Model Selection in Reinforcement Learning with General Function Approximations

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Abstract. We³ consider model selection for classic Reinforcement Learning (RL) environments – Multi Armed Bandits (MABs) and Markov Decision Processes (MDPs) – under general function approximations. In the model selection framework, we do not know the function classes, denoted by \mathcal{F} and \mathcal{M} , where the true models – reward generating function for MABs and and transition kernel for MDPs – lie, respectively. Instead, we are given M nested function (hypothesis) classes such that true models are contained in at-least one such class. In this paper, we propose and analyze efficient model selection algorithms for MABs and MDPs, that adapt to the smallest function class (among the nested M classes) containing the true underlying model. Under a separability assumption on the nested hypothesis classes, we show that the cumulative regret of our adaptive algorithms match to that of an oracle which knows the correct function classes (i.e., \mathcal{F} and \mathcal{M}) a priori. Furthermore, for both the settings, we show that the cost of model selection is an additive term in the regret having weak (logarithmic) dependence on the learning horizon T.

Keywords: Model Selection · Bandits · Reinforcement Learning

1 Introduction

We study the problem of model selection for Reinforcement Learning problems, which refers to choosing the appropriate hypothesis class, to model the mapping from actions to expected rewards. We choose two particular frameworks—(a) Multi-Armaed Bandits (MAB) and (b) markov Decision Processes (MDP). Specifically, we are interested in studying the model selection problems for these frameworks without any function approximations (like linear, generalized linear etc.). Note that, the problem of model selection plays an important role in applications such as personalized recommendations, autonomous driving, robotics as we explain in the sequel. Formally, a family of nested hypothesis classes \mathcal{H}_f , $f \in \mathcal{F}$ is specified, where each class posits a plausible model for mapping actions to expected rewards. Furthermore, the family \mathcal{F} is totally ordered, i.e., if $f_1 \leq f_2$, then $\mathcal{H}_{f_1} \subseteq \mathcal{H}_{f_2}$. It is assumed that the true model is contained in

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at least one of these specified families. Model selection guarantees then refer to algorithms whose regret scales in the complexity of the *smallest hypothesis class containing the true model*, even though the algorithm was not aware apriori.

Multi-Armed Bandits (MAB) [7] and Markov decision processes (MDP) [25] are classical frameworks to model a reinforcement learning (RL) environment, where an agent interacts with the environment by taking successive decisions and observe rewards generated by those decisions. One of the objectives in RL is to maximize the total reward accumulated over multiple rounds, or equivalently minimize the regret in comparison with an optimal policy [7]. Regret minimization is useful in several sequential decision-making problems such as portfolio allocation and sequential investment, dynamic resource allocation in communication systems, recommendation systems, etc. In these settings, there is no separate budget to purely explore the unknown environment; rather, exploration and exploitation need to be carefully balanced.

Optimization over large domains under restricted feedback is an important problem and has found applications in dynamic pricing for economic markets [6], wireless communication [8] and recommendation platforms (such as Netflix, Amazon Prime). Furthermore, in many applications (e.g., robotics, autonomous driving), the number of actions and the observable number of states can be very large or even infinite, which makes RL challenging, particularly in generalizing learnt knowledge across unseen states and actions. For example, the game of Go has a state space with size 3^{361} , and the state and action spaces of certain robotics applications can even be continuous. In recent years, we have witnessed an explosion in the RL literature to tackle this challenge, both in theory (see, e.g., [4,10,18,22,29]), and in practice (see, e.g., [21,31]).

In the first part of the paper, we focus on learning an unknown function $f^* \in \mathcal{F}$, supported over a compact domain, via online noisy observations. If the function class \mathcal{F} is known, the optimistic algorithm of [26] learns f^* , yielding a regret that depends on eluder dimension (a complexity measure of function classes) of \mathcal{F} . However, in the applications mentioned earlier, it is not immediately clear how one estimates \mathcal{F} . Naive estimation techniques may yield an unnecessarily big \mathcal{F} , and as a consequence, the regret may suffer. On the other hand, if the estimated class, $\widehat{\mathcal{F}}$ is such that $\widehat{\mathcal{F}} \subset \mathcal{F}$, then the learning algorithm might yield a linear regret because of this infeasibility. Hence, it is important to estimate the function class properly, and here is where the question of model selection appears. The problem of model selection is formally stated as followswe are given a family of M hypothesis classes $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \ldots \subset \mathcal{F}_M$, and the unknown function f^* is assumed to be contained in the family of nested classes. In particular, we assume that f^* lies in \mathcal{F}_{m^*} , where m^* is unknown. Model selection guarantees refer to algorithms whose regret scales in the complexity of the smallest model class containing the true function f^* , i.e., \mathcal{F}_{m^*} , even though the algorithm is not aware of that a priori.

In the second part of the paper, we address the model selection problem for generic MDPs without function approximation. The most related work to ours is by [4], which proposes an algorithm, namely UCRL-VTR, for model-based RL

without any structural assumptions, and it is based on the upper confidence RL and value-targeted regression principles. The regret of UCRL-VTR depends on the eluder dimension [26] and the metric entropy of the corresponding family of distributions \mathcal{P} in which the unknown transition model P^* lies. In most practical cases, however, the class \mathcal{P} given to (or estimated by) the RL agent is quite pessimistic; meaning that P^* actually lies in a small subset of \mathcal{P} (e.g., in the game of Go, the learning is possible without the need for visiting all the states [27]). We are given a family of M nested hypothesis classes $\mathcal{P}_1 \subset \mathcal{P}_2 \subset \ldots \subset \mathcal{P}_M$, where each class posits a plausible model class for the underlying RL problem. The true model P^* lies in a model class \mathcal{P}_{m*} , where m^* is unknown apriori. Similar to the functional bandits framework, we propose learning algorithms whose regret depends on the smallest model class containing the true model P^* .

The problem of model selection have received considerable attention in the last few years. Model selection is well studied in the contextual bandit setting. In this setting, minimax optimal regret guarantees can be obtained by exploiting the structure of the problem along with an eigenvalue assumption [9,12,15] We provide a comprehensive list of recent works on bandit model selection in Section 1.2. However, to the best of our knowledge, this is the first work to address the model selection question for generic (functional) MAB without imposing any assumptions on the reward structure.

In the RL framework, the question of model selection has received little attention. In a series of works, [23,24] consider the corralling framework of [2] for contextual bandits and reinforcement learning. While the corralling framework is versatile, the price for this is that the cost of model selection is multiplicative rather than additive. In particular, for the special case of linear bandits and linear reinforcement learning, the regret scales as \sqrt{T} in time with an additional multiplicative factor of \sqrt{M} , while the regret scaling with time is strictly larger than \sqrt{T} in the general contextual bandit. These papers treat all the hypothesis classes as bandit arms, and hence work in a (restricted) partial information setting, and as a consequence explore a lot, yielding worse regret. On the other hand, we consider all M classes at once (full information setting) and do inference, and hence explore less and obtain lower regret.

Very recently, [20] study the problem of model selection in RL with function approximation. Similar to the active-arm elimination technique employed in standard multi-armed bandit (MAB) problems [11], the authors eliminate the model classes that are dubbed misspecified, and obtain a regret of $\mathcal{O}(T^{2/3})$. On the other hand, our framework is quite different in the sense that we consider model selection for RL with general transition structure. Moreover, our regret scales as $\mathcal{O}(\sqrt{T})$. Note that the model selection guarantees we obtain in the linear MDPs are partly influenced by [15], where model selection for linear contextual bandits are discussed. However, there are a couple of subtle differences: (a) for linear contextual framework, one can perform pure exploration, and [15] crucially leverages that and (b) the contexts in linear contextual framework is assumed to be i.i.d, whereas for linear MDPs, the contexts are implicit and depend on states, actions and transition probabilities.

1.1 Our Contributions

In this paper, our setup considers any general model class (for both MAB and MDP settings) that are totally bounded, i.e., for arbitrary precision, the metric entropy is bounded. Note that this encompasses a significantly larger class of environments compared to the problems with function approximation. Assuming nested families of reward function and transition kernels, respectively for MABs and MDPs, we propose adaptive algorithms, namely Adaptive Bandit Learning (ABL) and Adaptive Reinforcement Learning (ARL). Assuming the hypothesis classes are separated, both ABL and ARL construct a test statistic and thresholds it to identify the correct hypothesis class. We show that these simple schemes achieve the regret of $\tilde{\mathcal{O}}(d^* + \sqrt{d^*\mathbb{M}^*T})$ for MABs and $\tilde{\mathcal{O}}(d^*H^2 + \sqrt{d^*\mathbb{M}^*H^2T})$ for MDPs (with episode length H), where $d_{\mathcal{E}}^*$ is the eluder dimension and \mathbb{M}^* is the metric entropy corresponding to the smallest model classes containing true models (f^* for MAB and P^* for MDP). The regret bounds show that both ABL and ARL adapts to the true problem complexity, and the cost of model section is only $\mathcal{O}(\log T)$, which is minimal compared to the total regret.

Notation For a positive integer n, we denote by [n] the set of integers $\{1, 2, ..., n\}$. For a set \mathcal{X} and functions $f, g: \mathcal{X} \to \mathbb{R}$, we denote (f - g)(x) := f(x) - g(x) and $(f - g)^2(x) := (f(x) - g(x))^2$ for any $x \in \mathcal{X}$. For any $P: \mathcal{Z} \to \Delta(\mathcal{X})$, we denote $(Pf)(z) := \int_{\mathcal{X}} f(x)P(x|z)dx$ for any $z \in \mathcal{Z}$, where $\Delta(\mathcal{X})$ denotes the set of signed distributions over \mathcal{X} .

1.2 Related Work

Model Selection in Online Learning: Model selection for bandits are only recently being studied [9,13]. These works aim to identify whether a given problem instance comes from contextual or standard setting. For linear contextual bandits, with the dimension of the underlying parameter as a complexity measure, [12,15] propose efficient algorithms that adapts to the *true* dimension of the problem. While [12] obtains a regret of $\mathcal{O}(T^{2/3})$, [15] obtains a $\mathcal{O}(\sqrt{T})$ regret (however, the regret of [15] depends on several problem dependent quantities and hence not instance uniform). Later on, these guarantees are extended to the generic contextual bandit problems without linear structure [16,19], where $\mathcal{O}(\sqrt{T})$ regret guarantees are obtained. The algorithm Corral was proposed in [2], where the optimal algorithm for each model class is casted as an expert, and the forecaster obtains low regret with respect to the best expert (best model class). The generality of this framework has rendered it fruitful in a variety of different settings; see, for example [2,3].

RL with Function Approximation: Regret minimization in RL under function approximation is first considered in [22]. It makes explicit model-based assumptions and the regret bound depends on the eluder dimensions of the models. In contrast, [32] considers a low-rank linear transition model and propose a model-based algorithm with regret $\mathcal{O}(\sqrt{d^3H^3T})$. Another line of work parameterizes the *Q*-functions directly, using state-action feature maps, and develop model-free algorithms with regret $\mathcal{O}(\text{poly}(dH)\sqrt{T})$ bypassing the need for fully

learning the transition model [17, 30, 35]. A recent line of work [29, 33] generalize these approaches by designing algorithms that work with general and neural function approximations, respectively.

2 Model Selection in Functional Multi-armed Bandits

Consider the problem of sequentially maximizing an unknown function $f^*: \mathcal{X} \to \mathbb{R}$ over a compact domain $\mathcal{X} \subset \mathbb{R}^d$. For example, in a machine learning application, $f^*(x)$ can be the validation accuracy of a learning algorithm and $x \in \mathcal{X}$ is a fixed configuration of (tunable) hyper-parameters of the training algorithm. The objective is to find the hyper-parameter configuration that achieves the highest validation accuracy. An algorithm for this problem chooses, at each round t, an input (also called action or arm) $x_t \in \mathcal{X}$, and subsequently observes a function evaluation (also called reward) $y_t = f^*(x_t) + \varepsilon_t$, which is a noisy version of the function value at x_t . The action x_t is chosen causally depending upon the history $\{x_1, y_1, \ldots, x_{t-1}, y_{t-1}\}$ of arms and reward sequences available before round t.

Assumption 1 (Sub-Gaussian noise) The noise sequence $\{\varepsilon_t\}_{t\geq 1}$ is conditionally zero-mean, i.e., $\mathbb{E}\left[\varepsilon_t|\mathcal{F}_{t-1}\right]=0$ and σ -sub-Gaussian for known σ , i.e.,

$$\forall t \geq 1, \ \forall \lambda \in \mathbb{R}, \ \mathbb{E}\left[\exp(\lambda \varepsilon_t) | \mathcal{F}_{t-1}\right] \leq \exp\left(\frac{\lambda^2 \sigma^2}{2}\right)$$

almost surely, where $\mathcal{F}_{t-1} := \sigma(x_1, y_1, \dots, x_{t-1}, y_{t-1}, x_t)$ is the σ -field summarizing the information available just before y_t is observed.

This is a mild assumption on the noise (it holds, for instance, for distributions bounded in $[-\sigma, \sigma]$) and is standard in the literature [1, 26, 28].

Regret: The learner's goal is to maximize its (expected) cumulative reward $\sum_{t=1}^{t} f^*(x_t)$ over a time horizon T (not necessarily known a priori) or, equivalently, minimize its cumulative regret

$$\mathcal{R}_T := \sum_{t=1}^T (f^*(x^*) - f^*(x_t)),$$

where $x^* \in \operatorname{argmax}_{x \in \mathcal{X}} f(x)$ is a maximizer of f (assuming the maximum is attained; not necessarily unique). A sublinear growth of \mathcal{R}_T implies the time-average regret $\mathcal{R}_T/T \to 0$ as $T \to \infty$, implying the algorithm eventually chooses actions that attain function values close to the optimum most of the time.

2.1 Model Selection Objective

In the literature, it is assumed that f^* belongs to a known class of functions \mathcal{F} . In this work, in contrast to the standard setting, we do not assume the knowledge of \mathcal{F} . Instead, we are given M nested function classes $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \ldots \subset \mathcal{F}_M$. Among the nested classes $\mathcal{F}_1, \ldots \mathcal{F}_M$, the ones containing f^* is denoted as realizable classes, and the ones not containing f^* are dubbed as non-realizable classes. The

smallest such family where the unknown function f^* lies is denoted by \mathcal{F}_{m^*} , where $m^* \in [M]$. However, we do not know the index m^* , and our goal is to propose adaptive algorithms such that the regret depends on the complexity of the function class \mathcal{F}_{m^*} . In order to achieve this, we need a separability condition on the nested models.

Assumption 2 (Local Separability) There exist $\Delta > 0$ and $\eta > 0$ such that

$$\inf_{f \in \mathcal{F}_{m^*-1}} \inf_{x_1 \neq x_2: D^*(x_1, x_2) \leqslant \eta} |f(x_1) - f^*(x_2)| \ge \Delta,$$

where⁴,
$$D^*(x_1, x_2) = |f^*(x_1) - f^*(x_2)|$$
.

The above assumption⁵ ensures that for action pairs (x_1, x_2) , where the obtained (expected) rewards are close (since it is generated by f^*), there is a gap between the true function f^* and the ones belonging to the function classes not containing f^* (i.e., the non-realizable function classes). Note that we do not require this separability to hold for all actions – just the ones which are indistinguishable from observing the rewards. Note that separability is needed for model selection since we neither assume any structural assumption on f^* , nor on the set \mathcal{X} .

We emphasize that separability is quite standard and assumptions of similar nature appear in a wide range of model selection problems, specially in the setting of contextual bandits [16, 19]. It is also quite standard in statistics, specifically in the area of clustering and latent variable modelling [5, 14, 34].

Separability for Lipschitz f^* : If the true function f^* is 1-Lipschitz. In that setting, the separability assumption takes the following form: for $\Delta > 0$ and $\eta > 0$,

$$\inf_{f \in \mathcal{F}_{m^*-1}} \inf_{x_1 \neq x_2 : ||x_1 - x_2|| \le \eta} |f(x_1) - f^*(x_2)| \ge \Delta$$

However, note that the above assumption is quite strong – any (random) arbitrary algorithm can perform model selection (with the knowledge of η and Δ)⁶ in the following way: first choose action x_1 . Using $||x_1-x_2|| \leq \eta$, choose x_2 . Pick any function f belonging to some class \mathcal{F}_m in the nested family and evaluate $|f(x_1) - y_t(x_2)|$, which is a good proxy for $|f(x_1) - f^*(x_2)|$. The algorithm continues to pick different $f \in \mathcal{F}_m$. With the knowledge of Δ , depending on how big \mathcal{F}_m is, the algorithm would be able to identify whether \mathcal{F}_m is realizable or not. Continuing it for all hypothesis classes, it would identify the correct class \mathcal{F}_{m^*} . Hence, for structured f^* , the problem of model selection with separation is not interesting and we do not consider that setup in this paper.

⁴ Here the roles of x_1 and x_2 are interchangeable without loss of generality.

⁵ We assume that the action set \mathcal{X} is compact and continuous, and so such action pairs (x_1, x_2) always exist, i.e., given any $x_1 \in \mathcal{X}$, an action x_2 such that $D^*(x_1, x_2) \leq \eta$ always exists.

⁶ This can be found using standard trick like doubling.

Separability for Linear f^* : If f^* is linear, the separability assumption is not necessary for model selection. In this setting, f^* is parameterized by some properties of the parameter, such as sparsity and norm, denotes the nested function classes. [12,15] addresses the linear bandit model selection problem without the separability assumption.

2.2 Algorithm: Adaptive Bandit Learning (ABL)

In this section, we provide a novel model selection algorithm (Algorithm 2) that, over multiple epochs, successively refine the estimate of the true model class \mathcal{F}_{m^*} where the unknown function f^* lies. At each epoch, we run a fresh instance of a base bandit algorithm for the estimated function class, which we call Bandit Learning. Note that our model selection algorithm works with any provable bandit learning algorithm, and is agnostic to the particular choice of such base algorithm. In what follows, we present a generic description of the base algorithm and then specialize to a special case.

The Base Algorithm Bandit Learning (Algorithm 1), in its general form, takes a function class \mathcal{F} and a confidence level $\delta \in (0,1]$ as its inputs. At each time t, it maintains a (high-probability) confidence set $\mathcal{C}_t(\mathcal{F},\delta)$ for the unknown function f^* , and chooses the most optimistic action with respect to this confidence set,

$$x_t \in \operatorname*{argmax} \max_{x \in \mathcal{X}} \max_{f \in \mathcal{C}_t(\mathcal{F}, \delta)} f(x) \ .$$
 (1)

The confidence set $C_t(\mathcal{F}, \delta)$ is constructed using all the data $\{x_s, y_s\}_{s < t}$ gathered in the past. First, a regularized least square estimate of f^* is computed as $\hat{f}_t \in \operatorname{argmin}_{f \in \mathcal{F}} \mathcal{L}_{t-1}(f)$, where $\mathcal{L}_t(f) := \sum_{s=1}^t (y_s - f(x_s))^2$ is the cumulative squared prediction error. The confidence set $C_t(\mathcal{F}, \delta)$ is then defined as the set of all functions $f \in \mathcal{F}$ satisfying

$$\sum_{s=1}^{t-1} \left(f(x_s) - \widehat{f}_t(x_s) \right)^2 \le \beta_t(\mathcal{F}, \delta) , \qquad (2)$$

where $\beta_t(\mathcal{F}, \delta)$ is an appropriately chosen confidence parameter. We now specialize to the bandit learning algorithm of [26] by setting the confidence parameter

$$\beta_t(\mathcal{F}, \delta) := 8\sigma^2 \log \left(2\mathcal{N} \left(\mathcal{F}, 1/T, \left\| \cdot \right\|_{\infty} \right) / \delta \right) + 2 \left(8 + \sqrt{8\sigma^2 \log \left(8t(t+1)/\delta \right)} \right),$$

where $\mathcal{N}(\mathcal{F}, \alpha, \|\cdot\|_{\infty})$ is the $(\alpha, \|\cdot\|_{\infty})$ -covering number⁷ of \mathcal{F} , one can ensure that f^* lies in the confidence set $\mathcal{C}_t(\mathcal{F}, \delta)$ at all time instant $t \geq 1$ with probability at least $1 - \delta$. The theoretical guarantees presented in the paper are also for this particular choice of base algorithm.

For any $\alpha > 0$, we call \mathcal{F}^{α} an $(\alpha, \|\cdot\|_{\infty})$ cover of the function class \mathcal{F} if for any $f \in \mathcal{F}$ there exists an f' in \mathcal{F}^{α} such that $\|f' - f\|_{\infty} := \sup_{x \in \mathcal{X}} |f'(x) - f(x)| \leq \alpha$.

Algorithm 1 Bandit Learning

- 1: **Input:** Function class \mathcal{F} , confidence level $\delta \in (0,1]$
- 2: **for** time $t = 1, 2, 3, \dots do$
- Compute an estimate f_t of f^*
- 4: Construct confidence set $C_t(\mathcal{F}, \delta)$ using (2)
- Choose an action x_t using (1) 5:
- 6: Observe reward y_t
- 7: end for

Algorithm 2 Adaptive Bandit Learning (ABL)

- 1: Input: Nested function classes $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \ldots \subset \mathcal{F}_M$, confidence level $\delta \in (0,1]$, threshold $\gamma_i > 0$
- 2: **for** epochs i = 1, 2 ... do
- **Model Selection:** 3:
- Compute elapsed time $\tau_{i-1} = \sum_{j=1}^{i-1} t_j$ for function classes $m = 1, 2 \dots, M$ do 4:
- 5:
- Compute the minimum average squared prediction error using (3) 6:
- 7:
- Choose index $m^{(i)} = \min\{m \in [M] : T_m^{(i)} \le \gamma_i\}$ 8:
- Model Learning: 9:
- Set epoch length $t_i = 2^i$, confidence level $\delta_i = \delta/2^i$ 10:
- Run Bandit Learning (Algorithm 1) over a time horizon t_i with function 11: class $\mathcal{F}_{m^{(i)}}$ and confidence level δ_i as its inputs
- 12: **end for**

Our Approach-Adaptive Bandit Learning (ABL): The description of our model selection algorithm is given in Algorithm 2. We consider doubling epochs – at each epoch $i \geq 1$, the base algorithm is run over time horizon $t_i = 2^i$. At the beginning of i-th epoch, using all the data of the previous epochs, we employ a model selection module as follows. First, we compute, for each class \mathcal{F}_m , the minimum average squared prediction error (via an offline regression oracle)

$$T_m^{(i)} = \min_{f \in \mathcal{F}_m} \frac{1}{\tau_{i-1}} \sum_{s=1}^{\tau_{i-1}} (y_s - f(x_s))^2 , \qquad (3)$$

where $\tau_{i-1} := \sum_{j=1}^{i-1} t_j$ denotes the total time elapsed before epoch *i*. Finally, we compare $T_m^{(i)}$ to a pre-calculated threshold γ , and pick the function class for which $T_m^{(i)}$ falls below such threshold (with smallest m, see Algorithm 2). After selecting the function class, we run the base algorithm for this class with confidence level $\delta_i = \delta/2^i$. We call the complete procedure Adaptive Bandit Learning (ABL).

2.3 Performance Guarantee of ABL

We now provide model selection and regret guarantees of ABL (Algorithm 2), when the base algorithm is chosen as [26]. Though the results to be presented in this section are quite general, they do not apply to any arbitrary function classes. In what follows, we will make the following boundedness assumption.

Assumption 3 (Bounded functions) We assume that $f(x) \in [0,1] \ \forall \ x \in \mathcal{X}$ and $f \in \mathcal{F}_m \ (\forall \ m \in [M]).^8$

It is worth noting that this same assumption is also required in the standard setting, i.e., when the true model class is known ($\mathcal{F}_{m^*} = \mathcal{F}$).

We denote by $\log \mathcal{N}(\mathcal{F}_m) = \log (\mathcal{N}(\mathcal{F}_m, 1/T, \|\cdot\|_{\infty}))$ the metric entropy (with scale 1/T) of the class \mathcal{F}_m . We have the following guarantee for ABL.

Lemma 1 (Model selection of ABL). Fix a $\delta \in (0,1]$ and $\lambda > 0$. Suppose, Assumptions 1, 2 and 3 hold and we set the threshold $\gamma_i = T_M^{(i)} + C_1$, for a sufficiently small constant C_1 . Then, with probability at least $1 - O(M\delta)$, ABL identifies the correct model class \mathcal{F}_{m^*} from epoch $i \geq i^*$ when the time elapsed before epoch i^* satisfies

$$\tau_{i^*-1} \ge C\sigma^4(\log T) \max \left\{ \frac{\log(1/\delta)}{(\frac{\Delta^2}{2} - 4\eta)^2}, \log\left(\frac{\mathcal{N}(\mathcal{F}_M)}{\delta}\right) \right\},$$

provided $\Delta \geqslant 2\sqrt{2\eta}$, where C > 1 is a sufficiently large universal constant.

Remark 1 (Dependence on the biggest class). Note that we choose a threshold that depends on the epoch number and the test statistic of the biggest class. Here we crucially exploit the fact that the biggest class always contains the true model class and use this to design the threshold.

We characterize the complexity of each function class \mathcal{F}_m by its *eluder dimension*, first introduced by [26] in the standard setting.

Definition 1 (Eluder dimension). The ε -eluder dimension $\dim_{\varepsilon}(\mathcal{F}_m, \varepsilon)$ of a function class \mathcal{F} is the length of the longest sequence $\{x_i\}_{i=1}^n \subseteq \mathcal{X}$ of input points such that for some $\varepsilon' \geq \varepsilon$ and for each $i \in \{2, \ldots, n\}$,

$$\sup_{f_1, f_2 \in \mathcal{F}} \left\{ (f_1 - f_2)(x_i) \mid \sqrt{\sum_{j=1}^{i-1} (f_1 - f_2)^2(x_i)} \le \varepsilon' \right\} > \varepsilon' .$$

Define $\mathcal{F}^* = \mathcal{F}_{m^*}$. Denote by $d_{\mathcal{E}}(\mathcal{F}^*) = \dim_{\mathcal{E}}(\mathcal{F}^*, 1/T)$, the (1/T)-eluder dimension of the (realizable) function class \mathcal{F}^* , where T is the time horizon. Then, armed with Lemma 1, we obtain the following regret bound for ABL.

⁸ We can extent the range to [0, c] without loss of generality.

Theorem 1 (Cumulative regret of ABL). Suppose the condition of Lemma 1 holds. Then, for any $\delta \in (0,1]$, the regret of ABL for horizon T is

$$\mathcal{R}_{T} \leq \mathcal{O}\left(\sigma^{4}(\log T) \max\left\{\frac{\log(1/\delta)}{(\frac{\Delta^{2}}{2} - 4\eta)^{2}}, \log\left(\frac{\mathcal{N}(\mathcal{F}_{M})}{\delta}\right)\right\}\right) + \mathcal{O}\left(d_{\mathcal{E}}(\mathcal{F}^{*}) \log T + c\sqrt{T}d_{\mathcal{E}}(\mathcal{F}^{*}) \log(\mathcal{N}(\mathcal{F}^{*})/\delta) \log^{2}(T/\delta)}\right),$$

with probability at least 9 $1 - O(M\delta)$.

Remark 2 (Cost of model selection). We retain the regret bound of [26] in the standard setting, and the first term in the regret bound captures the cost of model selection – the cost suffered before accumulating enough samples to infer the correct model class (with high probability). It has weak (logarithmic) dependence on horizon T and hence considered as a minor term, in the setting where T is large. Hence, model selection is essentially free upto log factors. Let us now have a close look at this term. It depends on the metric entropy of the biggest model class \mathcal{F}_M . This stems from the fact that the thresholds $\{\gamma_i\}_{i\geq 1}$ depend on the test statistic of \mathcal{F}_M (see Remark 1). We believe that, without additional assumptions, one can't get rid of this (minor) dependence on the complexity of the biggest class.

The second term is the major one (\sqrt{T} dependence on total number of steps), which essentially is the cost of learning the true kernel f^* . Since in this phase, we basically run the base algorithm for the correct model class, our regret guarantee matches to that of an oracle with the apriori knowledge of the correct class. Note that if we simply run a non model-adaptive algorithm for this problem, the regret would be $\widetilde{\mathcal{O}}(H\sqrt{Td_{\mathcal{E}}(\mathcal{F}_M)\log\mathcal{N}(\mathcal{F}_M)})$, where $d_{\mathcal{E}}(\mathcal{F}_M)$ denotes the eluder dimension of the largest model class \mathcal{F}_M . In contrast, by successively testing and thresholding, our algorithm adapts to the complexity of the smallest function class containing the true model class.

Remark 3 (Requires no knowledge of (Δ, η)). Our algorithm ABL doesn't require the knowledge of Δ and η . Rather, it automatically adapts to these parameters, and the dependence is reflected in the regret expression. The separation Δ implies how complex the job of model selection is. If the separation is small, it is difficult for ABL to separate out the model classes. Hence, it requires additional exploration, and as a result the regret increases. Another interesting fact of Theorem 1 is that it does not require any minimum separation across model classes. This is in sharp contrast with existing results in statistics (see, e.g. [5,34]). Even if Δ is quite small, Theorem 1 gives a model selection guarantee. Now, the cost of separation appears anyways in the minor term, and hence in the long run, it does not effect the overall performance of the algorithm.

⁹ One can choose $\delta = 1/\text{poly}(M)$ to obtain a high-probability bound which only adds an extra log M factor.

3 Model Selection in Markov Decision Processes

An (episodic) MDP is denoted by $\mathcal{M}(\mathcal{S}, \mathcal{A}, H, P^*, r)$, where \mathcal{S} is the state space, \mathcal{A} is the action space (both possibly infinite), H is the length of each episode, $P^*: \mathcal{S} \times \mathcal{A} \to \mathcal{\Delta}(\mathcal{S})$ is an (unknown) transition kernel (a function mapping state-action pairs to signed distribution over the state space) and $r: \mathcal{S} \times \mathcal{A} \to [0,1]$ is a (known) reward function. In episodic MDPs, a (deterministic) policy π is given by a collection of H functions (π_1, \dots, π_H) , where each $\pi_h: \mathcal{S} \to \mathcal{A}$ maps a state s to an action a. In each episode, an initial state s_1 is first picked by the environment (assumed to be fixed and history independent). Then, at each step $h \in [H]$, the agent observes the state s_h , picks an action a_h according to π_h , receives a reward $r(s_h, a_h)$, and then transitions to the next state s_{h+1} , which is drawn from the conditional distribution $P^*(\cdot|s_h, a_h)$. The episode ends when the terminal state s_{H+1} is reached. For each state-action pair $(s, a) \in \mathcal{S} \times \mathcal{A}$ and step $h \in [H]$, we define action values $Q_h^{\pi}(s, a)$ and and state values $V_h^{\pi}(s)$ corresponding to a policy π as

where the expectation is with respect to the randomness of the transition distribution P^* . It is not hard to see that Q_h^{π} and V_h^{π} satisfy the Bellman equations:

$$Q_h^{\pi}(s,a) = r(s,a) + (P^*V_{h+1}^{\pi})(s,a), \ \forall h \in [H], \text{ with } V_{H+1}^{\pi}(s) = 0 \text{ for all } s \in \mathcal{S}.$$

A policy π^* is said to be optimal if it maximizes the value for all states s and step h simultaneously, and the corresponding optimal value function is denoted by $V_h^*(s) = \sup_{\pi} V_h^{\pi}(s)$ for all $h \in [H]$, where the supremum is over all (non-stationary) policies. The agent interacts with the environment for K episodes to learn the unknown transition kernel P^* and thus, in turn, the optimal policy π^* . At each episode $k \geq 1$, the agent chooses a policy $\pi^k := (\pi_1^k, \dots, \pi_H^k)$ and a trajectory $(s_h^k, a_h^k, r(s_h^k, a_h^k), s_{h+1}^k)_{h \in [H]}$ is generated. The performance of the learning agent is measured by the cumulative (pseudo) regret accumulated over K episodes, defined as

$$\mathcal{R}(T) := \sum\nolimits_{k = 1}^K {\left[{V_1^*(s_1^k) - V_1^{\pi^k}(s_1^k)} \right],}$$

where T = KH is total steps in K episodes.

In this work, we consider general MDPs without any structural assumption on the unknown transition kernel P^* . In the standard setting [4], it is assumed that P^* belongs to a known family of transition models \mathcal{P} . Here, in contrast to the standard setting, we do not have the knowledge of \mathcal{P} . Instead, we are given M nested families of transition kernels $\mathcal{P}_1 \subset \mathcal{P}_2 \subset \ldots \subset \mathcal{P}_M$. The smallest such family where the true transition kernel P^* lies is denoted by \mathcal{P}_{m^*} , where $m^* \in [M]$. However, we do not know the index m^* , and our goal is to propose adaptive algorithms such that the regret depends on the complexity of the family \mathcal{P}_{m^*} . We assume a similar separability condition on these nested model classes.

Assumption 4 (Local Separability) There exist constants $\Delta > 0$ and $\eta > 0$ such that for any function $V : \mathcal{S} \to \mathbb{R}$,

$$\inf_{P \in \mathcal{P}_{m^*-1}} \inf_{D*((s_1,a_1),(s_2,a_2)) \leqslant \eta} |PV(s_1,a_1) - P^*V(s_2,a_2)| \ge \Delta,$$

where
$$(s_1, a_1) \neq (s_2, a_2)$$
 and $D^*((s_1, a_1), (s_2, a_2)) = |P^*V(s_1, a_1) - P^*V(s_2, a_2)|$.

This assumption ensures that expected values under the true model is wellseparated from those under models from non-realizable classes for two distinct state-action pairs for which values are close under true model. Once again, we need state and action spaces to be compact and continuous to guarantee such pairs always exist. Note that the assumption might appear to break down for any constant function V. However, we will be invoking this assumption with the value functions computed by the learning algorithm (see (4)). For reward functions that vary sufficiently across states and actions, and transition kernels that admit densities, the chance of getting hit by constant value functions is admissibly low. In case the rewards are constant, every policy would anyway incur zero regret rendering the learning problem trivial. The value functions appear in the separability assumption in the first place since we are interested in minimizing the regret. Instead, if one cares only about learning the true model, then separability of transition kernels under some suitable notion of distance (e.g., the KL-divergence) might suffice. Note that in [16,19], the regret is defined in terms of the regression function and hence the separability is assumed on the regression function itself. Model selection without separability is kept as an interesting future work.

3.1 Algorithm: Adaptive Reinforcement Learning (ARL)

In this section, we provide a novel model selection algorithm ARL (Algorithm 2) that use successive refinements over epochs. We use UCRL-VTR algorithm of [4] as our base algorithm, and add a model selection module at the beginning of each epoch. In other words, over multiple epochs, we successively refine our estimates of the proper model class where the true transition kernel P^* lies.

The Base Algorithm: UCRL-VTR, in its general form, takes a family of transition models \mathcal{P} and a confidence level $\delta \in (0,1]$ as its input. At each episode k, it maintains a (high-probability) confidence set $\mathcal{B}_{k-1} \subset \mathcal{P}$ for the unknown model P^* and use it for optimistic planning. First, it finds the transition kernel $P_k = \underset{P \in \mathcal{B}_{k-1}}{\operatorname{argmax}}_{P \in \mathcal{B}_{k-1}} V_{P,1}^*(s_1^k)$, where $V_{P,h}^*$ denote the optimal value function of an MDP with transition kernel P at step h. UCRL-VTR then computes, at each step h, the optimal value function $V_h^k := V_{P_k,h}^*$ under the kernel P_k using dynamic programming. Specifically, starting with $V_{H+1}^k(s,a) = 0$ for all pairs (s,a), it defines for all steps h = H down to 1,

$$Q_h^k(s,a) = r(s,a) + (P_k V_{h+1}^k)(s,a), \quad V_h^k(s) = \max_{a \in \mathcal{A}} Q_h^k(s,a).$$
 (4)

Then, at each step h, UCRL-VTR takes the action that maximizes the Q-function estimate, i.e. it chooses $a_h^k = \operatorname{argmax}_{a \in \mathcal{A}} Q_h^k(s_h^k, a)$. Now, the confidence set is updated using all the data gathered in the episode. First, UCRL-VTR computes an estimate of P^* by employing a non-linear value-targeted regression model with data $\left(s_h^j, a_h^j, V_{h+1}^j(s_{h+1}^j)\right)_{j \in [k], h \in [H]}$. Note that $\mathbb{E}[V_{h+1}^k(s_{h+1}^k)|\mathcal{G}_{h-1}^k] = (P^*V_{h+1}^k)(s_h^k, a_h^k)$, where \mathcal{G}_{h-1}^k denotes the σ -field summarizing the information available just before s_{h+1}^k is observed. This naturally leads to the estimate $\widehat{P}_k = \operatorname{argmin}_{P \in \mathcal{P}} \mathcal{L}_k(P)$, where

$$\mathcal{L}_{k}(P) := \sum_{j=1}^{k} \sum_{h=1}^{H} \left(V_{h+1}^{j}(s_{h+1}^{j}) - (PV_{h+1}^{j})(s_{h}^{j}, a_{h}^{j}) \right)^{2}. \tag{5}$$

The confidence set \mathcal{B}_k is then updated by enumerating the set of all transition kernels $P \in \mathcal{P}$ satisfying $\sum_{j=1}^k \sum_{h=1}^H \left((PV_{h+1}^j)(s_h^j, a_h^j) - (\widehat{P}_k V_{h+1}^j)(s_h^j, a_h^j) \right)^2 \le \beta_k(\delta)$ with the confidence width being defined as $\beta_k(\delta) := 8H^2 \log \left(\frac{2\mathcal{N}(\mathcal{P}, \frac{1}{kH}, \|\cdot\|_{\infty, 1})}{\delta} \right) + 4H^2 \left(2 + \sqrt{2 \log \left(\frac{4kH(kH+1)}{\delta} \right)} \right)$, where $\mathcal{N}(\mathcal{P}, \cdot, \cdot)$ denotes the covering number of the family \mathcal{P} . Then, one can show that P^* lies in the confidence set \mathcal{B}_k in all episodes k with probability at least $1 - \delta$. Here, we consider a slight different expression of $\beta_k(\delta)$ as compared to [4], but the proof essentially follows the same technique. Please refer to Appendix B for further details.

Our Approach: We consider doubling epochs - at each epoch $i \geq 1$, UCRL-VTR is run for $k_i = 2^i$ episodes. At the beginning of i-th epoch, using all the data of previous epochs, we add a model selection module as follows. First, we compute, for each family \mathcal{P}_m , the transition kernel $\widehat{P}_m^{(i)}$, that minimizes the empirical loss $\mathcal{L}_{\tau_{i-1}}(P)$ over all $P \in \mathcal{P}_m$ (see (5)), where $\tau_{i-1} := \sum_{j=1}^{k-1} k_j$ denotes the total number of episodes completed before epoch i. Next, we compute the average empirical loss $T_m^{(i)} := \frac{1}{\tau_{i-1}H}\mathcal{L}_{\tau_{i-1}}(\widehat{P}_m^{(i)})$ for the model $\widehat{P}_m^{(i)}$. Finally, we compare $T_m^{(i)}$ to a pre-calculated threshold γ_i , and pick the transition family for which $T_m^{(i)}$ falls below such threshold (with smallest m, see Algorithm 3). After selecting the family, we run UCRL-VTR for this family with confidence level $\delta_i = \frac{\delta}{2^i}$, where $\delta \in (0,1]$ is a parameter of the algorithm.

3.2 Performance Guarantee of ARL

First, we present our main result which states that the model selection procedure of ARL (Algorithm 3) succeeds with high probability after a certain number of epochs. To this end, we denote by $\log \mathcal{N}(\mathcal{P}_m) = \log(\mathcal{N}(\mathcal{P}_m, 1/T, \|\cdot\|_{\infty,1}))$ the metric entropy (with scale 1/T) of the family \mathcal{P}_m . We also use the shorthand notation $\mathcal{P}^* = \mathcal{P}_{m^*}$.

For any $\alpha > 0$, \mathcal{P}^{α} is an $(\alpha, \|\cdot\|_{\infty, 1})$ cover of \mathcal{P} if for any $P \in \mathcal{P}$ there exists an P' in \mathcal{P}^{α} such that $\|P' - P\|_{\infty, 1} := \sup_{s, a} \int_{\mathcal{S}} |P'(s'|s, a) - P(s'|s, a)| ds' \leq \alpha$.

Algorithm 3 Adaptive Reinforcement Learning - ARL

```
1: Input: Parameter \delta, function classes \mathcal{P}_1 \subset \mathcal{P}_2 \subset \ldots \subset \mathcal{P}_M, thresholds \{\gamma_i\}_{i\geq 1}

2: for epochs i=1,2\ldots do

3: Set \tau_{i-1} = \sum_{j=1}^{i-1} k_j

4: for function classes m=1,2\ldots,M do

5: Compute \widehat{P}_m^{(i)} = \operatorname{argmin}_{P\in\mathcal{P}_m} \sum_{k=1}^{\tau_{i-1}} \sum_{h=1}^{H} \left(V_{h+1}^k(s_{h+1}^k) - (PV_{h+1}^k)(s_h^k, a_h^k)\right)^2

6: Compute T_m^{(i)} = \frac{1}{\tau_{i-1}H} \sum_{k=1}^{\tau_{i-1}} \sum_{h=1}^{H} \left(V_{h+1}^k(s_{h+1}^k) - (\widehat{P}_m^{(i)}V_{h+1}^k)(s_h^k, a_h^k)\right)^2

7: end for

8: Set m^{(i)} = \min\{m \in [M] : T_m^{(i)} \leq \gamma_i\}, k_i = 2^i and \delta_i = \delta/2^i

9: Run UCRL-VTR for the family \mathcal{P}_{m^{(i)}} for k_i episodes with confidence level \delta_i

10: end for
```

Lemma 2 (Model selection of ARL). Fix a $\delta \in (0,1]$ and suppose Assumption 2 holds. Suppose the thresholds are set as $\gamma_i = T_M^{(i)} + C_2$, for some sufficiently small constant C_2 . Then, with probability at least $1 - O(M\delta)$, ARL identifies the correct model class \mathcal{P}_{m^*} from epoch $i \geq i^*$, where epoch length of i^* satisfies

$$2^{i^*} \geqslant C' \log K \max \left\{ \frac{H^3}{(\frac{1}{2}\Delta^2 - 2H\eta)^2} \log(2/\delta), 4H \log \left(\frac{\mathcal{N}(\mathcal{P}_M)}{\delta}\right) \right\},$$

provided $\Delta \geqslant 2\sqrt{H\eta}$, for a sufficiently large universal constant C' > 1.

Regret Bound: In order to present our regret bound, we define, for each model model class \mathcal{P}_m , a collection of functions $\mathcal{M}_m := \{f : \mathcal{S} \times \mathcal{A} \times \mathcal{V}_m \to \mathbb{R}\}$ such that any $f \in \mathcal{M}_m$ satisfies f(s, a, V) = (PV)(s, a) for some $P \in \mathcal{P}_m$ and $V \in \mathcal{V}_m$, where $\mathcal{V}_m := \{V_{P,h}^* : P \in \mathcal{P}_m, h \in [H]\}$ denotes the set of optimal value functions under the transition family \mathcal{P}_m . By one-to-one correspondence, we have $\mathcal{M}_1 \subset \mathcal{M}_2 \subset \ldots \subset \mathcal{M}_M$, and the complexities of these function classes determine the learning complexity of the RL problem under consideration. We characterize the complexity of each function class \mathcal{M}_m by its eluder dimension, which is defined similarly as Definition 1. (We take domain of function class \mathcal{M}_m to be $\mathcal{S} \times \mathcal{A} \times \mathcal{V}_m$.)

We define $\mathcal{M}^* = \mathcal{M}_{m^*}$, and denote by $d_{\mathcal{E}}(\mathcal{M}^*) = \dim_{\mathcal{E}}(\mathcal{M}^*, 1/T)$, the (1/T)-eluder dimension of the (realizable) function class \mathcal{M}^* , where T is the time horizon. Then, armed with Lemma 2, we obtain the following regret bound.

Theorem 2 (Cumulative regret of ARL). Suppose the conditions of Lemma 2 hold. Then, for any $\delta \in (0,1]$, running ARL for K episodes yields a regret bound

$$\mathcal{R}(T) = \mathcal{O}\left(\log K \max\left\{\frac{H^4 \log(1/\delta)}{(\frac{\Delta^2}{2} - 2H\eta)^2}, H^2 \log\left(\frac{\mathcal{N}(\mathcal{P}_M)}{\delta}\right)\right\}\right) + \mathcal{O}\left(H^2 d_{\mathcal{E}}(\mathcal{M}^*) \log K + H\sqrt{T d_{\mathcal{E}}(\mathcal{M}^*) \log(\mathcal{N}(\mathcal{P}^*)/\delta) \log K \log(T/\delta)}\right).$$

with probability at least $1 - O(M\delta)$.

Similar to Theorem 1, the first term in the regret bound captures the cost of model selection, having weak (logarithmic) dependence on the number of episodes K and hence considered as a minor term, in the setting where K is large. Hence, model selection is essentially *free* upto log factors. The second term is the major one (\sqrt{T} dependence on total number of steps), which essentially is the cost of learning the true kernel P^* . Since in this phase, we basically run UCRL-VTR for the correct model class, our regret guarantee matches to that of an oracle with the apriori knowledge of the correct class. ARL doesnot require the knowledge of (Δ, η) and it adapts to the complexity of the problem.

4 Conclusion

We address the problem of model selection for MAB and MDP and propose algorithms that obtains regret similar to an oracle who knows the true model class apriori. Our algorithms leverage the separability conditions crucially, and removing them is kept as a future work.

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