^\varepsilon\}_{k=1}^K$ over Θ^{Lin} such that for any $k \in [K]$ and $\mathcal{E}_1, \mathcal{E}_2 \in \Theta_k$,*

$$V_{1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(s_1) - V_{1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}(s_1) \le \varepsilon \,,$$

and the log covering number satisfies $\log(K) \le Hd \log(H^2 C_\psi/\varepsilon + 1)$.

For linear MDPs, the mutual information can be bounded by

$$\mathbb{I}(\zeta; \mathcal{D}_{L+1}) \le \mathbb{H}(\zeta) \le \log(K) \le Hd \log(H^2 C_\psi/\varepsilon + 1) \,.$$

Lemma 4.9. *The surrogate information ratio of linear MDPs is upper bounded by $\mathbb{E}[\widetilde{\Gamma}] \le 4H^3 d$.*

Theorem 4.10 (Regret bound for linear MDPs)**.** *By choosing $\varepsilon = 1/L$, the regret bound of surrogate IDS for linear MDPs satisfies*

$$\mathfrak{BR}_L(\pi_{\textit{s-IDS}}) \le \sqrt{4H^4 d^2 L \log(H^2 C_\psi L + 1)} + 1 \,.$$

This Bayesian bound improves the $O(d^{3/2} H^2 \sqrt{L})$ frequentist regret of LSVI-UCB [Jin et al., 2020] by a factor of $\sqrt{d}$ and matches the existing minimax lower bound $O(\sqrt{H^3 d^2 L})$ [Zhou et al., 2021] up to a H factor. However, we would like to emphasize that this is not an apples-to-apples comparison, since in general frequentist regret bound is stronger than Bayesian regret bound.

4.4 Regret bounds for TS

As a direct application of our rate-distortion analysis, we provide Bayesian regret bounds for Thompson sampling.

Theorem 4.11. *A generic regret bound for TS is*

$$\mathfrak{BR}_L(\pi_{TS}) \le \sqrt{\mathbb{E}[\widetilde{\Gamma}] \mathbb{I}(\zeta; \mathcal{D}_{L+1}) L} + L\varepsilon \,.$$

This implies for tabular and linear MDPs, TS has the same regret bound as `surrogate-IDS`. However, when the worst-case information ratio cannot be optimally bounded by the information ratio of TS, IDS demonstrates better regret bounds than TS, such as bandits with graph feedback [Hao et al., 2022] and sparse linear bandits [Hao et al., 2021].

5 Conclusion

In this paper, we derive the first prior-free Bayesian regret bounds for information-directed RL under tabular and linear MDPs. Theoretically, it will be of great interest to see if any version of IDS can achieve the $O(\sqrt{SAH^3 L})$ minimax lower bounds for tabular MDPs.

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Checklist

The checklist follows the references. Please read the checklist guidelines carefully for information on how to answer these questions. For each question, change the default **[TODO]** to [Yes] , [No] , or [N/A] . You are strongly encouraged to include a **justification to your answer**, either by referencing the appropriate section of your paper or providing a brief inline description. For example:

- Did you include the license to the code and datasets? [N/A]
- Did you include the license to the code and datasets? [N/A]
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Please do not modify the questions and only use the provided macros for your answers. Note that the Checklist section does not count towards the page limit. In your paper, please delete this instructions block and only keep the Checklist section heading above along with the questions/answers below.

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [N/A]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [N/A]
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [N/A]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [N/A]
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [N/A]
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(d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]

(e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]

5. If you used crowdsourcing or conducted research with human subjects...

(a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]

(b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]

(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

A Implementation and Experiment

In this section, we provide a practical implementation and experiments for `regularized-IDS`. In practice, the KL-distance could be hard to calculated. Following the idea from Russo and Van Roy [2018], we could lower bound the KL-distance by a variance term as follows. By Pinsker's inequality,

$$\begin{aligned}\int D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s,a)||P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s,a)\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E}) &\geq \int \left\|P_h^{\mathcal{E}}(\cdot|s,a)-P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s,a)\right\|_2^2 \mathrm{d}\mathbb{P}_\ell(\mathcal{E}) \\ &\geq \int \sum_{s'}\left(P_h^{\mathcal{E}}(s'|s,a)-P_h^{\bar{\mathcal{E}}_\ell}(s'|s,a)\right)^2 \mathrm{d}\mathbb{P}_\ell(\mathcal{E}) \\ &= \sum_{s'} \mathrm{Var}\left(P_h^{\mathcal{E}}(s'|s,a)\right) .\end{aligned}$$

Then the *augmented* reward function in terms of variance terms is

$$r'_h(s,a) = r_h(s,a) + \lambda \sum_{s'} \mathrm{Var}\left(P_h^{\mathcal{E}}(s'|s,a)\right) .$$

When the prior distribution of $P_h^{\mathcal{E}}(\cdot|s,a)$ follows an independent Dirichlet distribution with parameter $\beta_{s,a}^h \in \mathbb{R}^{|\mathcal{S}|}$, the posterior parameter $(\beta_{s,a,1}^h,\ldots,\beta_{s,a,S}^h)$ can be computed recursively. For example, if we observe a transition from (s,a) to the first state, we update the posterior parameter to be $(\beta_{s,a,1}^h+1,\ldots,\beta_{s,a,S}^h)$. We provide a detailed implementation of `regularized-IDS` in Algorithm 1.

Algorithm 1 Tabular `regularized-IDS`

Input: prior parameters $\{\beta_{s,a}^h\}_{h\in[H],s\in\mathcal{S},a\in\mathcal{A}}$, number of episodes L, the regularization parameter λ.
Initialize: $\mathcal{H}_{1,1}=\emptyset$
for episodes $\ell = 1,\ldots,L$ **do**
  for $h\in[H], s\in\mathcal{S}, a\in\mathcal{A}$ **do**
    Compute $P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s,a) = \mathbb{E}_\ell[P_h^{\mathcal{E}}(\cdot|s,a)]$
    Compute $r'_h(s,a) = r_h(s,a) + \lambda\sum_{s'}\mathrm{Var}\left(P_h^{\mathcal{E}}(s'|s,a)\right)$
  end for
  Compute $\pi_{\text{r-IDS}}^\ell$ through value iteration based on $\{P_h^{\bar{\mathcal{E}}_\ell}, r'_h\}_{h=1}^H$
  for layers $h=1,\ldots,H$ **do**
    Sample and apply a_{h+1}^ℓ according to $\pi_{\text{r-IDS},h}^\ell(\cdot|s_h)$
    Observe s_{h+1}^ℓ
    $\mathcal{H}_{\ell,h+1} = \mathcal{H}_{\ell,h}\cup\{a_{h+1}^\ell, s_{h+1}^\ell\}$
  end for
end for

A.1 Experiment

We compare performance of `regularized-IDS` and PSRL [Osband et al., 2013] using RiverSwim and stochastic Chain MDP environment, where the state is reset every 20 steps. RiverSwim consists of six states arranged in a chain. The agent begins at the far left state and at every time step has the choice to swim left or right. The agent receives a small reward for reaching the leftmost state, but the optimal policy is to attempt to swim right and receive a much larger reward.

We use Dirichlet prior for both `regularized-IDS` and PSRL and repeat the experiment for 50 runs. We report the cumulative empirical regret over 10000 episodes. As suggested in Theorem 3.9, the regularization parameter should be proportion to $\sqrt{L}$. Thus we choose $\lambda = \lambda_0\sqrt{L}$ where λ_0 is chosen across $\{0.1, 0.5, 1\}$. Figure 1 shows that for a proper choice of the tuning parameter, `regularized-IDS` can outperform PSRL.

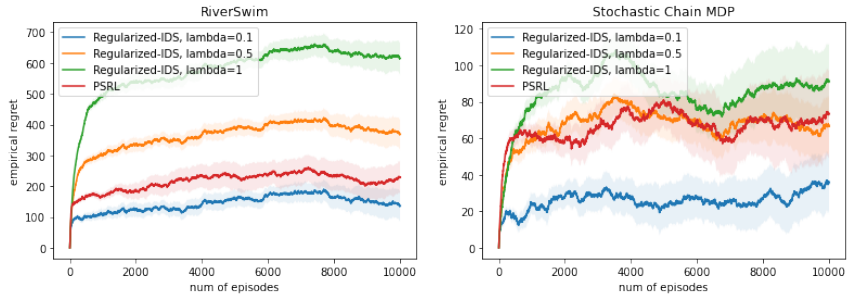

Figure 1: Cumulative empirical regret.

B Proofs of learning the whole environment

B.1 Proof of Theorem 3.1

Proof. We follow the standard information-theoretical regret decomposition:

$$\begin{aligned}
\mathfrak{BR}_L(\pi_{\text{IDS}}) &= \sum_{\ell=1}^{L} \mathbb{E}\left[\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi^\ell_{\text{IDS}}}(s^\ell_1)\right]\right] \\
&= \sum_{\ell=1}^{L} \mathbb{E}\left[\sqrt{\frac{\left(\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi^\ell_{\text{IDS}}}(s^\ell_1)\right]\right)^2}{\mathbb{I}^{\pi^\ell_{\text{IDS}}}_\ell(\mathcal{E};\mathcal{H}_{\ell,H})}\mathbb{I}^{\pi^\ell_{\text{IDS}}}_\ell(\mathcal{E};\mathcal{H}_{\ell,H})}\right] \\
&\le \sqrt{\mathbb{E}\left[\sum_{\ell=1}^{L}\Gamma_\ell(\pi^\ell_{\text{IDS}})\right]}\sqrt{\mathbb{E}\left[\sum_{\ell=1}^{L}\mathbb{I}^{\pi^\ell_{\text{IDS}}}_\ell(\mathcal{E};\mathcal{H}_{\ell,H})\right]} = \sqrt{\mathbb{I}\left(\mathcal{E};\mathcal{D}_{L+1}\right)\sum_{\ell=1}^{L}\mathbb{E}[\Gamma_\ell(\pi^\ell_{\text{IDS}})]}\,,
\end{aligned}$$

where the first inequality is from the Cauchy–Schwarz inequality and the last equation is due to the chain rule of mutual information

$$\mathbb{I}\left(\mathcal{E};\mathcal{D}_{L+1}\right) = \mathbb{I}\left(\mathcal{E};(\mathcal{H}_{1,H},\ldots,\mathcal{H}_{L,H})\right) = \sum_{\ell=1}^{L}\mathbb{E}\left[\mathbb{I}^{\pi^\ell_{\text{IDS}}}_\ell(\mathcal{E};\mathcal{H}_{\ell,H})\right]\,.$$

According to the definition of Γ^*, we have $\Gamma_\ell(\pi^\ell_{\text{IDS}}) \le \Gamma^*$ for any $\ell \in [L]$. □

B.2 Proof of Lemma 3.2

Proof. From the definition of IDS policy stated in Eq. (3.2), for any $\ell \in [L]$,

$$\Gamma_\ell(\pi^\ell_{\text{IDS}}) \le \Gamma_\ell(\pi^\ell_{\text{TS}}) = \frac{\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1)\right]^2}{\mathbb{I}^{\pi^\ell_{\text{TS}}}_\ell\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)}\,.$$

We first decompose the one-step regret as follows,

$$\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1)\right] = \underbrace{\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\bar{\mathcal{E}}_\ell}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1)\right]}_{I_1} + \underbrace{\mathbb{E}_\ell\left[V^{\bar{\mathcal{E}}_\ell}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1)\right]}_{I_2}\,. \tag{B.1}$$

Bounding I_1 Note that conditional on $\mathcal{D}_\ell$, the law of π^ℓ_{TS} is the same as the law of π^* and both π^* and π^ℓ_{TS} are independent of $\bar{\mathcal{E}}_\ell$. This fact implies that

$$I_1 = \mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1) - V^{\bar{\mathcal{E}}_\ell}_{1,\pi^*}(s^\ell_1)\right]\,.$$

Denote

$$\Delta_h^{\mathcal{E}}(s,a) = \mathbb{E}_{s'\sim P_h^{\mathcal{E}}(\cdot|s,a)}[V_{h+1,\pi^*}^{\mathcal{E}}(s')] - \mathbb{E}_{s'\sim P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s,a)}[V_{h+1,\pi^*}^{\mathcal{E}}(s')]\,.$$

Applying Lemma E.3, we have

$$\begin{aligned}
I_1 &= \mathbb{E}_\ell\left[\sum_{h=1}^H \mathbb{E}_{\pi^*}^{\bar{\mathcal{E}}_\ell}\left[\Delta_h^{\mathcal{E}}(s_h^\ell, a_h^\ell)\right]\right] = \mathbb{E}_\ell\left[\sum_{h=1}^H \mathbb{E}\left[\mathbb{E}_{\pi^*}^{\bar{\mathcal{E}}_\ell}\left[\Delta_h^{\mathcal{E}}(s_h^\ell, a_h^\ell)\right]\Big|\mathcal{E}\right]\right] \\
&= \sum_{h=1}^H \mathbb{E}_\ell\left[\mathbb{E}\left[\sum_{(s,a)} d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)\Delta_h^{\mathcal{E}}(s,a)\Big|\mathcal{E}\right]\right]\,, \\
&= \sum_{h=1}^H \mathbb{E}_\ell\left[\sum_{(s,a)} d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)\Delta_h^{\mathcal{E}}(s,a)\right]\,, \\
&= \sum_{h=1}^H \mathbb{E}_\ell\left[\sum_{(s,a)} \frac{d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)}{(\mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)])^{1/2}}(\mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)])^{1/2}\Delta_h^{\mathcal{E}}(s,a)\right]\,.
\end{aligned}$$

Here we just divide the element that corresponds to $d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a) > 0$.

Applying Cauchy–Schwarz inequality and using the fact that $d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a) \le 1$, we have

$$\begin{aligned}
I_1 &\le \left(\sum_{h=1}^H \mathbb{E}_\ell\left[\sum_{(s,a)} \frac{(d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a))^2}{\mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)]}\right]\right)^{1/2}\left(\sum_{h=1}^H \mathbb{E}_\ell\left[\sum_{(s,a)} \mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)](\Delta_h^{\mathcal{E}}(s,a))^2\right]\right)^{1/2} \\
&\le \left(\sum_{h=1}^H \mathbb{E}_\ell\left[\sum_{(s,a)} \frac{d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)}{\mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)]}\right]\right)^{1/2}\left(\sum_{h=1}^H \mathbb{E}_\ell\left[\sum_{(s,a)} \mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)](\Delta_h^{\mathcal{E}}(s,a))^2\right]\right)^{1/2}\,.
\end{aligned} \tag{B.2}$$

First, note that

$$\sum_{h=1}^H \mathbb{E}_\ell\left[\sum_{(s,a)} \frac{d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)}{\mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)]}\right] = \sum_{h=1}^H\left[\sum_{(s,a)} \frac{\mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)]}{\mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)]}\right] \le HSA\,. \tag{B.3}$$

Second, since the law of π^* is the same as π_{TS}^ℓ conditional on $\mathcal{D}_\ell$, we have

$$\mathbb{E}_\ell\left[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)\right] = \mathbb{E}_\ell\left[d_{h,\pi_{\text{TS}}^\ell}^{\bar{\mathcal{E}}_\ell}(s,a)\right]\,.$$

Then we can obtain

$$\begin{aligned}
\mathbb{E}_\ell\left[\sum_{(s,a)} \mathbb{E}_\ell[d_{h,\pi^*}^{\bar{\mathcal{E}}_\ell}(s,a)](\Delta_h^{\mathcal{E}}(s,a))^2\right] &= \mathbb{E}_\ell\left[\sum_{(s,a)} \mathbb{E}_\ell\left[d_{h,\pi_{\text{TS}}^\ell}^{\bar{\mathcal{E}}_\ell}(s,a)\right](\Delta_h^{\mathcal{E}}(s,a))^2\right] \\
&= \mathbb{E}_\ell\left[\sum_{(s,a)} d_{h,\pi_{\text{TS}}^\ell}^{\bar{\mathcal{E}}_\ell}(s,a)\right]\mathbb{E}_\ell\left[(\Delta_h^{\mathcal{E}}(s,a))^2\right]\,.
\end{aligned}$$

Given $\mathcal{D}_\ell$, we have $d_{h,\pi_{\text{TS}}^\ell}^{\bar{\mathcal{E}}_\ell}(s,a)$ and $\Delta_h^{\mathcal{E}}(s,a)$ are independent. This implies

$$\begin{aligned}
&\mathbb{E}_\ell\left[\sum_{(s,a)} d_{h,\pi_{\text{TS}}^\ell}^{\bar{\mathcal{E}}_\ell}(s,a)\right]\mathbb{E}_\ell\left[(\Delta_h^{\mathcal{E}}(s,a))^2\right] = \mathbb{E}_\ell\left[\sum_{(s,a)} d_{h,\pi_{\text{TS}}^\ell}^{\bar{\mathcal{E}}_\ell}(s,a)(\Delta_h^{\mathcal{E}}(s,a))^2\right] \\
&= \mathbb{E}_\ell\left[\mathbb{E}_{\pi_{\text{TS}}^\ell}^{\bar{\mathcal{E}}_\ell}\left[(\Delta_h^{\mathcal{E}}(s_h^\ell, a_h^\ell))^2\right]\right] \\
&= H^2\mathbb{E}_\ell\left[\mathbb{E}_{\pi_{\text{TS}}^\ell}^{\bar{\mathcal{E}}_\ell}\left[\left(\mathbb{E}_{s'\sim P_h^{\mathcal{E}}(\cdot|s_h^\ell,a_h^\ell)}\left[V_{h+1,\pi^*}^{\mathcal{E}}(s')/H\right] - \mathbb{E}_{s'\sim P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s_h^\ell,a_h^\ell)}\left[V_{h+1,\pi^*}^{\mathcal{E}}(s')/H\right]\right)^2\right]\right]\,,
\end{aligned} \tag{B.4}$$

where $\mathbb{E}^{\bar{\mathcal{E}}_\ell}_{\pi^\ell_{\text{TS}}}$ is taken with respect to s^ℓ_h, a^ℓ_h and $\mathbb{E}_\ell$ is taken with respect to π^ℓ_{TS} and $\mathcal{E}$.

Combining Eqs. (B.2)-(B.4) together and applying Lemma E.2 which is a variant of Pinsker's inequality,

$$I_1 \leq \sqrt{SAH^3}\left(\sum_{h=1}^{H}\mathbb{E}_\ell\mathbb{E}^{\bar{\mathcal{E}}_\ell}_{\pi^\ell_{\text{TS}}}\left[\frac{1}{2}D_{\text{KL}}\left(P^{\mathcal{E}}_h(\cdot|s^\ell_h,a^\ell_h)||P^{\bar{\mathcal{E}}_\ell}_h(\cdot|s^\ell_h,a^\ell_h)\right)\right]\right)^{1/2}. \tag{B.5}$$

The next lemma establishes the relationship between the cumulative KL-distance in Eq. (B.5) and mutual information $\mathbb{I}^{\pi^\ell_{\text{TS}}}_\ell(\mathcal{E};\mathcal{H}_{\ell,H})$. This lemma will be frequently used later.

Lemma B.1. *For environment $\mathcal{E}$ and its corresponding mean of posterior measure $\bar{\mathcal{E}}_\ell$, the following holds for any policy π,*

$$\sum_{h=1}^{H}\mathbb{E}_\ell\mathbb{E}^{\bar{\mathcal{E}}_\ell}_{\pi}\left[D_{\text{KL}}\left(P^{\mathcal{E}}_h(\cdot|s^\ell_h,a^\ell_h)||P^{\bar{\mathcal{E}}_\ell}_h(\cdot|s^\ell_h,a^\ell_h)\right)\right] = \mathbb{I}^{\pi}_\ell\left(\mathcal{E};\mathcal{H}_{\ell,H}\right).$$

Together with Eq. (B.5),

$$I_1 \leq \sqrt{\frac{1}{2}SAH^3\mathbb{I}^{\pi^\ell_{\text{TS}}}_\ell\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)}. \tag{B.6}$$

Bounding I_2 The upper bound for I_2 is similar. Applying Lemma E.3 and repeating the steps of showing Eq. (B.5),

$$\begin{aligned}
&\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1) - V^{\bar{\mathcal{E}}_\ell}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1)\right]\\
&= \mathbb{E}_\ell\left[\sum_{h=1}^{H}\mathbb{E}^{\bar{\mathcal{E}}_\ell}_{\pi^\ell_{\text{TS}}}\left[\mathbb{E}_{s'\sim P^{\mathcal{E}}_h(\cdot|s^\ell_h,a^\ell_h)}[V^{\mathcal{E}}_{h+1,\pi^\ell_{\text{TS}}}(s')] - \mathbb{E}_{s'\sim P^{\bar{\mathcal{E}}_\ell}_h(\cdot|s^\ell_h,a^\ell_h)}[V^{\mathcal{E}}_{h+1,\pi^\ell_{\text{TS}}}(s')]\right]\right]\\
&\leq \sqrt{SAH^3}\left(\sum_{h=1}^{H}\mathbb{E}_\ell\mathbb{E}^{\bar{\mathcal{E}}_\ell}_{\pi^\ell_{\text{TS}}}\left[\frac{1}{2}D_{\text{KL}}\left(P^{\mathcal{E}}_h(\cdot|s^\ell_h,a^\ell_h)||P^{\bar{\mathcal{E}}_\ell}_h(\cdot|s_h,a_h)\right)\right]\right)^{1/2}.
\end{aligned}$$

Applying Lemma B.1 again, we obtain

$$I_2 \leq \sqrt{SAH^3\mathbb{I}^{\pi^\ell_{\text{TS}}}_\ell\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)} \tag{B.7}$$

Combining Eqs. (B.1), (B.6) and (B.7) together, we have

$$\Gamma^* \leq \max_{\ell\in[L]}\Gamma_\ell(\pi^\ell_{\text{TS}}) = \frac{\left(\mathbb{E}_\ell\left[V^{\mathcal{E}}_{1,\pi^\ell_{\text{TS}}}(s^\ell_1) - V^{\mathcal{E}}_{1,\pi^*}(s^\ell_1)\right]\right)^2}{\mathbb{I}^{\pi^\ell_{\text{TS}}}_\ell\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)} \leq 2SAH^3.$$

This ends the proof. □

B.3 Proof of Lemma 3.3

Proof. Now we start to bound $\mathbb{I}\left(\mathcal{E};\mathcal{D}_{L+1}\right)$. Assume the prior probability measure of $\mathcal{E}$ is $\rho(\mathcal{E})$ that takes the value in Θ and suppose the Bayes mixture density $p_\rho(\mathcal{D}_{L+1}) = \int_{\mathcal{E}\in\Theta}p(\mathcal{D}_{L+1}|\mathcal{E})d\rho(\mathcal{E})$. Let $\{\Theta_k\}_{k=1}^K$ be a partition of Θ. We choose ρ_1 as an uniform distribution over $\{\Theta_k\}_{k=1}^K$ such that $q(\mathcal{D}_{L+1}) = p_{\rho_1}(\mathcal{D}_{L+1}) = \int_{\theta\in\Theta}p(\mathcal{D}_{L+1}|\theta)\,\mathrm{d}\rho_1(\theta)$ and we denote $\mathbb{Q}_{\mathcal{D}_{L+1}}$ as the corresponding probability measure. Based on the equivalent form of mutual information,

$$\begin{aligned}
\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1}) &= \mathbb{E}_{\mathcal{E}}\left[D_{\text{KL}}(\mathbb{P}_{\mathcal{D}_{L+1}|\mathcal{E}}||\mathbb{P}_{\mathcal{D}_{L+1}})\right]\\
&= \int_{\mathcal{E}\in\Theta}\int p(\mathcal{D}_{L+1}|\mathcal{E})\log\left(\frac{p(\mathcal{D}_{L+1}|\mathcal{E})}{p_\rho(\mathcal{D}_{L+1})}\right)\mu(\mathrm{d}\mathcal{D}_{L+1})\,\mathrm{d}\rho(\mathcal{E})\\
&\leq \int_{\mathcal{E}\in\Theta}\int p(\mathcal{D}_{L+1}|\mathcal{E})\log\left(\frac{p(\mathcal{D}_{L+1}|\mathcal{E})}{q(\mathcal{D}_{L+1})}\right)\mu(\mathrm{d}\mathcal{D}_{L+1})\,\mathrm{d}\rho(\mathcal{E})\\
&= \int_{\mathcal{E}\in\Theta}D_{\text{KL}}(\mathbb{P}_{\mathcal{D}_{L+1}|\mathcal{E}}||\mathbb{Q}_{\mathcal{D}_{L+1}})\,\mathrm{d}\rho(\mathcal{E}).
\end{aligned} \tag{B.8}$$

where the inequality is due to the fact that Bayes mixture density $p_\rho(\mathcal{D}_{L+1})$ minimizes the average KL divergences over any choice of densities $q(\mathcal{D}_{L+1})$.

According to the definition of the KL-divergence term,

$$\begin{aligned} D_{\mathrm{KL}}\left(\mathbb{P}_{\mathcal{D}_{L+1}|\mathcal{E}}||\mathbb{Q}_{\mathcal{D}_{L+1}}\right) &= \mathbb{E}\left[\log \frac{p(\mathcal{D}_{L+1}|\mathcal{E})}{1/K\sum_{\widetilde{\mathcal{E}}\in\Theta_k} p(\mathcal{D}_{L+1}|\widetilde{\mathcal{E}})}\right] \\ &\leq \mathbb{E}\left[\log \frac{p(\mathcal{D}_{L+1}|\mathcal{E})}{1/K p(\mathcal{D}_{L+1}|\widetilde{\mathcal{E}})}\right] \\ &\leq \log(K) + D_{\mathrm{KL}}\left(\mathbb{P}_{\mathcal{D}_{L+1}|\mathcal{E}}||\mathbb{P}_{\mathcal{D}_{L+1}|\widetilde{\mathcal{E}}}\right) . \end{aligned} \tag{B.9}$$

By the chain rule of KL-divergence,

$$\begin{aligned} D_{\mathrm{KL}}\left(\mathbb{P}_{\mathcal{D}_{L+1}|\mathcal{E}}||\mathbb{P}_{\mathcal{D}_{L+1}|\widetilde{\mathcal{E}}}\right) &= \mathbb{E}\left[\sum_{\ell=1}^{L}\sum_{h=1}^{H} D_{\mathrm{KL}}\left(P(\cdot|s_h^\ell, a_h^\ell, \mathcal{E})||P(\cdot|s_h^\ell, a_h^\ell, \widetilde{\mathcal{E}})\right)\right] \\ &= \mathbb{E}\left[\sum_{\ell=1}^{L}\sum_{h=1}^{H} D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s_h^\ell, a_h^\ell)||P_h^{\widetilde{\mathcal{E}}}(\cdot|s_h^\ell, a_h^\ell)\right)\right] . \end{aligned}$$

It remains to construct a partition of $\{\Theta_k\}_{k=1}^K$ such that for any $\mathcal{E}\in\Theta$, there always exists $\widetilde{\mathcal{E}}\in\Theta_k$ such that for any s, a, h,

$$D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s,a)||P_h^{\widetilde{\mathcal{E}}}(\cdot|s,a)\right) \leq \varepsilon .$$

The existence of such partition is shown in the following theorem.

Theorem B.2 (Divergence covering number)**.** *For any $0<\varepsilon<1$, suppose $\mathcal{N}(k,\varepsilon)$ is a divergence covering set over k-dimensional probability simplex such that for any P, there exists $\widetilde{P}\in\mathcal{N}(k,\varepsilon)$ such that*

$$D_{\mathrm{KL}}(P||\widetilde{P}) \leq \varepsilon .$$

Then there exists such set whose covering number can be bounded by

$$|\mathcal{N}(k,\varepsilon)| \leq 8^{k-1}\left(\frac{k-1}{\varepsilon}\right)^{\frac{k-1}{2}} .$$

The proof could be found in Tang and Polyanskiy [2021, Theorem 4]. For each s, a, h, we construct such divergence covering set $\mathcal{N}_{sa}^h(S,\varepsilon)$ and the partition $\{\Theta_k\}_{k=1}^K$ is constructed such that $\mathcal{E}\in\Theta_k$ if for any s, a, h, $P_h^{\mathcal{E}}(\cdot|s,a)\in\mathcal{N}_{sa}^h(S,\varepsilon)$. According to Theorem B.2,

$$\log(K) \leq \log\left(|\mathcal{N}_{sa}^h(S,\varepsilon)|^{SAH}\right) \leq (S-1)SAH\log(8) + (S-1)SAH\log\left(\frac{S-1}{\varepsilon}\right) .$$

Therefore, together with Eq. (B.9),

$$\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1}) \leq LH\varepsilon + S^2AH\log\left(S/\varepsilon\right) .$$

By choosing $\varepsilon = 1/LH$,

$$\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1}) \leq 2S^2AH\log\left(SLH\right) .$$

This ends the proof. □

B.4 Proof of Proposition 3.8

According to the linearity of expectation and independence of priors over different layers, we can obtain $\mathbb{E}_\ell[V_{1,\pi}^{\mathcal{E}}(s_1^\ell)] = V_{1,\pi}^{\bar{\mathcal{E}}_\ell}(s_1^\ell)$ which implies

$$\mathbb{E}_\ell[V_{1,\pi}^{\mathcal{E}}(s_1^\ell)] = \mathbb{E}_\pi^{\bar{\mathcal{E}}_\ell}\left[\sum_{h=1}^{H} r_h(s_h,a_h)\right] .$$

According to the proof of Lemma B.1 in Appendix D.1

$$\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)=\sum_{h=1}^{H}\mathbb{E}_\pi^{\bar{\mathcal{E}}_\ell}\left[\int D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s_h,a_h)||P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s_h,a_h)\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E})\right].$$

Combining them together,

$$\begin{aligned}&\mathbb{E}_\ell[V_{1,\pi}^{\mathcal{E}}(s_1^\ell)]+\lambda\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)\\=&\mathbb{E}_\pi^{\bar{\mathcal{E}}_\ell}\left[\sum_{h=1}^{H}\left(r_h(s_h,a_h)+\lambda\int D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s_h,a_h)||P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s_h,a_h)\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E})\right)\right].\end{aligned}$$

B.5 Proof of Theorem 3.9

Proof. Using the fact that $2ab\le a^2+b^2$, we have for any policy π

$$\frac{\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell)-V_{1,\pi}^{\mathcal{E}}(s_1^\ell)\right]\sqrt{\lambda\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)}}{\sqrt{\lambda\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)}}\le\frac{\left(\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell)-V_{1,\pi}^{\mathcal{E}}(s_1^\ell)\right]\right)^2}{2\lambda\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)}+\frac{\lambda}{2}\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right).$$

This implies

$$\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell)-V_{1,\pi}^{\mathcal{E}}(s_1^\ell)\right]-\frac{\lambda}{2}\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)\le\frac{\left(\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell)-V_{1,\pi}^{\mathcal{E}}(s_1^\ell)\right]\right)^2}{2\lambda\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)}.$$

We follow the regret decomposition as

$$\begin{aligned}\mathfrak{BR}_L(\pi_{\text{r-IDS}})&=\sum_{\ell=1}^{L}\mathbb{E}\left[\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell)-V_{1,\pi_{\text{r-IDS}}^\ell}^{\mathcal{E}}(s_1^\ell)\right]\right]\\&=\mathbb{E}\left[\sum_{\ell=1}^{L}\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell)-V_{1,\pi_{\text{r-IDS}}^\ell}^{\mathcal{E}}(s_1^\ell)\right]-\lambda\sum_{\ell=1}^{L}\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)\right]+\mathbb{E}\left[\lambda\sum_{\ell=1}^{L}\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)\right]\\&\le\frac{1}{2\lambda}\sum_{\ell=1}^{L}\mathbb{E}\left[\frac{\left(\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell)-V_{1,\pi}^{\mathcal{E}}(s_1^\ell)\right]\right)^2}{\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right)}\right]+\lambda\mathbb{I}\left(\mathcal{E};\mathcal{D}_{L+1}\right)\\&\le\frac{L\mathbb{E}[\Gamma^*]}{2\lambda}+\lambda\mathbb{I}\left(\mathcal{E};\mathcal{D}_{L+1}\right),\end{aligned}$$

where Γ^* is the worst-case information ratio. Letting $\lambda=\sqrt{L\mathbb{E}[\Gamma^*]/\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1})}$, we have

$$\mathfrak{BR}_L(\pi^{\text{r-IDS}})\le\sqrt{\frac{3}{2}L\mathbb{E}[\Gamma^*]\mathbb{I}(\mathcal{E};\mathcal{D}_{L+1})}.$$

This ends the proof. □

C Proofs of learning a surrogate environment

C.1 Proof of Lemma 4.1

Proof. Conditional on $\mathcal{D}_\ell$, let $\mathcal{E}_\ell$ be an independent sample of $\mathcal{E}$. Note that

$$\begin{aligned}\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_\ell}(s_1^\ell)\middle|\mathcal{E}_\ell\in\Theta_k\right]&=\sum_{\mathcal{E}\in\Theta_k}\mathbb{P}\left(\mathcal{E}_\ell=\mathcal{E}|\mathcal{E}_\ell\in\Theta_k\right)\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}}(s_1^\ell)\middle|\mathcal{E}_\ell\in\Theta_k\right]\\&=\sum_{\mathcal{E}\in\Theta_k}\mathbb{P}\left(\mathcal{E}_\ell=\mathcal{E}|\mathcal{E}_\ell\in\Theta_k\right)\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}}(s_1^\ell)\right],\end{aligned}$$

where the last equation is due to the independence between $\mathcal{E}_\ell$ and $\mathcal{E}$. For each $k\in[K]$, according to Lemma E.1, there exists $\mathcal{E}_1^{k,\ell},\mathcal{E}_2^{k,\ell}\in\Theta_k$ and $r_{k,\ell}\in[0,1]$ such that

$$\begin{aligned}r_{k,\ell}\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_1^{k,\ell}}(s_1^\ell)\right]+(1-r_{k,\ell})\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_2^{k,\ell}}(s_1^\ell)\right]&\le\sum_{\mathcal{E}\in\Theta_k}\mathbb{P}\left(\mathcal{E}_\ell=\mathcal{E}|\mathcal{E}_\ell\in\Theta_k\right)\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}}(s_1^\ell)\right]\\&=\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_\ell}(s_1^\ell)\middle|\mathcal{E}_\ell\in\Theta_k\right].\end{aligned}$$

Recall that ζ is a discrete random variable taking values in $\{1, \dots, K\}$ that indicates the region $\mathcal{E}$ lies such that $\zeta = k$ if and only if $\mathcal{E} \in \Theta_k$. The surrogate learning target $\widetilde{\mathcal{E}}_\ell^*$ is a random variable such that

$$\mathbb{P}_\ell\left(\widetilde{\mathcal{E}}_\ell^* = \mathcal{E}_1^{k,\ell} | \zeta = k\right) = r_{k,\ell}, \mathbb{P}_\ell\left(\widetilde{\mathcal{E}}_\ell^* = \mathcal{E}_2^{k,\ell} | \zeta = k\right) = 1 - r_{k,\ell}\,. \tag{C.1}$$

This implies the law of $\widetilde{\mathcal{E}}_\ell^*$ only depends on ζ and conditional on ζ, $\widetilde{\mathcal{E}}_\ell^*$ is independent of $\mathcal{E}$.

We also need to ensure learning towards $\widetilde{\mathcal{E}}_\ell^*$ will not occur too much additional regret. Let $\widetilde{\mathcal{E}}_\ell$ be an independent sample of $\widetilde{\mathcal{E}}_\ell^*$. From the law of total expectations,

$$\begin{aligned}
&\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\widetilde{\mathcal{E}}_\ell}(s_1^\ell) - V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_\ell}(s_1^\ell)\right] \\
&= \sum_{k=1}^K \mathbb{P}\left(\mathcal{E}_\ell \in \Theta_k\right) \mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\widetilde{\mathcal{E}}_\ell}(s_1^\ell) - V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_\ell}(s_1^\ell) | \mathcal{E}_\ell \in \Theta_k\right] \\
&= \sum_{k=1}^K \mathbb{P}\left(\mathcal{E}_\ell \in \Theta_k\right) \left(r_{k,\ell}\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_1^{k,\ell}}(s_1^\ell)\right] + (1 - r_{k,\ell})\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_2^{k,\ell}}(s_1^\ell)\right] - \mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_\ell}(s_1^\ell) | \mathcal{E}_\ell \in \Theta_k\right]\right) \\
&\leq 0\,.
\end{aligned}$$

On the other hand, we have $\mathbb{E}_\ell[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}_\ell}(s_1^\ell)] = \mathbb{E}_\ell[V_{1,\pi_{\text{TS}}^\ell}^{\mathcal{E}}(s_1^\ell)]$ and this implies

$$\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\widetilde{\mathcal{E}}_\ell}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\mathcal{E}}(s_1^\ell)\right] \leq 0\,. \tag{C.2}$$

When $\mathcal{E} \in \Theta_k$, then $\zeta = k$ which implies $\widetilde{\mathcal{E}}_\ell^* \in \Theta_k$ either. That means $\mathcal{E}$ and $\widetilde{\mathcal{E}}^*$ are in the same partition and

$$\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}}(s_1^\ell) - V_{1,\pi_{\mathcal{E}}^*}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell)\right] \leq \varepsilon\,. \tag{C.3}$$

Putting Eqs. (C.2)-(C.3) together,

$$\mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\mathcal{E}}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\mathcal{E}}(s_1^\ell)\right] - \mathbb{E}_\ell\left[V_{1,\pi_{\mathcal{E}}^*}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) - V_{1,\pi_{\mathcal{E}}^*}^{\widetilde{\mathcal{E}}_\ell}(s_1^\ell)\right] \leq \varepsilon\,. \tag{C.4}$$

Noticing that $\mathbb{E}_\ell[V_{1,\pi_{\mathcal{E}}^*}^{\widetilde{\mathcal{E}}_\ell}(s_1^\ell)] = \mathbb{E}_\ell[V_{1,\pi_{\text{TS}}^\ell}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell)]$, this ends the proof. □

C.2 Proof of Theorem 4.2

Proof. We decompose

$$\begin{aligned}
\mathfrak{BR}_L(\pi_{\text{s-IDS}}) &= \sum_{\ell=1}^L \mathbb{E}\left[\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell) - V_{1,\pi_{\text{s-IDS}}^\ell}^{\mathcal{E}}(s_1^\ell)\right] - \varepsilon\right] + L\varepsilon \\
&\leq \sqrt{\mathbb{E}\left[\sum_{\ell=1}^L \frac{\left(\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell) - V_{1,\pi_{\text{s-IDS}}^\ell}^{\mathcal{E}}(s_1^\ell)\right] - \varepsilon\right)^2}{\mathbb{I}_\ell^{\pi_{\text{s-IDS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})}\right]} \sqrt{\mathbb{E}\left[\sum_{\ell=1}^L \mathbb{I}_\ell^{\pi_{\text{s-IDS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})\right]} + L\varepsilon\,.
\end{aligned}$$

From the definition of $\pi_{\text{s-IDS}}^\ell$ in Eq. (4.3),

$$\mathfrak{BR}_L(\pi_{\text{s-IDS}}) \leq \sqrt{\mathbb{E}\left[\sum_{\ell=1}^L \frac{\left(\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\mathcal{E}}(s_1^\ell)\right] - \varepsilon\right)^2}{\mathbb{I}_\ell^{\pi_{\text{TS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})}\right]} \sqrt{\mathbb{E}\left[\sum_{\ell=1}^L \mathbb{I}_\ell^{\pi_{\text{r-IDS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})\right]} + L\varepsilon\,.$$

According to Lemma 4.1,

$$\mathbb{E}_\ell\left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\mathcal{E}}(s_1^\ell)\right] - \varepsilon \leq \mathbb{E}_\ell\left[V_{1,\pi^*}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell)\right]\,.$$

For any $\ell \in [L]$, conditional on ζ, we have $\widetilde{\mathcal{E}}_\ell^*$ and $\mathcal{H}_{\ell,H}$ are independent under the law of $\mathbb{P}_{\ell,\pi^\ell_{\text{s-IDS}}}$. By the data processing inequality, we have

$$\mathbb{I}_\ell^{\pi^\ell_{\text{s-IDS}}}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H}) \le \mathbb{I}_\ell^{\pi^\ell_{\text{s-IDS}}}(\zeta; \mathcal{H}_{\ell,H}) \,.$$

Therefore,

$$\begin{aligned}
\mathfrak{BR}_L(\pi_{\text{s-IDS}}) &\le \sqrt{\mathbb{E}\left[\sum_{\ell=1}^L \frac{\left(\mathbb{E}_\ell\left[V^{\widetilde{\mathcal{E}}_\ell^*}_{1,\pi^*}(s_1^\ell) - V^{\widetilde{\mathcal{E}}_\ell^*}_{1,\pi^\ell_{\text{TS}}}(s_1^\ell)\right]\right)^2}{\mathbb{I}_\ell^{\pi^\ell_{\text{TS}}}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})}\right]} \sqrt{\mathbb{E}\left[\sum_{\ell=1}^L \mathbb{I}_\ell^{\pi^\ell_{\text{s-IDS}}}(\zeta; \mathcal{H}_{\ell,H})\right]} + L\varepsilon \\
&= \sqrt{\mathbb{E}\left[\sum_{\ell=1}^L \frac{\left(\mathbb{E}_\ell\left[V^{\widetilde{\mathcal{E}}_\ell^*}_{1,\pi^*}(s_1^\ell) - V^{\widetilde{\mathcal{E}}_\ell^*}_{1,\pi^\ell_{\text{TS}}}(s_1^\ell)\right]\right)^2}{\mathbb{I}_\ell^{\pi^\ell_{\text{TS}}}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})}\right]} \sqrt{\mathbb{I}(\zeta; \mathcal{D}_{L+1})} + L\varepsilon \,.
\end{aligned}$$

This ends the proof. □

C.3 Proof of Lemma 4.3

Proof. We construct a partition over Θ such that Eq. (4.1) holds. For any $\mathcal{E}_1, \mathcal{E}_2 \in \Theta_k$, we use Lemma E.3,

$$\begin{aligned}
& V^{\mathcal{E}_1}_{1,\pi^*_{\mathcal{E}_1}}(s_1) - V^{\mathcal{E}_2}_{1,\pi^*_{\mathcal{E}_1}}(s_1) \\
=& \sum_{h=1}^H \mathbb{E}^{\mathcal{E}_2}_{\pi^*_{\mathcal{E}_1}}\left[\mathbb{E}_{s'\sim P_h^{\mathcal{E}_1}(\cdot|s_h^\ell,a_h^\ell)}[V^{\mathcal{E}_1}_{h+1,\pi^*_{\mathcal{E}_1}}(s')] - \mathbb{E}_{s'\sim P_h^{\mathcal{E}_2}(\cdot|s_h^\ell,a_h^\ell)}[V^{\mathcal{E}_1}_{h+1,\pi^*_{\mathcal{E}_1}}(s')]\right] \\
=& \sum_{h=1}^H \mathbb{E}^{\mathcal{E}_2}_{\pi^*_{\mathcal{E}_1}}\left[P_h^{\mathcal{E}_1}(\cdot|s_h^\ell,a_h^\ell)^\top V^{\mathcal{E}_1}_{h+1,\pi^*_{\mathcal{E}_1}}(\cdot) - P_h^{\mathcal{E}_2}(\cdot|s_h^\ell,a_h^\ell)^\top V^{\mathcal{E}_2}_{h+1,\pi^*_{\mathcal{E}_1}}(\cdot)\right] \\
&+ \sum_{h=1}^H \mathbb{E}^{\mathcal{E}_2}_{\pi^*_{\mathcal{E}_1}}\left[P_h^{\mathcal{E}_2}(\cdot|s_h^\ell,a_h^\ell)^\top\left(V^{\mathcal{E}_2}_{h+1,\pi^*_{\mathcal{E}_1}}(\cdot) - V^{\mathcal{E}_1}_{h+1,\pi^*_{\mathcal{E}_1}}(\cdot)\right)\right] \\
\le& \sum_{h=1}^H \mathbb{E}^{\mathcal{E}_2}_{\pi^*_{\mathcal{E}_1}} \underbrace{\left[P_h^{\mathcal{E}_1}(\cdot|s_h^\ell,a_h^\ell)^\top V^{\mathcal{E}_1}_{h+1,\pi^*_{\mathcal{E}_1}}(\cdot) - P_h^{\mathcal{E}_2}(\cdot|s_h^\ell,a_h^\ell)^\top V^{\mathcal{E}_2}_{h+1,\pi^*_{\mathcal{E}_1}}(\cdot)\right]}_{I_1} \\
&+ \sum_{h=1}^H \mathbb{E}^{\mathcal{E}_2}_{\pi^*_{\mathcal{E}_1}} \underbrace{\left[\left\|V^{\mathcal{E}_2}_{h+1,\pi^*_{\mathcal{E}_1}}(\cdot) - V^{\mathcal{E}_1}_{h+1,\pi^*_{\mathcal{E}_1}}(\cdot)\right\|_2\right]}_{I_2} \,.
\end{aligned}$$

The construction follows the following steps.

- First, we construct a cover for I_1. Since the reward is assumed to be bounded by 1, we have $P_h^{\mathcal{E}}(\cdot|s_h^\ell,a_h^\ell)^\top V^{\mathcal{E}}_{h+1,\pi^*_{\mathcal{E}}}(\cdot) \in [0,H]$ for any $\mathcal{E}$. For each (s,a,h), we construct a covering set $\{\mathcal{I}^1_{sah},\ldots,\mathcal{I}^m_{sah}\}$ for $[0,1]$ where $m = H/\varepsilon$. Thus, each set is of length ε.
- Second, let $\{\mathcal{C}_1,\ldots,\mathcal{C}_M\}$ be an ε-covering of a S-dimensional ℓ_2-ball.
- Third, we construct the partition $\{\Theta_k\}_{k=1}^K$ in the way that $\mathcal{E} \in \Theta_k$ if for any s,a,h,

$$\left\langle P_h^{\mathcal{E}}(\cdot|s,a), V^{\mathcal{E}}_{h+1,\pi^*_{\mathcal{E}}}(\cdot)\right\rangle \in \mathcal{I}^{k_1}_{sah}, V^{\mathcal{E}}_{h+1,\pi^*_{\mathcal{E}}}(\cdot)/H \in \mathcal{C}_{k_2} \,,$$

  where $k_1 \in [m], k_2 \in [M]$. The existence of k_1, k_2 holds trivially.

Apparently, $\{\Theta_k\}_{k=1}^K$ is a partition of Θ. For any $k \in [K]$ and $\mathcal{E}_1, \mathcal{E}_2 \in \Theta_k$, the following holds for any s, a, h,

$$\left|\left\langle P_h^{\mathcal{E}_1}(\cdot|s,a), V_{h+1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(\cdot)\right\rangle - \left\langle P_h^{\mathcal{E}_2}(\cdot|s,a), V_{h+1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}(\cdot)\right\rangle\right| \le \varepsilon\,,$$

and

$$\left\|\left(V_{h+1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(\cdot) - V_{h+1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}(\cdot)\right)/H\right\|_2 \le \varepsilon\,.$$

Therefore, we have constructed a partition $\{\Theta_k\}_{k=1}^K$ over Θ such that for any $\mathcal{E}_1, \mathcal{E}_2 \in \Theta_k$,

$$V_{1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(s_1) - V_{1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}(s_1) \le \varepsilon\,,$$

with the covering number bounded by

$$K \le \left(\frac{H^2}{\varepsilon}\right)^{SAH} + \left(\frac{H^2}{\varepsilon}+1\right)^{S} \le 2(2H^2/\varepsilon)^{SAH}\,.$$

This ends the proof. □

C.4 Proof of Lemma 4.8

Proof. We construct a partition $\{\Theta_k\}_{k=1}^K$ over Θ^{Lin} such that Eq. (4.1) holds. For any $\mathcal{E}_1, \mathcal{E}_2 \in \Theta_k$, by Lemma E.3,

$$\begin{aligned}
&V_{1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(s_1) - V_{1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}(s_1)\\
=&\sum_{h=1}^H \mathbb{E}_{\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}\left[P_h^{\mathcal{E}_1}(\cdot|s_h^\ell,a_h^\ell)^\top V_{h+1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(\cdot) - P_h^{\mathcal{E}_2}(\cdot|s_h^\ell,a_h^\ell)^\top V_{h+1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(\cdot)\right]\\
=&\sum_{h=1}^H \mathbb{E}_{\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}\left[\phi(s_h^\ell,a_h^\ell)^\top \sum_{s'} V_{h+1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(s')\psi_h^{\mathcal{E}_1}(s') - \phi(s_h^\ell,a_h^\ell)^\top \sum_{s'} V_{h+1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(s')\psi_h^{\mathcal{E}_2}(s')\right]\,,
\end{aligned}$$

where the last equation is from the definition of linear MDP. Moreover, since the value function is always bounded by H, we have

$$\begin{aligned}
&V_{1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_1}(s_1) - V_{1,\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}(s_1) = H\sum_{h=1}^H \mathbb{E}_{\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}\left[\phi(s_h^\ell,a_h^\ell)^\top\left(\sum_{s'}\psi_h^{\mathcal{E}_1}(s') - \sum_{s'}\psi_h^{\mathcal{E}_2}(s')\right)\right]\\
&\le H\sum_{h=1}^H \mathbb{E}_{\pi^*_{\mathcal{E}_1}}^{\mathcal{E}_2}\left[\left\|\phi(s_h^\ell,a_h^\ell)\right\|_2\right]\left\|\sum_{s'}\psi_h^{\mathcal{E}_1}(s') - \sum_{s'}\psi_h^{\mathcal{E}_2}(s')\right\|_2\\
&\le H\sum_{h=1}^H\left\|\sum_{s'}\psi_h^{\mathcal{E}_1}(s') - \sum_{s'}\psi_h^{\mathcal{E}_2}(s')\right\|_2\,.
\end{aligned}$$

From Definition 4.7,

$$\left\|\sum_{s'}\psi_h^{\mathcal{E}}(s')\right\|_2 \le C_\psi\,.$$

For each $h \in [H]$, let $\{\mathcal{C}_1^h, \ldots, \mathcal{C}_K^h\}$ be an ε-covering of a d-dimensional ℓ_2-ball. We construct the partition $\{\Theta_k\}_{k=1}^K$ in the way that $\mathcal{E} \in \Theta_k$ if

$$\frac{1}{C_\psi}\sum_{s'}\psi_h^{\mathcal{E}}(s') \in \mathcal{C}_k^h\,.$$

Apparently, $\{\Theta_k\}_{k=1}^K$ is a partition of Θ. For any $k \in [K]$ and $\mathcal{E}_1, \mathcal{E}_2 \in \Theta_k$, the following holds

$$\left\|\frac{1}{C_\psi}\sum_{s'}\psi_h^{\mathcal{E}_1}(s') - \frac{1}{C_\psi}\sum_{s'}\psi_h^{\mathcal{E}_2}(s')\right\|_2 \le \varepsilon\,,$$

which implies

$$V^{\mathcal{E}_1}_{1,\pi^*_{\mathcal{E}_1}}(s_1) - V^{\mathcal{E}_2}_{1,\pi^*_{\mathcal{E}_1}}(s_1) \le H^2 C_\psi \varepsilon\,.$$

Letting $\varepsilon' = H^2 C_\psi \varepsilon$, the covering number can be bounded by

$$K \le \left(\frac{H^2 C_\psi}{\varepsilon'} + 1\right)^{Hd}.$$

This ends the proof. □

C.5 Proof of Lemma 4.9

Proof. We write $\bar{\mathcal{E}}^*_\ell$ as the MDP consisted by the mean of posterior measure of $\widetilde{\mathcal{E}}^*_\ell$. Noting that $\mathbb{E}_\ell[V^{\widetilde{\mathcal{E}}_\ell}_{1,\pi^*_{\mathcal{E}}}(s^\ell_1)] = \mathbb{E}_\ell[V^{\widetilde{\mathcal{E}}^*_\ell}_{1,\pi^\ell_{\mathrm{TS}}}(s^\ell_1)]$, we decompose the regret as

$$\begin{aligned}
\mathbb{E}_\ell\left[V^{\widetilde{\mathcal{E}}^*_\ell}_{1,\pi^*}(s^\ell_1) - V^{\widetilde{\mathcal{E}}^*_\ell}_{1,\pi^\ell_{\mathrm{TS}}}(s^\ell_1)\right] &= \mathbb{E}_\ell\left[V^{\widetilde{\mathcal{E}}^*_\ell}_{1,\pi^*}(s^\ell_1) - V^{\widetilde{\mathcal{E}}_\ell}_{1,\pi^*}(s^\ell_1)\right] \\
&= \underbrace{\mathbb{E}_\ell\left[V^{\widetilde{\mathcal{E}}^*_\ell}_{1,\pi^*}(s^\ell_1) - V^{\bar{\mathcal{E}}^*_\ell}_{1,\pi^*}(s^\ell_1)\right]}_{I_1} + \underbrace{\mathbb{E}_\ell\left[V^{\bar{\mathcal{E}}^*_\ell}_{1,\pi^*}(s^\ell_1) - V^{\widetilde{\mathcal{E}}_\ell}_{1,\pi^*}(s^\ell_1)\right]}_{I_2},
\end{aligned}$$

According to Lemma E.3,

$$I_1 = \mathbb{E}_\ell\left[\sum_{h=1}^H \mathbb{E}^{\bar{\mathcal{E}}_\ell}_{\pi^*}\left[P^{\widetilde{\mathcal{E}}^*_\ell}_h(\cdot|s^\ell_h,a^\ell_h)^\top V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(\cdot) - P^{\bar{\mathcal{E}}^*_\ell}_h(\cdot|s^\ell_h,a^\ell_h)^\top V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(\cdot)\right]\right].$$

Using the definition of linear MDPs in Definition 4.7,

$$\begin{aligned}
I_1 &= \mathbb{E}_\ell\left[\sum_{h=1}^H \mathbb{E}^{\bar{\mathcal{E}}^*_\ell}_{\pi^*}\left[\sum_{s'}\phi(s^\ell_h,a^\ell_h)^\top \psi^{\widetilde{\mathcal{E}}^*_\ell}_h(s')V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(s') - \sum_{s'}\phi(s^\ell_h,a^\ell_h)^\top \psi^{\bar{\mathcal{E}}^*_\ell}_h(s')V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(s')\right]\right] \\
&= \mathbb{E}_\ell\left[\sum_{h=1}^H \mathbb{E}^{\bar{\mathcal{E}}^*_\ell}_{\pi^*}\left[\phi(s^\ell_h,a^\ell_h)^\top\right]\sum_{s'}(\psi^{\widetilde{\mathcal{E}}^*_\ell}_h(s') - \psi^{\bar{\mathcal{E}}^*_\ell}_h(s'))V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(s')\right].
\end{aligned}$$

Denoting

$$\Sigma_h = \mathbb{E}_\ell\left[\mathbb{E}^{\bar{\mathcal{E}}^*_\ell}_{\pi^*}\left[\phi(s^\ell_h,a^\ell_h)\right]\mathbb{E}^{\bar{\mathcal{E}}^*_\ell}_{\pi^*}\left[\phi(s^\ell_h,a^\ell_h)^\top\right]\right],$$

we have

$$I_1 = \sum_{h=1}^H \mathbb{E}_\ell\left[\mathbb{E}^{\bar{\mathcal{E}}^*_\ell}_{\pi^*}\left[\phi(s^\ell_h,a^\ell_h)^\top\right]\Sigma_h^{-1/2}\Sigma_h^{1/2}\sum_{s'}(\psi^{\widetilde{\mathcal{E}}^*_\ell}_h(s') - \psi^{\bar{\mathcal{E}}^*_\ell}_h(s'))V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(s')\right]$$

By Cauchy–Schwarz inequality, we have

$$I_1 \le \sqrt{\sum_{h=1}^H \mathbb{E}_\ell\left[\left\|\Sigma_h^{1/2}\sum_{s'}(\psi^{\widetilde{\mathcal{E}}^*_\ell}_h(s') - \psi^{\bar{\mathcal{E}}^*_\ell}_h(s'))V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(s')\right\|_2^2\right]}\sqrt{\sum_{h=1}^H \mathbb{E}_\ell\left[\left\|\Sigma_h^{-1/2}\mathbb{E}^{\bar{\mathcal{E}}^*_\ell}_{\pi^*}\left[\phi(s^\ell_h,a^\ell_h)\right]\right\|_2^2\right]}.$$

- For the first part,

$$\begin{aligned}
&\sum_{h=1}^H \mathbb{E}_\ell\left[\left\|\Sigma_h^{1/2}\sum_{s'}(\psi^{\widetilde{\mathcal{E}}^*_\ell}_h(s') - \psi^{\bar{\mathcal{E}}^*_\ell}_h(s'))V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(s')\right\|_2^2\right] \\
&= \sum_{h=1}^H \mathbb{E}_\ell\left[\left(\mathbb{E}^{\bar{\mathcal{E}}^*_\ell}_{\pi^*}\left[\phi(s^\ell_h,a^\ell_h)^\top\right]\sum_{s'}(\psi^{\widetilde{\mathcal{E}}^*_\ell}_h(s') - \psi^{\bar{\mathcal{E}}^*_\ell}_h(s'))V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(s')\right)^2\right] \\
&= H^2\sum_{h=1}^H \mathbb{E}_\ell\left(\mathbb{E}^{\bar{\mathcal{E}}^*_\ell}_{\pi^*}\left[P^{\widetilde{\mathcal{E}}^*_\ell}_h(\cdot|s^\ell_h,a^\ell_h)^\top V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(\cdot)/H - P^{\bar{\mathcal{E}}^*_\ell}_h(\cdot|s^\ell_h,a^\ell_h)^\top V^{\widetilde{\mathcal{E}}^*_\ell}_{h+1,\pi^*}(\cdot)/H\right]\right)^2.
\end{aligned}$$

Applying Lemma B.1, we have

$$H^2 \sum_{h=1}^{H} \mathbb{E}_\ell \left[\left\| \Sigma_h^{1/2} \sum_{s'} (\psi_h^{\widetilde{\mathcal{E}}_\ell^*}(s') - \psi_h^{\bar{\mathcal{E}}_\ell^*}(s')) V_{h+1,\pi^*}^{\widetilde{\mathcal{E}}_\ell^*}(s') \right\|_2^2 \right] = H^2 \mathbb{I}_\ell^{\pi^*} \left(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H} \right) .$$

- For the second part, we can rewrite

$$\begin{aligned} &\mathbb{E}_\ell \left[\left\| \Sigma_h^{-1/2} \mathbb{E}_{\pi^*}^{\bar{\mathcal{E}}_\ell^*} \left[\phi(s_h^\ell, a_h^\ell) \right] \right\|_2^2 \right] \\ &= \left\langle \mathbb{E}_\ell \left[\mathbb{E}_{\pi^*}^{\bar{\mathcal{E}}_\ell^*} \left[\phi(s_h^\ell, a_h^\ell) \right] \mathbb{E}_{\pi^*}^{\bar{\mathcal{E}}_\ell^*} \left[\phi(s_h^\ell, a_h^\ell)^\top \right] \right], \Sigma_h^{-1} \right\rangle = \langle \Sigma_h, \Sigma_h^{-1} \rangle = d . \end{aligned}$$

Therefore, putting them together,

$$I_1 \leq \sqrt{H^3 d \mathbb{I}_\ell^{\pi^*} \left(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H} \right)} .$$

The derivation of bounding I_2 is similar so we omit the detailed proof here. This ends the proof. □

C.6 Proof of Theorem 4.11

Directly using Lemma 4.1, we can decompose

$$\begin{aligned} \mathfrak{BR}_L(\pi_{\text{TS}}) &= \sum_{\ell=1}^{L} \mathbb{E} \left[\mathbb{E}_\ell \left[V_{1,\pi^*}^{\mathcal{E}}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\mathcal{E}}(s_1^\ell) \right] \right] \\ &\leq \sum_{\ell=1}^{L} \mathbb{E} \left[\mathbb{E}_\ell \left[V_{1,\pi^*}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) \right] \right] + L\varepsilon \\ &\leq \sqrt{\mathbb{E} \left[\sum_{\ell=1}^{L} \frac{\left(\mathbb{E}_\ell \left[V_{1,\pi^*}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) \right] \right)^2}{\mathbb{I}_\ell^{\pi_{\text{TS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})} \right]} \sqrt{\mathbb{E} \left[\sum_{\ell=1}^{L} \mathbb{I}_\ell^{\pi_{\text{TS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H}) \right]} + L\varepsilon . \end{aligned}$$

By the construction of $\widetilde{\mathcal{E}}_\ell^*$, $\widetilde{\mathcal{E}}_\ell^*$ and $\mathcal{E}$ are independent conditional on ζ. Thus $\widetilde{\mathcal{E}}_\ell^*$ and $\mathcal{H}_{\ell,H}$ are independent under the law $\mathbb{P}_{\ell,\pi_{\text{TS}}^\ell}$ given ζ. By the data processing inequality, we have

$$\mathbb{I}_\ell^{\pi_{\text{TS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H}) \leq \mathbb{I}_\ell^{\pi_{\text{TS}}^\ell}(\zeta; \mathcal{H}_{\ell,H}) .$$

Therefore,

$$\begin{aligned} \mathfrak{BR}_L(\pi_{\text{TS}}) &\leq \sqrt{\mathbb{E} \left[\sum_{\ell=1}^{L} \frac{\left(\mathbb{E}_\ell \left[V_{1,\pi^*}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) \right] \right)^2}{\mathbb{I}_\ell^{\pi_{\text{TS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})} \right]} \sqrt{\mathbb{E} \left[\sum_{\ell=1}^{L} \mathbb{I}_\ell^{\pi_{\text{TS}}^\ell}(\zeta; \mathcal{H}_{\ell,H}) \right]} + L\varepsilon \\ &= \sqrt{\mathbb{E} \left[\sum_{\ell=1}^{L} \frac{\left(\mathbb{E}_\ell \left[V_{1,\pi^*}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) - V_{1,\pi_{\text{TS}}^\ell}^{\widetilde{\mathcal{E}}_\ell^*}(s_1^\ell) \right] \right)^2}{\mathbb{I}_\ell^{\pi_{\text{TS}}^\ell}(\widetilde{\mathcal{E}}_\ell^*; \mathcal{H}_{\ell,H})} \right]} \sqrt{\mathbb{I}(\zeta; \mathcal{D}_{L+1})} + L\varepsilon . \end{aligned}$$

This ends the proof.

D Proofs of technical lemmas

D.1 Proof of Lemma B.1

Proof. Using the chain rule of mutual information,

$$\begin{aligned}\mathbb{I}_\ell^\pi\left(\mathcal{E};\mathcal{H}_{\ell,H}\right) &= \sum_{h=1}^{H}\mathbb{E}_\ell\left[\mathbb{I}_\ell^\pi\left(\mathcal{E};(s_h^\ell,a_h^\ell,r_h^\ell)\middle|\mathcal{H}_{\ell,h-1}\right)\right]\\ &= \sum_{h=1}^{H}\mathbb{E}_\ell\left[\mathbb{I}_\ell^\pi\left(\mathcal{E};s_h^\ell\middle|\mathcal{H}_{\ell,h-1}\right)\right]+\sum_{h=1}^{H}\mathbb{E}_\ell\left[\mathbb{I}_\ell^\pi\left(\mathcal{E};a_h^\ell\middle|s_h^\ell,\mathcal{H}_{\ell,h-1}\right)\right]\\ &\quad+\sum_{h=1}^{H}\mathbb{E}_\ell\left[\mathbb{I}_\ell^\pi\left(\mathcal{E};r_h^\ell\middle|s_h^\ell,a_h^\ell,\mathcal{H}_{\ell,h-1}\right)\right]\,.\end{aligned} \tag{D.1}$$

- For the first term in Eq. (D.1), by the definition of conditional mutual information and Markov property, we have

$$\begin{aligned}&\mathbb{I}_\ell^\pi\left(\mathcal{E};s_h^\ell\middle|\mathcal{H}_{\ell,h-1}\right)\\ &=\int D_{\mathrm{KL}}\left(\mathbb{P}_{\ell,\pi}\left(s_h^\ell=\cdot|\mathcal{H}_{\ell,h-1},\mathcal{E}\right)||\mathbb{P}_{\ell,\pi}\left(s_h^\ell=\cdot|\mathcal{H}_{\ell,h-1}\right)\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E}|\mathcal{H}_{\ell,h-1})\\ &=\int D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}\left(\cdot|s_{h-1}^\ell,a_{h-1}^\ell\right)||\mathbb{P}_{\ell,\pi}\left(s_h^\ell=\cdot|\mathcal{H}_{\ell,h-1}\right)\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E}|\mathcal{H}_{\ell,h-1})\,.\end{aligned} \tag{D.2}$$

  Since the priors of transition probability kernel are independent over different layers, $\mathbb{P}_\ell(\mathcal{E}|\mathcal{H}_{\ell,h-1})=\mathbb{P}_\ell(\mathcal{E})$ such that

$$\begin{aligned}\mathbb{P}_{\ell,\pi}\left(s_h^\ell=\cdot|\mathcal{H}_{\ell,h-1}\right) &= \int\mathbb{P}_{\ell,\pi}\left(s_h^\ell=\cdot|\mathcal{H}_{\ell,h-1},\mathcal{E}\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E}|\mathcal{H}_{\ell,h-1})\\ &=\int P_h^{\mathcal{E}}(\cdot|s_{h-1}^\ell,a_{h-1}^\ell)\,\mathrm{d}\mathbb{P}_\ell(\mathcal{E}|\mathcal{H}_{\ell,h-1})\\ &=\int P_h^{\mathcal{E}}(\cdot|s_{h-1}^\ell,a_{h-1}^\ell)\,\mathrm{d}\mathbb{P}_\ell(\mathcal{E})\\ &=P_h^{\bar{\mathcal{E}}_\ell}\left(\cdot|s_{h-1}^\ell,a_{h-1}^\ell\right)\,,\end{aligned} \tag{D.3}$$

  where the last equation is by the definition of probability kernel $P_h^{\bar{\mathcal{E}}_\ell}$. Combining Eqs. (D.2) and (D.3) together,

$$\mathbb{I}_\ell^\pi\left(\mathcal{E};s_h^\ell\middle|\mathcal{H}_{\ell,h-1}\right)=\int D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s_{h-1}^\ell,a_{h-1}^\ell)||P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s_{h-1}^\ell,a_{h-1}^\ell)\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E})\,.$$

  Therefore,

$$\begin{aligned}&\mathbb{E}_\ell\left[\mathbb{I}_\ell^\pi\left(\mathcal{E};s_h^\ell\middle|\mathcal{H}_{\ell,h-1}\right)\right]\\ &=\mathbb{E}_\ell\left[\int D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s_{h-1}^\ell,a_{h-1}^\ell)||P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s_{h-1}^\ell,a_{h-1}^\ell)\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E})\right]\\ &=\sum_{(s,a)}\mathbb{P}_{\ell,\pi}(s_{h-1}^\ell=s,a_{h-1}^\ell=a)\int D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s,a)||P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s,a)\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E})\\ &=\sum_{(s,a)}\int\mathbb{P}_{\ell,\pi}(s_{h-1}^\ell=s,a_{h-1}^\ell=a|\mathcal{E})\,\mathrm{d}\mathbb{P}_\ell(\mathcal{E})\int D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s,a)||P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s,a)\right)\mathrm{d}\mathbb{P}_\ell(\mathcal{E})\,.\end{aligned}$$

  Using the linearity of expectation and the independence of priors over different layers, we can show

$$\int\mathbb{P}_{\ell,\pi}(s_{h-1}^\ell=s,a_{h-1}^\ell=a|\mathcal{E})\,\mathrm{d}\mathbb{P}_\ell(\mathcal{E})=\mathbb{P}_\pi^{\bar{\mathcal{E}}_\ell}(s_{h-1}^\ell=s,a_{h-1}^\ell=a)\,.$$

This implies

$$
\begin{aligned}
&\mathbb{E}_\ell\left[\mathbb{I}_\ell^\pi\left(\mathcal{E}; s_h^\ell \middle| \mathcal{H}_{\ell,h-1}\right)\right] \\
&= \sum_{(s,a)} \mathbb{P}_\pi^{\bar{\mathcal{E}}_\ell}(s_{h-1}^\ell = s, a_{h-1}^\ell = a) \int D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s,a) || P_h^{\bar{\mathcal{E}}}(\cdot|s,a)\right) \mathrm{d}\mathbb{P}_\ell(\mathcal{E}) \\
&= \int \mathbb{E}_\pi^{\bar{\mathcal{E}}_\ell}\left[D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s_{h-1}^\ell, a_{h-1}^\ell) || P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s_{h-1}^\ell, a_{h-1}^\ell)\right)\right] \mathrm{d}\mathbb{P}_\ell(\mathcal{E}) \\
&= \mathbb{E}_\ell\left[\mathbb{E}_\pi^{\bar{\mathcal{E}}_\ell}\left[D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s_{h-1}^\ell, a_{h-1}^\ell) || P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s_{h-1}^\ell, a_{h-1}^\ell)\right)\right]\right] ,
\end{aligned}
$$

where $\mathbb{E}_\pi^{\bar{\mathcal{E}}_\ell}$ is taken with respect to $s_{h-1}^\ell, a_{h-1}^\ell$ and $\mathbb{E}_\ell$ is taken with respect to $\mathcal{E}$.

- For the second term of Eq. (D.1), we have

$$
\begin{aligned}
&\mathbb{I}_\ell^\pi\left(\mathcal{E}; a_h^\ell \middle| s_h^\ell, \mathcal{H}_{\ell,h-1}\right) \\
&= \int D_{\mathrm{KL}}\left(\mathbb{P}_{\ell,\pi}\left(a_h^\ell = \cdot|\mathcal{H}_{\ell,h-1}, s_h^\ell, \mathcal{E}\right) || \mathbb{P}_{\ell,\pi}\left(a_h^\ell = \cdot|s_h^\ell, \mathcal{H}_{\ell,h-1}\right)\right) \mathrm{d}\mathbb{P}_\ell(\mathcal{E}) .
\end{aligned}
$$

  When $\mathcal{H}_{\ell,h-1}^\pi$ is fixed, both sides of the KL term are equal to $\pi(\cdot|s_h^\ell)$ and thus $\mathbb{I}_\ell^\pi(\mathcal{E}; a_h^\ell | s_h^\ell, \mathcal{H}_{\ell,h-1}) = 0$.

- For the third term of Eq. (D.1), since the reward function is deterministic and known, we have

$$
\mathbb{I}_\ell^\pi\left(\mathcal{E}; r_h^\ell \middle| s_h^\ell, a_h^\ell, \mathcal{H}_{\ell,h-1}^\pi\right) = 0 .
$$

This suffices to show

$$
\sum_{h=1}^H \mathbb{E}_\ell \mathbb{E}_{\pi_{\mathrm{TS}}^\ell}^{\bar{\mathcal{E}}_\ell}\left[D_{\mathrm{KL}}\left(P_h^{\mathcal{E}}(\cdot|s_h,a_h) || P_h^{\bar{\mathcal{E}}_\ell}(\cdot|s_h,a_h)\right)\right] = \mathbb{I}_\ell^\pi\left(\mathcal{E}; \mathcal{H}_{\ell,H}\right) . \tag{D.4}
$$

This ends the proof.

□

E Supporting lemmas

Lemma E.1 (Lemma 1 in Dong and Roy [2018]). *Let $\{a_i\}_{i=1}^N$ and $\{b_i\}_{i=1}^N$ be two sequences of real numbers, where $N < \infty$. Let $\{p_i\}_{i=1}^N$ be such that $p_i \geq 0$ for all i and $\sum_{i=1}^N p_i = 1$. Then there exists indices $j, k \in [N]$ and $r \in [0,1]$ such that*

$$
r a_j + (1-r) a_k \leq \sum_{i=1}^N a_i p_i, r b_j + (1-r) b_k \leq \sum_{i=1}^L b_i p_i .
$$

Lemma E.2 (Fact 9 in Russo and Van Roy [2014]). *For any distribution P and Q such that P is absolutely continuous with respect to Q, any random variable $X : \Omega \to \mathcal{X}$ and any $g : \mathcal{X} \to \mathbb{R}$ such that $\sup g - \inf g \leq 1$, we have*

$$
\mathbb{E}_P[g(x)] - \mathbb{E}_Q[g(x)] \leq \sqrt{\frac{1}{2} D_{\mathrm{KL}}(P||Q)} ,
$$

which is a variant of Pinsker's inequality.

Lemma E.3. *For any two environments $\mathcal{E}, \mathcal{E}'$, any policy π and a fixed set of reward functions $\{r_h\}_{h=1}^H$, we have*

$$
V_{1,\pi}^{\mathcal{E}}(s_1) - V_{1,\pi}^{\mathcal{E}'}(s_1) = \sum_{h=1}^H \mathbb{E}_\pi^{\mathcal{E}'}\left[\mathbb{E}_{s' \sim P_h^{\mathcal{E}}(\cdot|s_h,a_h)}[V_{h+1,\pi}^{\mathcal{E}}(s')] - \mathbb{E}_{s' \sim P_h^{\mathcal{E}'}(\cdot|s_h,a_h)}[V_{h+1,\pi}^{\mathcal{E}}(s')]\right] ,
$$

where we define $V_{H+1,\pi^*}^{\mathcal{E}}(\cdot) = 0$ and the outer expectation $\mathbb{E}_\pi^{\mathcal{E}'}$ is with respect to s_h, a_h.

Proof. Similar proofs can be found in Osband et al. [2013], Foster et al. [2021]. For the self-completeness, we include a full proof here. First, we realize

$$\begin{aligned}
&\sum_{h=1}^{H} \mathbb{E}_{\pi}^{\mathcal{E}'} \left[Q_{h,\pi}^{\mathcal{E}}(s_h, a_h) - r_h(s_h, a_h) - V_{h+1,\pi}^{\mathcal{E}}(s_{h+1}) \right] \\
&= \sum_{h=1}^{H} \mathbb{E}_{\pi}^{\mathcal{E}'} \left[Q_{h,\pi}^{\mathcal{E}}(s_h, a_h) - V_{h+1,\pi}^{\mathcal{E}}(s_{h+1}) \right] - \sum_{h=1}^{H} \mathbb{E}_{\pi}^{\mathcal{E}'} \left[r_h(s_h, a_h) \right] \\
&= \sum_{h=1}^{H} \mathbb{E}_{\pi}^{\mathcal{E}'} \left[Q_{h,\pi}^{\mathcal{E}}(s_h, a_h) - V_{h+1,\pi}^{\mathcal{E}}(s_{h+1}) \right] - V_{1,\pi}^{\mathcal{E}'}(s_1) \,.
\end{aligned} \tag{E.1}$$

Since $V_{h,\pi}^{\mathcal{E}}(s) = \mathbb{E}_{a \sim \pi_h(\cdot|s)}[Q_{h,\pi}^{\mathcal{E}}(s, a)]$, we have

$$\begin{aligned}
&\sum_{h=1}^{H} \mathbb{E}_{\pi}^{\mathcal{E}'} \left[Q_{h,\pi}^{\mathcal{E}}(s_h, a_h) - V_{h+1,\pi}^{\mathcal{E}}(s_{h+1}) \right] = \sum_{h=1}^{H} \mathbb{E}_{\pi}^{\mathcal{E}'} \left[V_{h,\pi}^{\mathcal{E}}(s_h) - V_{h+1,\pi}^{\mathcal{E}}(s_{h+1}) \right] \\
&= \mathbb{E}_{\pi}^{\mathcal{E}'} \left[V_{1,\pi}^{\mathcal{E}}(s_1) \right] = V_{1,\pi}^{\mathcal{E}}(s_1) \,.
\end{aligned} \tag{E.2}$$

Using the Bellman equation, we have

$$\begin{aligned}
&V_{1,\pi}^{\mathcal{E}}(s_1) - V_{1,\pi}^{\mathcal{E}'}(s_1) \\
&= \sum_{h=1}^{H} \mathbb{E}_{\pi}^{\mathcal{E}'} \left[\mathbb{E}_{s' \sim P_h^{\mathcal{E}}(\cdot|s_h, a_h)}[V_{h+1,\pi}^{\mathcal{E}}(s')] - \mathbb{E}_{s' \sim P_h^{\mathcal{E}'}(\cdot|s_h, a_h)}[V_{h+1,\pi}^{\mathcal{E}}(s')] \right] \,.
\end{aligned}$$

This ends the proof. □