No-Regret Reinforcement Learning with Value Function Approximation: A Kernel Embedding Approach

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Abstract

We consider the regret minimization problem in reinforcement learning (RL) in the episodic setting. In many real-world RL environments, the state and action spaces are continuous or very large. Existing approaches establish regret guarantees by either a low-dimensional representation of the stochastic transition model or an approximation of the Q-functions. However, the understanding of function approximation schemes for state-value functions largely remains missing. In this paper, we propose an online model-based RL algorithm, namely the CME-RL, that learns representations of transition distributions as embeddings in a reproducing kernel Hilbert space while carefully balancing the exploitation-exploration tradeoff. We demonstrate the efficiency of our algorithm by proving a frequentist (worst-case) regret bound that is of order $\tilde{O}(H\gamma_N\sqrt{N})$, where $H$ is the episode length, $N$ is the total number of time steps and $\gamma_N$ is an information theoretic quantity relating the effective dimension of the state-action feature space. Our method bypasses the need for estimating transition probabilities and applies to any domain on which kernels can be defined. It also brings new insights into the general theory of kernel methods for approximate inference and RL regret minimization.

Keywords: Model-based RL, Value function approximation, Kernel mean embedding.

1. Introduction

Reinforcement learning (RL) is concerned with learning to take actions to maximize rewards, by trial and error, in environments that can evolve in response to actions. A Markov decision process (MDP) (Puterman, 2014) is a popular framework to model decision making in RL environments. In the MDP, starting from an initial observed state, an agent repeatedly (a) takes an action, (b) receives a reward, and (c) observes the next state of the MDP. The traditional RL objective is a search goal – find a policy (a rule to select an action for each state) with high total reward using as few interactions with the environment as possible, also known as the sample complexity of RL (Strehl et al., 2009). This is, however, quite different from the corresponding optimization goal, where the learner seeks to maximize the total reward earned from all its decisions, or equivalently, minimize the regret or shortfall in total reward compared to that of an optimal policy (Jaksch et al., 2010). This objective is relevant in many practical sequential decision-making settings in which every decision that is taken carries utility or value – recommendation systems, sequential investment and portfolio allocation, dynamic resource allocation in communication systems etc. In such online optimization settings, there is no separate budget or time devoted to purely exploring the unknown environment; rather, exploration and exploitation must be carefully balanced.

1. $\tilde{O}(\cdot)$ hides only absolute constant and poly-logarithmic factors.
Several studies have considered the task of regret minimization in tabular MDPs, in which the state and action spaces are finite, and the value function is represented by a table (Jaksch et al., 2010; Osband et al., 2013; Gheshlaghi Azar et al., 2017; Dann et al., 2017; Jin et al., 2018; Efroni et al., 2019; Zanette and Brunskill, 2019). The regret bound achieved by these works essentially is proportional to $\sqrt{SAN}$, where $S$ and $A$ denote the numbers of states and actions, respectively, and $N$ the total number of steps. In many practical applications, however, the number of states and actions is enormous. 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. These continuous state and action spaces make RL a challenging task, especially in terms of generalizing learnt knowledge across unseen states and actions. In such cases, the tabular model suffers from the “curse of dimensionality” problem. To tackle this issue, the popular “optimism in the face of uncertainty” principle from Jaksch et al. (2010) has been extended to handle continuous MDPs, when assuming some Lipschitz-like smoothness or regularity on the rewards and dynamics (Ortner and Ryabko, 2012; Domingues et al., 2020).

Another line of work considers function approximation, i.e., they use features to parameterize reward and transition models, with the hope that the features can capture leading structures of the MDP (Osband and Van Roy, 2014; Chowdhury and Gopalan, 2019). The model-based algorithms developed in these works assume oracle access to an optimistic planner to facilitate the learning. The optimistic planning step is quite prohibitive and often becomes computationally intractable for continuous state and action spaces. Yang and Wang (2019) considers a low-rank bilinear transition model bypassing the complicated planning step; however, their algorithm potentially needs to compute the value function across all states. This suffers an $\Omega(S)$ computational complexity and as a consequence cannot directly handle continuous state spaces. To alleviate the computational burden intrinsic to these model-based approaches, a recent body of work parameterizes the value functions directly, using $d$-dimensional state-action feature maps, and develop model-free algorithms bypassing the need for fully learning the reward and transition models (Jin et al., 2019; Wang et al., 2019; Zanette et al., 2020a). Under the assumption that the (action-)value function can be approximated by a linear or a generalized linear function of the feature vectors, these papers develop algorithms with regret bound proportional to $\text{poly}(d)\sqrt{T}$, which is independent of the size of the state and action spaces. Wang et al. (2020) generalizes this approach by designing an algorithm that works with general (non-linear) value function approximators and prove a similar regret guarantee that depends on the eluder dimension (Russo and Van Roy, 2013) and log-covering number of the underlying function class. Recently, Yang et al. (2020) consider kernel and neural function approximations and designed algorithms with regret characterized by intrinsic complexity of the function classes. Nevertheless, there is a lack of theoretical understanding in designing provably efficient model-based RL algorithms with (non-linear) value function approximation.

In this work, we revisit function approximation in RL by modelling the value functions as elements of a reproducing kernel Hilbert space (RKHS) (Sch"{o}lkopf and Smola, 2002) compatible with a (possibly infinite dimensional) state feature map. The main motivation behind this formulation is that the conditional expectations of any function in the RKHS become a linear operation, via the RKHS inner product with an appropriate distribution embedding, known as the conditional mean embedding (Muandet et al., 2016). In recent years, conditional mean embeddings (CMEs) have found extensive applications in many machine learning tasks (Song et al., 2009, 2010a,b, 2013; Fukumizu et al., 2008, 2009; Hsu and Ramos, 2019; Chowdhury et al., 2020). The foremost advantage of CMEs in our setup is that one can directly compute conditional expectations of the
value functions based only on the observed data, since the alternative approach of estimating the transition probabilities as an intermediate step scales poorly with the dimension of the state space (Grünewälder et al., 2012). The convergence of conditional mean estimates to the true embeddings in the RKHS norm has been established by Grünewälder et al. (2012) assuming access to independent and identically distributed (i.i.d.) transition samples (the “simulator” setting). However, in the online RL environment like the one considered in this work, one collects data based on past observations, and hence the existing result fails to remain useful. Against this backdrop, we make the following contributions:

- In the online RL environment, we derive a concentration inequality for mean embedding estimates of the transition distribution around the true embeddings as a function of the uncertainties around these estimates (Theorem 1). This bound not only serves as a key tool in designing our model-based RL algorithm but also is of independent interest.

- Focusing on the value function approximation in the RKHS setting, we present the first model based RL algorithm, namely the Conditional Mean Embedding RL (CME-RL), that is provably efficient in regret performance and does not require any additional oracle access or stronger computational assumptions (Algorithm 1). Concretely, in the general setting of an episodic MDP, we prove that CME-RL enjoys a regret bound of $\tilde{O}(H\gamma_N\sqrt{N})$, where $H$ is the length of each episode, $\gamma_N$ is a complexity measure relating the effective dimension of the RKHS compatible with the state-action features (Theorem 2).

- Our approach is also robust to the RKHS modelling assumption: when the value functions are not elements of the RKHS, but $\zeta$-close to some RKHS element in the $\ell_{\infty}$ norm, then (a modified version of) CME-RL achieves a $\tilde{O}(H\gamma_N\sqrt{N} + \zeta N)$ regret, where the linear regret term arises due to the function class misspecification (Theorem 3).

2. Preliminaries

Notations We begin by introducing some notations. We let $\mathcal{H}$ be a arbitrary Hilbert space with inner product $\langle \cdot, \cdot \rangle_\mathcal{H}$ and corresponding norm $\|\cdot\|_\mathcal{H}$. When $\mathcal{G}$ is another Hilbert space, we denote by $\mathcal{L}(\mathcal{G}, \mathcal{H})$ the Banach space of bounded linear operators from $\mathcal{G}$ to $\mathcal{H}$, with the operator norm $\|A\| := \sup_{\|g\|_\mathcal{G}=1} \|Ag\|_\mathcal{H}$. We let $\text{HS}(\mathcal{G}, \mathcal{H})$ denote the subspace of operators in $\mathcal{L}(\mathcal{G}, \mathcal{H})$ with bounded Hilbert-Schmidt norm $\|A\|_{\text{HS}} := \left( \sum_{i,j=1}^{\infty} \langle f_i, A g_j \rangle_\mathcal{H}^2 \right)^{1/2}$, where the $f_i$’s form a complete orthonormal system (CONS) for $\mathcal{G}$ and the $g_j$’s form a CONS for $\mathcal{H}$. In the case $\mathcal{G} = \mathcal{H}$, we set $\mathcal{L}(\mathcal{H}) := \mathcal{L}(\mathcal{H}, \mathcal{H})$. We denote by $\mathcal{L}_+(\mathcal{H})$ the set of all bounded, positive-definite linear operators on $\mathcal{H}$, i.e., $A \in \mathcal{L}_+(\mathcal{H})$ if, for any $h \in \mathcal{H}$, $\langle h, Ah \rangle_\mathcal{H} > 0$.

Regret minimization in finite-horizon episodic MDPs We consider episodic reinforcement learning in a finite-horizon Markov decision process (MDP) of episode length $H$ with (possibly infinite) state and action spaces $\mathcal{S}$ and $\mathcal{A}$, respectively, reward function $R : \mathcal{S} \times \mathcal{A} \rightarrow [0,1]$, and transition probability measure $P : \mathcal{S} \times \mathcal{A} \rightarrow \Delta(\mathcal{S})$, where $\Delta(\mathcal{S})$ denotes the probability simplex on $\mathcal{S}$. The learning agent interacts with the MDP in episodes and, at each episode $t$, a trajectory $(s^t_1, a^t_1, r^t_1, \ldots, s^t_H, a^t_H, r^t_H, s^t_{H+1})$ is generated. Here $a^t_h$ denotes the action taken at state $s^t_h$, $r^t_h := R(s^t_h, a^t_h)$ denotes the immediate reward, and $s^t_{h+1} \sim P(\cdot|s^t_h, a^t_h)$ denotes the random next state. The initial state $s^t_1$ is assumed to be fixed and history independent, and can even be possibly chosen by an adversary. The episode terminates when $s^t_{H+1}$ is reached, where the agent
cannot take any action and hence receives no reward. The actions are chosen following some policy
π = (π₁, ..., π₇₇), where each π₇₇ is a mapping from the state space S into the action space A.
The agent would like to find a policy π that maximizes the long-term expected cumulative reward
starting from every state s ∈ S and every step h ∈ [H], defined as:

\[ V_h^π(s) := \mathbb{E} \left[ \sum_{j=h}^{H} R(s_j, π_j(s_j)) \mid s_h = s \right] . \]

We call Vₜ: S → ℝ the value function of policy π at step h. Accordingly, we also define the
action-value function, or Q-function, Qₜ: S × A → ℝ as:

\[ Q_h^{π}(s, a) := R(s, a) + \mathbb{E} \left[ \sum_{j=h+1}^{H} R(s_j, π_j(s_j)) \mid s_h = s, a_h = a \right] , \]

which gives the expected value of cumulative rewards starting from a state-action pair at the h-th
step and following the policy π afterwards. Note that Vₜ⁺(s) = Qₜ⁺(s, πₜ(s)) and it satisfies the
Bellman optimality equation:

\[ V_h^{π⁺}(s) = R(s, π(h)) + \mathbb{E}_{X \sim P(\cdot \mid s, π(h))} \left[ V_{h+1}^{π⁺}(X) \right] , \quad \forall h \in [H] , \]

with Vₜ⁺₁(s) = 0 for all s ∈ S. We denote by π⁺ an optimal policy satisfying:

\[ V_h^{π⁺}(s) = \max_{π \in Π} V_h^{π}(s) , \quad \forall s ∈ S , \forall h \in [H] , \]

where Π is the set of all non-stationary policies. Since the episode length is finite, such a policy
exists when the action space A is large but finite (Puterman, 2014). We denote the optimal value
function by Vₜ⁺(s) := Vₜ⁺⁺(s). We also denote the optimal action-value function (or Q-function) as
Qₜ⁺(s, a) = maxπ Qₜ⁺(s, a). It is easily shown that the optimal action-value function satisfies the
Bellman optimality equation:

\[ Q_h^{π⁺}(s, a) := R(s, a) + \mathbb{E}_{X \sim P(\cdot \mid s, a)} \left[ V_{h+1}^{π⁺}(X) \right] , \quad \forall h \in [H] , \]

with Vₜ⁺(s) = maxₐ∈A Qₜ⁺(s, a). This implies that the optimal policy is the greedy policy with
respect to the optimal action-value functions. Thus, to find the optimal policy π⁺, it suffices to
estimate the optimal action-value functions (Qₜ⁺ₗ)ₗ∈[H].

The agent aims to learn the optimal policy by interacting with the environment during a set of
episodes. We measure performance of the agent by the cumulative (pseudo) regret accumulated
over T episodes, defined as:

\[ \mathcal{R}(N) := \sum_{t=1}^{T} \left[ V_1^{π⁺}(s_1) - V_1^{π⁺}(s_1) \right] , \]

where π is the policy chosen by the agent at episode t and N = TH is the total number of steps.
The regret measures the quantum of reward that the learner gives up by not knowing the MDP in
advance and applying the optimal policy π⁺ from the start. We seek algorithms that attain sublinear
regret \( \mathcal{R}(N) = o(N) \) in the number of steps they face, since, for instance, an algorithm that does
not adapt its policy selection behavior depending on past experience can easily be seen to achieve
linear (Ω(\(N\))) regret (Lai and Robbins, 1985).

**Value function approximation in episodic MDPs** A very large or possibly infinite state and
action space makes reinforcement learning a challenging task. To obtain sub-linear regret
 guarantees, it is necessary to posit some regularity assumptions on the underlying function class. In
this paper, we use reproducing kernel Hilbert spaces to model the value functions. Let \( \mathcal{H}_ψ \) and
\( \mathcal{H}_φ \) be two RKHSs with continuous positive semi-definite kernel functions \( k_ψ: S × S → ℝ⁺ \) and
\( k_φ: (S × A) × (S × A) → ℝ⁺ \), with corresponding inner products \( \langle \cdot , \cdot \rangle_{\mathcal{H}_ψ} \) and \( \langle \cdot , \cdot \rangle_{\mathcal{H}_φ} \), respectively.
There exist feature maps $\psi: S \to \mathcal{H}_\psi$ and $\varphi: S \times A \to \mathcal{H}_\varphi$ such that $k_\psi(\cdot, \cdot) = \langle \psi(\cdot), \psi(\cdot) \rangle_{\mathcal{H}_\psi}$ and $k_\varphi(\cdot, \cdot) = \langle \varphi(\cdot, \cdot), \varphi(\cdot, \cdot) \rangle_{\mathcal{H}_\varphi}$, respectively (Steinwart and Christmann, 2008).

The weakest assumption one can pose on the value functions is realizability, which posits that the optimal value functions $(V^*_h)_{h \in [H]}$ lie in the RKHS $\mathcal{H}_\psi$, or at least are well-approximated by $\mathcal{H}_\psi$. For stateless MDPs or multi-armed bandits where $H = 1$, realizability alone suffices for provably efficient algorithms (Abbasi-Yadkori et al., 2011; Chowdhury and Gopalan, 2017). But it does not seem to be sufficient when $H > 1$, and in these settings it is common to make stronger assumptions (Jin et al., 2019; Wang et al., 2019, 2020). Following these works, our main assumption is a closure property for all value functions in the following class:

$$\mathcal{V} := \left\{ s \mapsto \min_{a \in A} \left\{ H, \max_{a \in A} \left\{ R(s, a) + \langle \varphi(s, a), \mu \rangle_{\mathcal{H}_\varphi} + \eta \sqrt{\langle \varphi(s, a), \Sigma^{-1} \varphi(s, a) \rangle_{\mathcal{H}_\varphi}} \right\} \right\} ,$$

where $0 < \eta < \infty$, $\mu \in \mathcal{H}_\varphi$ and $\Sigma \in \mathcal{L}_+(\mathcal{H}_\varphi)$ are the parameters of the function class.

**Assumption 1 (Optimistic closure)** For any $V \in \mathcal{V}$ (Equation 3), we have $V \in \mathcal{H}_\psi$. Furthermore, for a positive constant $B_V$, we have $\|V\|_{\mathcal{H}_\psi} \leq B_V$.

While this property seems quite strong, we note that related closure-type assumptions are common in the literature. We will relax this assumption later in Section 4.3. In addition, our results do not require explicit knowledge of $\mathcal{H}_\psi$ nor its kernel $k_\psi$, as we will only interact with elements of $\mathcal{V}$ via point evaluations and RKHS norm bounds.

### 3. RKHS embeddings of transition distribution

In order to find an estimate of the optimal value function, it is imperative to estimate the conditional expectations of the form $\mathbb{E}_{X \sim P(\cdot|s,a)}[f(X)]$. In the model-based approach considered in this work, we do so by estimating the mean embedding of the conditional distribution $P(\cdot|s,a)$, which is the focus of this section. For a bounded kernel $k_\psi$ on the state space $S$, the mean embedding of the conditional distribution $P(\cdot|s,a)$ in $\mathcal{H}_\psi$ is an element $\nu_{P}^{s,a} \in \mathcal{H}_\psi$ such that:

$$\forall f \in \mathcal{H}_\psi, \quad \mathbb{E}_{X \sim P(\cdot|s,a)}[f(X)] = \left\langle f, \nu_{P}^{s,a} \right\rangle_{\mathcal{H}_\psi} .$$

The mean embedding can be explicitly expressed as a function: $\nu_{P}^{s,a}(y) = \mathbb{E}_{X \sim P(\cdot|s,a)}[k_\psi(X,y)]$ for all $y \in S$. If the kernel $k_\psi$ is characteristic, such as a stationary kernel, then the mapping $P(\cdot|s,a) \mapsto \nu_{P}^{s,a}$ is injective, defining a one-to-one relationship between transition distributions and elements of $\mathcal{H}_\psi$ (Sriperumbudur et al., 2011). Following existing works (Song et al., 2009; Grünewälder et al., 2012), we now make a smoothness assumption on the transition distribution.

**Assumption 2** For any $f \in \mathcal{H}_\psi$, the function $(s,a) \mapsto \mathbb{E}_{X \sim P(\cdot|s,a)}[f(X)]$ is an element of $\mathcal{H}_\varphi$.

Under Assumption 2, the mean embeddings admit a linear representation in state-action features via an operator $\Theta_P \in \mathcal{L}(\mathcal{H}_\varphi, \mathcal{H}_\psi)$, known as the **conditional embedding operator**, such that:

$$\forall (s,a) \in S \times A, \quad \nu_{P}^{s,a} = \Theta_P \varphi(s,a) .$$

Assumption 2 always holds for finite domains with characteristic kernels. Though it is not necessarily true for continuous domains, we note that the CMEs for classical linear (Abbasi-Yadkori and Szepesvári, 2011) and non-linear (Kakade et al., 2020) dynamical systems satisfy this assumption.

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2. Boundedness of a kernel holds for any stationary kernel, e.g., the squared exponential kernel and the Matérn kernel (Rasmussen and Williams, 2006).
3.1. Sample estimate of conditional mean embedding

At the beginning of each episode $t$, given the data $D_t := (s_h^t, a_h^t, s_{h+1}^t)_{\tau < t, h \in H}$ containing all transition samples observed until episode $t - 1$, we consider a sample based estimate of the conditional embedding operator. This is achieved by solving the following ridge-regression problem: 

$$
\min_{\Theta \in \mathcal{H}(\mathcal{P}_0, \mathcal{K}_\psi)} \sum_{\tau < t, h \in H} \| \psi(s_{h+1}^t) - \Theta \varphi(s_h^t, a_h^t) \|_{\mathcal{H}_\psi}^2 + \lambda \| \Theta \|_{\mathcal{H}_\psi}^2 ,
$$

where $\lambda > 0$ is a regularising constant. The solution of Equation 6 is given by:

$$
\hat{\Theta}_t = \sum_{\tau < t, h \in H} \psi(s_{h+1}^t) \otimes \varphi(s_h^t, a_h^t) \left( \mathcal{C}_{\varphi,t} + \lambda I \right)^{-1} ,
$$

where $\mathcal{C}_{\varphi,t} := \sum_{\tau < t, h \in H} \varphi(s_h^t, a_h^t) \otimes \varphi(s_h^t, a_h^t)$. To simplify notations, we now let $n = (t - 1)H$ denote the total number of steps completed at the beginning of episode $t$. We denote a vector $k_{\varphi,t}(s, a) \in \mathbb{R}^n$ and a matrix $K_{\varphi,t} \in \mathbb{R}^{n \times n}$ by:

$$
k_{\varphi,t}(s, a) := [k_{\varphi}((s_h^t, a_h^t), (s, a))]_{\tau < t, h \in H} , \quad K_{\varphi,t} := [k_{\varphi}((s_h^t, a_h^t), (s_h', a_h'))]_{\tau, \tau' < t, h, h' \in H} .
$$

Then, via Equation 7, the conditional mean embeddings can be estimated as

$$
\hat{\vartheta}_t^{(s,a)} = \hat{\Theta}_t \varphi(s, a) = \sum_{\tau < t, h \in H} [\alpha_t(s, a)]_{(\tau, h)} \psi(s_{h+1}^t) ,
$$

where we define the weight vector $\alpha_t(s, a) := (K_{\varphi,t} + \lambda I)^{-1} k_{\varphi,t}(s, a)$.

3.2. Concentration of mean embedding estimates

In this section, we show that for any state-action pair $(s, a)$, the CME estimates $\hat{\vartheta}_t^{(s,a)}$ lies within a high-probability confidence region around the true embedding $\vartheta_P^{(s,a)}$. This eventually translates, via Equation 4, to a concentration property of $\langle f, \hat{\vartheta}_t^{(s,a)} \rangle_{\mathcal{H}_\psi}$ around $\mathbb{E}_{X \sim \mathbb{P}(s,a)}[f(X)]$ for any $f \in \mathcal{H}_\psi$. The uncertainty of CME estimates can be characterized by the expression $\sigma_{\varphi,t}^2(s, a) := \lambda \langle \varphi(s, a), M_t^{-1} \varphi(s, a) \rangle_{\mathcal{H}_\psi} = \lambda \| \varphi(s, a) \|^2_{M_t^{-1}}$, where $M_t := \mathcal{C}_{\varphi,t} + \lambda I$. To see this, we first note that an application of Sherman-Morrison formula yields:

$$
\sigma_{\varphi,t}^2(s, a) := k_{\varphi}((s, a), (s, a)) - k_{\varphi,t}(s, a)^\top (K_{\varphi,t} + \lambda I)^{-1} k_{\varphi,t}(s, a) ,
$$

which is equivalent to the predictive variance of a Gaussian process (GP) (Rasmussen and Williams, 2006). Although a sample from a GP is usually not an element of the RKHS defined by its kernel (Lukić and Beder, 2001), the following result allows us to use $\sigma_{\varphi,t}^2(s, a)$ as an error measure.

**Theorem 1 (Concentration of the conditional embedding operator)** Let $\sup_{s \in \mathcal{S}} \sqrt{k_\psi(s, s)} \leq B_\psi$. Then, under Assumption 2, the following holds for any $\lambda > 0$ and $\delta \in (0, 1)$:

$$
\mathbb{P} \left[ \forall t \in \mathbb{N}, \| (\Theta_P - \hat{\Theta}_t) M_t^{1/2} \|_{\mathcal{H}_\psi} \leq \beta_t(\delta) \right] \geq 1 - \delta ,
$$

where, for any $B_P \geq \| \Theta_P \|$, $\beta_t(\delta) := B_P \sqrt{\lambda + 2B_\psi \sqrt{2 \log(1/\delta) + \log \det(I + \lambda^{-1} K_{\varphi,t})}}$.

Theorem 1 implies a concentration inequality for the CME estimates, since, for all $t \geq 1$:

$$
\| \vartheta_P^{(s,a)} - \hat{\vartheta}_t^{(s,a)} \|_{\mathcal{H}_\psi} \leq \| (\Theta_P - \hat{\Theta}_t) M_t^{1/2} \| \| \varphi(s, a) \|_{M_t^{-1}} \leq \beta_t(\delta) \lambda^{-1/2} \sigma_{\varphi,t}(s, a), \forall (s, a) \in \mathcal{S} \times \mathcal{A} ,
$$

with probability at least $1 - \delta$. This result forms the core of our value function approximations.

**Remark 1** Considering the simulation setting, Grünewälder et al. (2012) assume access to a sample $(s_i, a_i, s'_i)_{i=1}^m$, drawn i.i.d. from a joint distribution $P_0$ such that the conditional probabilities
satisfy \( P_0(s'_i | s_i, a_i) = P(s'_i | s_i, a_i) \) for all \( i \in [m] \). Under Assumption 2, the authors establish the convergence of CME estimates \( \tilde{\Theta}^{(s,a)}_h \) to the true CMEs \( \varphi^{(s,a)}_h \) in \( P_0 \)-probability. This guarantee, however, does not apply to our setting, since we do not assume any simulator access.

**Proof sketch of Theorem 1** To derive this result, we note that \( \tilde{\Theta}^{(s,a)}_h \) is a least-squares estimator for \( \Theta^{(s,a)}_h : (s, a) \mapsto \mathbb{E}_{X \sim P(\cdot | s, a)}[f(X)] \), when \( f \in \mathcal{H}_\psi \), and apply Theorem 3.11 in Abbasi-Yadkori (2012) to bound the error in inner products. Taking a supremum over all \( f \in \mathcal{H}_\psi \), we arrive at a bound for the operator norm. The complete proof is given in Chowdhury and Oliveira (2020).

### 4. RL exploration using RKHS embeddings

In this section, we aim to develop an online RL algorithm using the conditional mean embedding estimates that balances exploration and exploitation (near) optimally. We realize this, at a high level, by following the Upper-Confidence Bound (UCB) principle and thus our algorithm falls in a similar framework as in Jaksch et al. (2010); Gheshtlaghi Azar et al. (2017); Yang and Wang (2019).

#### 4.1. The Conditional Mean Embedding RL (CME-RL) algorithm

At a high level, each episode \( t \) consists of two passes over all steps. In the first pass, we maintain the \( Q \)-function estimates via dynamic programming. To balance the exploration-exploitation trade-off, we first define a confidence set \( C_t \) that contains the set of conditional embedding operators that are deemed to be consistent with all the data that has been collected in the past. Specifically, for any \( \delta \in (0, 1] \), \( \lambda > 0 \) and constants \( B_P \) and \( B_\psi \), Theorem 1 governs us to define the confidence set

\[
C_t := \left\{ \Theta \in \mathcal{L}(\mathcal{H}_\varphi, \mathcal{H}_\psi) : \left\| (\Theta - \tilde{\Theta}_t) M_t^{1/2} \right\| \leq \beta_t(\delta/2) \right\},
\]

where \( \beta_t(\cdot) \) acts as a parameter governing the exploration-exploitation trade-off. This confidence set is then used to compute the optimistic \( Q \)-estimates, starting with \( V^t_{H+1}(s) = 0 \), and setting:

\[
\text{for } h = H, H-1, \ldots, 1, \quad V^t_{h}(s) = \min \left\{ H, \max_{a \in A} Q^t_h(s, a) \right\},
\]

\[
Q^t_h(s, a) = R(s, a) + \max_{\Theta_P, \varphi_\psi} \mathbb{E}_{X \sim P(\cdot | s, a)} \left[ V^t_{h+1}(X) \right].
\]

We note here that we only require an optimistic estimate of the optimal \( Q \)-function. Hence, it is not necessary to solve the maximization problem in Equation 12 explicitly. In fact, we can use a closed-form expression instead of searching for the optimal embedding operator \( \Theta^{(s,a)}_h \) in the confidence set \( C_t \). If the value estimate \( V^t_{h+1} \) lies in the RKHS \( \mathcal{H}_\psi \), we then have from Equation 4 that \( \mathbb{E}_{X \sim P(\cdot | s, a)} \left[ V^t_{h+1}(X) \right] = \left\langle V^t_{h+1}, \varphi^{(s,a)}_{h+1} \right\rangle_{\mathcal{H}_\varphi} \), and from Equation 8 that:

\[
\left\langle V^t_{h+1}, \varphi^{(s,a)}_{h+1} \right\rangle_{\mathcal{H}_\varphi} = \alpha_t(s, a)^\top v^t_{h+1} = k_{\varphi,t}(s, a)^\top (K_{\varphi,t} + \lambda I)^{-1} v^t_{h+1},
\]

where we define the vector \( v^t_{h+1} := [V^t_{h+1}(s_{h'+1})]_{t'<t', h'<H} \). Now, since the confidence set \( C_t \) is convex, the \( Q \)-updates given by Equation 12 admit the closed-form expression:

\[
Q^t_h(s, a) = R(s, a) + k_{\varphi,t}(s, a)^\top (K_{\varphi,t} + \lambda I)^{-1} v^t_{h+1} + \left\| V^t_{h+1} \right\|_{\mathcal{H}_\varphi} \beta_t(\delta/2) \lambda^{-1/2} \sigma_{\varphi,t}(s, a).
\]

We now note that, by the optimistic closure property (Assumption 1), the value estimate \( V^t_h \) given by Equation 11 lies in the RKHS \( \mathcal{H}_\psi \), rendering the closed-form expression in Equation 13 valid.

In the second pass over the steps, we execute the greedy policy with respect to the \( Q \)-function estimates obtained in the first pass. Specifically, at each step \( h \), we chose the action:

\[
a^t_h = \pi_h^t(s^t_h) \in \arg\max_{a \in A} Q^t_h(s^t_h, a).
\]
The pseudo-code of CME-RL is given in Algorithm 1. Note that, in order to implement CME-RL, we do not need to know the kernel $k_{\varphi}$; only the knowledge of the upper bound $B_V$ over the RKHS norm of $V_{h+1}^t$ suffices our purpose. For simplicity of representation, we assume that the agent, while not knowing the conditional mean embedding operator $\Theta_P$, knows the reward function $R$. When $R$ is unknown but an element of the RKHS $\mathcal{H}_\varphi$, our algorithm can be extended naturally with an optimistic reward estimation step at each episode, similar to the contextual bandit setting (Abbasi-Yadkori et al., 2011; Chowdhury and Gopalan, 2017).

**Algorithm 1: Conditional Mean Embedding RL (CME-RL)**

1. **Input:** Kernel $k_{\varphi}$, constants $B_P$, $B_V$ and $B_{\psi}$, parameters $\eta > 0$ and $\delta \in (0, 1]$

2. **for** episode $t = 1, \ldots, T$ **do**
   
   3. Receive the initial state $s_1^t$ and set $V_{H+1}^t(\cdot) = 0$

   4. **for** step $h = H, \ldots, 1$ **do** // Update value function estimates

   5. \[ Q_h^t(\cdot) = R(\cdot, \cdot) + k_{\varphi,t}(\cdot, \cdot) (K_{\varphi,t} + \lambda I)^{-1} v_{h+1}^t + B_V \beta_t(\delta/2) \lambda^{-1/2} \sigma_{\varphi,t}(\cdot, \cdot) \]

   6. \[ V_h^t(\cdot) = \min \left\{ H, \max_{a \in A} Q_h^t(\cdot, a) \right\} \]

   7. **for** step $h = 1, \ldots, H$ **do** // Run episode

   8. Take action $a_h^t \in \arg\max_{a \in A} Q_h^t(s_h^t, a)$ and observe next state $s_{h+1}^t \sim P(\cdot|s_h^t, a_h^t)$

---

**Computational complexity of CME-RL** The dominant cost is evaluating the Q-function estimates $Q_h^t$ (Equation 13). As typical in kernel methods (Schölkopf and Smola, 2002), it involves inversion of $tH \times tH$ matrices, which take $O(t^2H^3)$ time. In the policy execution phase (Equation 14), we do not need to compute the entire Q-function as the algorithm only queries Q-values at visited states. Hence, assuming a constant cost of optimizing over the actions, the per-episode running time is $O(t^2H^4)$. However, using standard sketching techniques like the Nyström approximation (Drineas and Mahoney, 2005) or the random Fourier features approximation (Rahimi and Recht, 2007), and by using the Sherman-Morrison formula to amortize matrix inversions, per-episode running cost can be reduced to $O(m^2H)$, where $m$ is the dimension of feature approximations.

**4.2. Regret bound for CME-RL**

In this section, we present the regret guarantee of our algorithm. We first define

\[
\gamma_N \equiv \gamma_{\varphi, \lambda, N} := \sup_{X \subseteq S \times A; |X| = N} \frac{1}{2} \log \det(I + \lambda^{-1} K_{\varphi,X}) \text{ ,}
\]

where $X = \{(s_i, a_i)\}_{i \in [N]}$ and $K_{\varphi,X} = [k_{\varphi}((s_i, a_i), (s_j, a_j))]_{i,j \in [N]}$ is the gram matrix over the data set $X$. $\gamma_N$ denotes the maximum information gain about a (random) function $f$ sampled from a zero-mean GP with covariance function $k_{\varphi}$ after $N$ noisy observations, obtained by passing $f$ through an i.i.d. Gaussian channel $N(0, \lambda)$. Consider the case when $k_{\varphi}$ is a squared exponential kernel on $\mathbb{R}^d$. Then it can be verified that $\gamma_N = O((\log N)^{d+1})$ (Srinivas et al., 2009).

**Theorem 2 (Cumulative regret of CME-RL)** Under assumptions 1 and 2, after interacting with the environment for $N = TH$ steps, with probability at least $1 - \delta$, CME-RL (Algorithm 1) achieves the regret bound

\[ \mathcal{R}(N) \leq 2B_V \alpha_{N, \delta} \sqrt{2(1 + \lambda^{-1} B_{\varphi}^2 H) N \gamma_N + 2H \sqrt{2N \log(2/\delta)}} \text{ ,} \]

where $B_{\varphi} \geq \sup_{s,a} \sqrt{k_{\varphi}((s,a), (s,a))}$, and $\alpha_{N, \delta} := B_P \sqrt{\lambda} + 2B_{\psi} \sqrt{2 \log(2/\delta) + \gamma_N}$.
Theorem 2 yields a $\hat{O}(H\gamma_N\sqrt{N})$ regret bound for CME-RL. Comparing to the minimax regret in tabular setting, $\Theta(H\sqrt{SAN})$ (Gheslaghan Azar et al., 2017), our bound replaces the sublinear dependency on the number of state-action pairs by a linear dependency on the intrinsic complexity measure, $\gamma_N$, of the feature space $\mathcal{H}_\varphi$, which is crucial in the large state-action space setting that entails function approximation. Additionally, in the kernelized bandit setting ($H = 1$), our bound matches the best known upper bound $O(\gamma_N\sqrt{N})$ (Chowdhury and Gopalan, 2017). We note, however, that while an MDP has state transitions, the bandits do not, and a naive adaptation of existing kernelized bandit algorithms to this setting would give a regret exponential in episode length $H$. Furthermore, due to the Markov transition structure, the lower bound for kernelized bandits (Scarlett et al., 2017) does not directly apply here. Hence, it remains an interesting future direction to determine the optimal dependency on $\gamma_N$.

Conversion to PAC guarantee Similarly to the discussion in Jin et al. (2019), our regret bound directly translates to a sample complexity or probably approximately correct (PAC) guarantee in the following sense. Assuming a fixed initial state $s_1^t = s$ for each episode $t$, with at least a constant probability, we can learn an $\varepsilon$-optimal policy $\pi$ that satisfies $V_\pi^*(s) - V_\pi^0(s) \leq \varepsilon$ by running CME-RL for $T = O(d_{\text{eff}}^2 H^2/\varepsilon^2)$ episodes, where $d_{\text{eff}}$ is a known upper bound over $\gamma_N$, and then output the greedy policy according to the $Q$-function at $t$-th episode, where $t$ is sampled uniformly from $[T]$. Here $d_{\text{eff}}$ effectively captures the number of significant dimensions of $\mathcal{H}_\varphi$.

Remark 2 Yang and Wang (2019) assumes the transition model $P(s'|s,a) = \langle \psi(s'), \Theta_P \varphi(s,a) \rangle_{\mathcal{H}_\varphi}$, and propose a model-based algorithm with regret $\hat{O}(H^2\gamma_N\sqrt{N})$. In comparison, we get an $O(H)$ factor improvement thanks to a tighter control over the sum of predictive variances. Furthermore, Yang and Wang (2019) need the $\Theta_P$ to be Hilbert-Schmidt, whereas we only need it be bounded. This is achieved through a tighter confidence set construction using the CME estimates (Theorem 1).

Remark 3 Considering linear function approximation ($\mathcal{H}_\varphi = \mathbb{R}^d$), Jin et al. (2019) assumes that for any $V \in \mathcal{V}$ (Equation 3), the map $(s,a) \mapsto \mathbb{E}_{X \sim P(\cdot|s,a)}[V(X)]$ lies in $\mathcal{H}_\varphi$, and propose a model-free algorithm with regret $\hat{O}(\sqrt{Hd^3N})$. For linear kernels, it can be verified that $\gamma_N = O(d \log N)$ and thus our regret (Theorem 2) is of the order $\hat{O}(Hd\sqrt{N})$. We note that this apparent improvement in our bound is a consequence of slightly stronger assumptions 1 and 2. While Jin et al. (2019) obtain the bound by proving a uniform concentration result over the set $\mathcal{V}$, we obtain the regret bound via a novel concentration property of CME estimates (Theorem 1).

Proof sketch of Theorem 2 We start with a control on the $Q$-function estimates $Q^t_h$, which in turn leads to the regret bound, as our policy is based on $Q^t_h$. We prove that as long as the transition distribution $P$ lies in the confidence set $C_t$, the $Q$-updates are optimistic estimates of the optimal $Q$-values, i.e., $Q^t_h(s,a) \leq Q^t_h(s,a)$ for all $(s,a)$. This implies $V^*_1(s^t_1) \leq V^*_1(s^t_1)$ and thus, in turn, the regret $R(N) \leq \sum_{t=1}^{T} (V^*_1(s^t_1) - V^*_1(s^t_1))$. At this point, we let $g^t_1(s^t_1) := V^*_1(s^t_1) - V^*_1(s^t_1)$ denote the gap between the optimal value and the actual value obtained at episode $t$. We then have $g^t_1(s^t_1) \leq \sum_{t=1}^{T} (Q^t_h(s^t_1,a^t_h) - (R(s^t_h,a^t_h) + \mathbb{E}_{X \sim P(\cdot|s^t_h,a^t_h)}[V^t_{h+1}(X)])) + m^t_h)$, where $(m^t_h)_{t,h}$ denotes a martingale difference sequence. We control this via the Azuma-Hoeffding inequality as $\sum_{t,h} m^t_h = O(H\sqrt{N})$. The rest of the terms inside the summation can be controlled, by Theorem 1 and by design of the confidence set $C_t$, using the predictive variances $\sigma_{\varphi,t}(s^t_h,a^t_h)$. Now, the proof can be completed by showing that $\sum_{t,h} \sigma_{\varphi,t}(s^t_h,a^t_h) = O(\sqrt{HN\gamma_N})$. Complete proof of this result is given in Chowdhury and Oliveira (2020).
4.3. Robustness to model misspecification

Theorem 2 hinges on the fact that any optimistic estimate of the value function can be specified as an element in $\mathcal{H}_\psi$. In this section, we study the case when there is a misspecification error. Formally, we consider the following assumption.

**Assumption 3 (Approximate optimistic closure)** There exists constants $\zeta > 0$ and $B_V > 0$, such that for any $V \in \mathcal{V}$ (Equation 3), there exists a function $\tilde{V} \in \mathcal{H}_\psi$ which satisfies $\|V - \tilde{V}\|_\infty \leq \zeta$ and $\|\tilde{V}\|_{\mathcal{H}_\psi} \leq B_V$. We call $\zeta$ the misspecification error.

The quality of this approximation will further depend upon how well any $V \in \mathcal{V}$ can be approximated by a low-norm function in $\mathcal{H}_\psi$. One specialization is to the case when $\mathcal{V} \subseteq C_b(S)$, the vector space of continuous and bounded functions on $S$, and $k_\psi$ is a $C_b(S)$-universal kernel (Steinwart and Christmann, 2008). In this case, we can choose $\tilde{V}$ such that $\|V - \tilde{V}\|_\infty$ is arbitrarily small. For technical reasons, we also make the following assumption.

**Assumption 4** The RKHS $\mathcal{H}_\psi$ contains the constant functions.

The following theorem states that our algorithm is in fact robust to a small model misspecification. To achieve this, we only need to adopt a different exploration term in Equation 13 to account for the misspecification error $\zeta$. In particular, we define the $Q$-function updates as

$$Q_h^t(s, a) := R(s, a) + k_{\varphi, t}(s, a) \top (K_{\varphi, t} + \lambda I)^{-1} h_{t+1} + \left( B_V + \zeta \|1\|_{\mathcal{H}_\psi} \right) \beta_t(\delta/2) \sigma_{\psi, t}(s, a),$$

where $\|1\|_{\mathcal{H}_\psi}$ denotes the norm of the all-one function $s \mapsto 1$ in $\mathcal{H}_\psi$.

**Theorem 3 (Cumulative regret under misspecification)** Under assumptions 2, 3 and 4, with probability at least $1 - \delta$, CME-RL achieves the regret bound

$$\mathcal{R}(N) \leq 2 \left( B_V + \zeta \|1\|_{\mathcal{H}_\psi} \right) \alpha_{N, \delta} \sqrt{2(1 + \lambda^{-1} B^2 \mathcal{P}^2) H N \gamma N + 4 \zeta N + 2 H \sqrt{2 N \log(2/\delta)}},$$

where $B_\varphi$ and $\alpha_{N, \delta}$ are as given in Theorem 2.

In comparison with Theorem 2, Theorem 3 asserts that CME-RL will incur at most an additional $O(\zeta \gamma N \sqrt{HN} + \zeta N)$ regret when the model is misspecified. This additional term is linear in $N$ due to the intrinsic bias introduced by the approximation. When $\zeta$ is sufficiently small (as is typical for universal kernels $k_\psi$), our algorithm will still enjoy good theoretical guarantees. Complete proof of Theorem 3 is given in Chowdhury and Oliveira (2020).

Similar to Theorem 2, we can also convert Theorem 3 to a PAC guarantee. Assuming a fixed initial state $s$, with at least a constant probability, we can learn an $\varepsilon$-optimal policy $\pi$ that satisfies $V^*_\pi(s) - V^{\text{opt}}(s) \leq \varepsilon + \zeta \gamma_1 H^{3/2}$ by running CME-RL for $T = O(d_{\text{eff}}^2 H^2 / \varepsilon^2)$ episodes.

5. Conclusion

In this paper, we have presented a novel model-based RL algorithm with sub-linear regret guarantees under an optimistic RKHS-closure assumption on the value functions, without requiring a “simulator” access. The algorithm essentially performs an optimistic value iteration step, which is derived from a novel concentration inequality for the mean embeddings of the transition distribution. We have also shown robustness of our algorithm to small model misspecifications. It remains an open research direction to relax the strong optimistic closure assumption to a milder one, like in Zanette et al. (2020b), without sacrificing on the computational and regret performances.

3. This is a mild assumption, because for any RKHS $\mathcal{H}_\psi$, the direct sum $\mathcal{H}_\psi + \mathbb{R}$, where $\mathbb{R}$ denotes the RKHS associated with the positive definite kernel $k(s, s') = 1$, is again a RKHS with reproducing kernel $k_\psi(s, s') + 1$. 
References

Yasin Abbasi-Yadkori. *Online Learning for Linearly Parametrized Control Problems*. Phd, University of Alberta, 2012.

Yasin Abbasi-Yadkori and Csaba Szepesvári. Regret bounds for the adaptive control of linear quadratic systems. In *Proceedings of the 24th Annual Conference on Learning Theory*, pages 1–26, 2011.

Yasin Abbasi-Yadkori, Dávid Pál, and Csaba Szepesvári. Improved algorithms for linear stochastic bandits. In *Advances in Neural Information Processing Systems*, pages 2312–2320, 2011.

Sayak Ray Chowdhury and Aditya Gopalan. On kernelized multi-armed bandits. In *Proceedings of the 34th Annual Conference on Learning Theory*, pages 1–26, 2011.

Sayak Ray Chowdhury and Aditya Gopalan. Online learning in kernelized markov decision processes. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 3197–3205, 2019.

Sayak Ray Chowdhury and Rafael Oliveira. No-Regret Reinforcement Learning with Value Function Approximation: a Kernel Embedding Approach. *arXiv e-prints*, art. arXiv:2011.07881, November 2020.

Sayak Ray Chowdhury, Rafael Oliveira, and Fabio Ramos. Active learning of conditional mean embeddings via bayesian optimisation. In *Conference on Uncertainty in Artificial Intelligence*, pages 1119–1128. PMLR, 2020.

Christoph Dann, Tor Lattimore, and Emma Brunskill. Unifying PAC and regret: Uniform PAC bounds for episodic reinforcement learning. In *Advances in Neural Information Processing Systems 30 (NIPS)*, pages 5711–5721, 2017.

Omar Darwiche Domingues, Pierre Ménard, Matteo Pirotta, Emilie Kaufmann, and Michal Valko. Regret bounds for kernel-based reinforcement learning. *arXiv preprint arXiv:2004.05599*, 2020.

Petros Drineas and Michael W Mahoney. On the nyström method for approximating a gram matrix for improved kernel-based learning. *Journal of Machine Learning Research*, 6:2153–2175, 2005.

Yonathan Efroni, Nadav Merlis, Mohammad Ghavamzadeh, and Shie Mannor. Tight regret bounds for model-based reinforcement learning with greedy policies. In *Advances in Neural Information Processing Systems*, pages 12203–12213, 2019.

Kenji Fukumizu, Arthur Gretton, Xiaohai Sun, and Bernhard Schölkopf. Kernel measures of conditional dependence. In *Advances in neural information processing systems*, pages 489–496, 2008.

Kenji Fukumizu, Francis R Bach, Michael I Jordan, et al. Kernel dimension reduction in regression. *The Annals of Statistics*, 37(4):1871–1905, 2009.
Mohammad Gheshlaghi Azar, Ian Osband, and Rémi Munos. Minimax regret bounds for reinforcement learning. In Proceedings of the 34th International Conference on Machine Learning (ICML), pages 263–272, 2017.

Steffen Grünewälder, Guy Lever, Luca Baldassarre, Massimilano Pontil, and Arthur Gretton. Modelling transition dynamics in mdps with rkhs embeddings. In Proceedings of the 29th International Conference on International Conference on Machine Learning, pages 1603–1610, 2012.

Kelvin Hsu and Fabio Ramos. Bayesian Learning of Conditional Kernel Mean Embeddings for Automatic Likelihood-Free Inference. In Proceedings of the 22nd International Conference on Artificial Intelligence and Statistics (AISTATS), Naha, Okinawa, Japan, 2019.

Thomas Jaksch, Ronald Ortner, and Peter Auer. Near-optimal regret bounds for reinforcement learning. Journal of Machine Learning Research, 11(Apr):1563–1600, 2010.

Chi Jin, Zeyuan Allen-Zhu, Sebastien Bubeck, and Michael I Jordan. Is q-learning provably efficient? In Advances in Neural Information Processing Systems, pages 4863–4873, 2018.

Chi Jin, Zhuoran Yang, Zhaoran Wang, and Michael I Jordan. Provably efficient reinforcement learning with linear function approximation. arXiv preprint arXiv:1907.05388, 2019.

Sham Kakade, Akshay Krishnamurthy, Kendall Lowrey, Motoya Ohnishi, and Wen Sun. Information theoretic regret bounds for online nonlinear control. arXiv preprint arXiv:2006.12466, 2020.

Tze Leung Lai and Herbert Robbins. Asymptotically efficient adaptive allocation rules. Advances in Applied Mathematics, 6(1):4–22, 1985.

M. N. Lukic and J. H. Beder. Stochastic processes with sample paths in reproducing kernel Hilbert spaces. Transactions of the American Mathematical Society, 353(10):3945–3969, 2001.

Krikamol Muandet, Kenji Fukumizu, Bharath Sriperumbudur, and Bernhard Schölkopf. Kernel Mean Embedding of Distributions: A Review and Beyond. arXiv, 2016.

Ronald Ortner and Daniil Ryabko. Online regret bounds for undiscounted continuous reinforcement learning. In Advances in Neural Information Processing Systems 25 (NIPS), pages 1763–1771, 2012.

Ian Osband and Benjamin Van Roy. Model-based reinforcement learning and the eluder dimension. In Advances in Neural Information Processing Systems 27 (NIPS), pages 1466–1474, 2014.

Ian Osband, Dan Russo, and Benjamin Van Roy. (more) efficient reinforcement learning via posterior sampling. In Advances in Neural Information Processing Systems 26 (NIPS), pages 3003–3011, 2013.

Martin L Puterman. Markov decision processes: discrete stochastic dynamic programming. John Wiley & Sons, 2014.
Ali Rahimi and Benjamin Recht. Random features for large-scale kernel machines. In John C. Platt, Daphne Koller, Yoram Singer, and Sam T. Roweis, editors, Proceedings of the 21st conference on advances in Neural Information Processing Systems, NIPS '07, Vancouver, British Columbia, Canada, dec 2007. MIT Press.

C. E. Rasmussen and C. K. I. Williams. Gaussian processes for machine learning. MIT Press, 2006.

Daniel Russo and Benjamin Van Roy. Eluder dimension and the sample complexity of optimistic exploration. In Advances in Neural Information Processing Systems, pages 2256–2264, 2013.

Jonathan Scarlett, Ilijia Bogunovic, and Volkan Cevher. Lower bounds on regret for noisy gaussian process bandit optimization. arXiv preprint arXiv:1706.00090, 2017.

Bernhard Schölkopf and Alexander J. Smola. Learning with kernels: support vector machines, regularization, optimization, and beyond. MIT Press, Cambridge, Mass, 2002.

Le Song, Jonathan Huang, Alex Smola, and Kenji Fukumizu. Hilbert space embeddings of conditional distributions with applications to dynamical systems. In Proceedings of the 26th Annual International Conference on Machine Learning, pages 961–968, 2009.

Le Song, Byron Boots, Sajid M Siddiqi, Geoffrey Gordon, and Alex Smola. Hilbert space embeddings of hidden markov models. In Proceedings of the 27th International Conference on International Conference on Machine Learning, pages 991–998, 2010a.

Le Song, Arthur Gretton, and Carlos Guestrin. Nonparametric tree graphical models. In Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, pages 765–772, 2010b.

Le Song, Kenji Fukumizu, and Arthur Gretton. Kernel embeddings of conditional distributions: A unified kernel framework for nonparametric inference in graphical models. IEEE Signal Processing Magazine, 30(4):98–111, 2013. ISSN 10535888. doi: 10.1109/MSP.2013.2252713.

Niranjan Srinivas, Andreas Krause, Sham M Kakade, and Matthias Seeger. Gaussian process optimization in the bandit setting: No regret and experimental design. arXiv preprint arXiv:0912.3995, 2009.

Bharath K. Sriperumbudur, Kenji Fukumizu, and Gert R. G. Lanckriet. Universality, Characteristic Kernels and RKHS Embedding of Measures. Journal of Machine Learning Research (JMLR), 12:2389–2410, 2011.

Ingo Steinwart and Andreas Christmann. Support vector machines. Springer Science & Business Media, 2008.

Alexander L Strehl, Lihong Li, and Michael L Littman. Reinforcement learning in finite mdps: PAC analysis. Journal of Machine Learning Research, 10(Nov):2413–2444, 2009.

Ruosong Wang, Ruslan Salakhutdinov, and Lin F Yang. Provably efficient reinforcement learning with general value function approximation. arXiv preprint arXiv:2005.10804, 2020.

Yining Wang, Ruosong Wang, Simon S Du, and Akshay Krishnamurthy. Optimism in reinforcement learning with generalized linear function approximation. arXiv preprint arXiv:1912.04136, 2019.
Lin F Yang and Mengdi Wang. Reinforcement leaning in feature space: Matrix bandit, kernels, and regret bound. arXiv preprint arXiv:1905.10389, 2019.

Zhuoran Yang, Chi Jin, Zhaoran Wang, Mengdi Wang, and Michael Jordan. Provably efficient reinforcement learning with kernel and neural function approximations. Advances in Neural Information Processing Systems, 33, 2020.

Andrea Zanette and Emma Brunskill. Tighter problem-dependent regret bounds in reinforcement learning without domain knowledge using value function bounds. In International Conference on Machine Learning, pages 7304–7312, 2019.

Andrea Zanette, David Brandfonbrener, Emma Brunskill, Matteo Pirotta, and Alessandro Lazaric. Frequentist regret bounds for randomized least-squares value iteration. In International Conference on Artificial Intelligence and Statistics, pages 1954–1964, 2020a.

Andrea Zanette, Alessandro Lazaric, Mykel Kochenderfer, and Emma Brunskill. Learning near optimal policies with low inherent bellman error. arXiv preprint arXiv:2003.00153, 2020b.

Appendix A. Auxiliary results

Our results are based on concentration bounds for the conditional mean embeddings. We start with a few auxiliary results derived from the theory of multi-armed bandits and RKHS’s.

A.1. Concentration of arbitrary inner products

We first need to define the data-generating process and its properties. Let $\mathcal{F}_h^t$ be the filtration induced by the sequence $\mathcal{D}_t \cup \{(s_{h_1}^t, a_{h_1}^t)\}_{h_1 < h}$, where $\mathcal{D}_t$ denotes the replay buffer at the beginning of episode $t$. Given any bounded, measurable function $f : S \to \mathbb{R}$, the evaluation noise defined by $\epsilon_{f,h}^t := f(s_{h+1}^t) - \mathbb{E}[f(s)|s_h^t, a_h^t]$, for $s, s_{h+1}^t \sim P(\cdot|s_h^t, a_h^t)$, is such that:

$$\mathbb{E}[\epsilon_{f,h}^t | s_h^t, a_h^t] = 0$$

$$|\epsilon_{f,h}^t| \leq 2 \|f\|_{\infty}, \quad \forall t \geq 1, \forall h \in \{1, \ldots, H\},$$

where $\|f\|_{\infty} := \sup_{s \in S} |f(s)|$. From Equation 16, we can see that $\{\epsilon_{f,h}^t\}_{t, h}$ is a martingale difference sequence adapted to the filtration $\{\mathcal{F}_h^t\}_{h, t}$ for any bounded, measurable function. In addition, due to its boundedness (cf. Equation 17), we have that $\epsilon_{f,h}^t$ is $\sigma_f$-sub-Gaussian, for $\sigma_f := 2 \|f\|_{\infty}$, i.e.:

$$\forall t \geq 1, \forall h \in \{1, \ldots, H\}, \quad \mathbb{E}[\exp(\lambda \epsilon_{f,h}^t)] \leq \exp \left( \frac{1}{2} \lambda^2 \sigma_f^2 \right), \quad \forall \lambda \in \mathbb{R}.$$  

The observations above hold for any bounded, measurable function $f : S \to \mathbb{R}$, so that we can consider functions in the RKHS $\mathcal{H}_\varphi$. Any $f \in \mathcal{H}_\varphi$ is bounded by:

$$\|f\|_{\infty} := \sup_{s \in S} |f(s)| = \sup_{s \in S} \langle f, \psi(s) \rangle_{\mathcal{H}_\varphi} \leq \|f\|_{\mathcal{H}_\varphi} \sup_{s \in S} \|\psi(s)\|_{\mathcal{H}_\varphi} \leq B_\varphi \|f\|_{\mathcal{H}_\varphi},$$

where we first applied the reproducing property and then the Cauchy-Schwarz inequality. From our assumption on $\Theta_P : \mathcal{H}_\varphi \to \mathcal{H}_\varphi$, we also know that $g_f := \Theta_P^* f \in \mathcal{H}_\varphi$ for any $f \in \mathcal{H}_\varphi$, where $\Theta_P^* : \mathcal{H}_\varphi \to \mathcal{H}_\varphi$ denotes the transpose of the linear operator $\Theta_P$. We can now derive the following lemma based on Abbasi-Yadkori (2012, Thr. 3.11).

4. Throughout the text we implicitly assume measurable feature maps $\psi : S \to \mathcal{H}_\varphi$ and $\varphi : S \times A \to \mathcal{H}_\varphi$. 

Lemma 1 For any \( f \in \mathcal{H}_\psi \) and any \( \delta \in (0, 1) \), with probability at least \( 1 - \delta \), we have:
\[
\forall t \geq 1, \quad \left| \left\langle q, \hat{\Theta}^T_t f \right\rangle_{\mathcal{H}_\psi} - \left\langle q, \Theta^P_t f \right\rangle_{\mathcal{H}_\psi} \right| \leq \beta_{f,t}(\delta) \| q \|_{M_t^{-1}}, \quad \forall q \in \mathcal{H}_\varphi,
\]
where \( M_t := \lambda I + \sum_{\tau < t, h \leq H} \varphi(s^t_h, a^t_h) \otimes \varphi(s^t_h, a^t_h) \), and:
\[
\beta_{f,t}(\delta) := \sqrt{\lambda} \left\| \Theta^P_t f \right\|_{\mathcal{H}_\psi} + 2 \| f \|_{\infty} \sqrt{2 \log \left( \frac{\det(I + \lambda^{-1} K_{\varphi,t})^{1/2}}{\delta} \right)}.
\]

Proof We first need to verify whether the linear model assumption in Abbasi-Yadkori (cf. 2012, Assumption A1) holds in our settings. From the definition of the data-generating process, we have that \( \varphi(s^t_h, a^t_h) \) is \( \mathcal{F}^{t}_{h} \)-measurable. Letting \( y^t_{f,h} := f(s^t_{h+1}) \), we have that \( y^t_{f,h} \) is \( \mathcal{F}^t_{h+1} \)-measurable, and:
\[
\varepsilon^t_{f,h} = y^t_{f,h} - \left( \varphi(s^t_{h}, a^t_{h}), g_f \right)_{\mathcal{H}_\psi}, \quad \forall t \geq 1, \forall h \in \{1, \ldots, H\},
\]
which defines a martingale difference sequence and is \( 2 \| f \|_{\infty} \)-sub-Gaussian for \( g_f := \Theta^P_t f \in \mathcal{H}_\varphi \). Lastly, note that the function \( \hat{\Theta}^T_t f \in \mathcal{H}_\varphi \) is equivalent to the least-squares estimator for \( g_f \) from samples \( \{y^t_{f,h}\}_{t,h} \), that is:
\[
\hat{\Theta}^T_t f = \Phi_t (K_{\varphi,t} + \lambda I)^{-1} f_t,
\]
where \( f_t := [f(s^t_{h+1})]_{\tau < t, h \leq H} = [y^t_{f,h}]_{\tau < t, h \leq H} \). The rest of the proof follows by a direct application of Theorem 3.11 in Abbasi-Yadkori (2012) for the function \( g_f \).

A.2. Closed-form solution for the operator optimization problem

In this section, we show that Equation 13 is a closed-form solution for the operator optimization problem in Equation 12, which is of the form:
\[
\max_{\Theta \in L_1^t} \mathbb{E}_P[f].
\]
Although the term corresponding to \( f \) in Equation 12 is not necessarily in the RKHS \( \mathcal{H}_\psi \), we may for now assume that \( f \in \mathcal{H}_\psi \). In this case, the problem above may be rewritten as a quadratically constrained linear program in \( L(\mathcal{H}_\varphi, \mathcal{H}_\psi) \):
\[
\max_{\Theta \in L(\mathcal{H}_\varphi, \mathcal{H}_\psi)} \langle f, \Theta \varphi(s, a) \rangle_{\mathcal{H}_\psi}
\]
\[
s.t. \quad \left\| (\Theta - \hat{\Theta}) M_t^{1/2} \right\| \leq \beta_t(\delta/2),
\]
where \( M_t := \hat{\Theta}_{\varphi,t} + \lambda I \in L(\mathcal{H}_\varphi, \mathcal{H}_\varphi) \). The problem above admits a closed-form solution by applying the Karush-Kuhn-Tucker (KKT) conditions. Directly solving this would require us to take derivatives of the operator norm. However, observe that for any operator \( M \in L(\mathcal{H}_\varphi, \mathcal{H}_\psi) \) we have:
\[
\| M \| \leq \sqrt{\text{tr}(M^T M)},
\]
where the latter corresponds to the Hilbert-Schmidt norm. Compared to the operator norm, we can easily take derivatives of the trace to compute the KKT conditions. In addition, due to the upper bound, any solution satisfying the Hilbert-Schmidt norm constraint is also a solution under the operator norm constraint.
We replace Equation 25 with the following problem:

\[
\max_{\Theta \in \mathcal{L}(\mathcal{H}_\varphi, \mathcal{H}_\psi)} \langle f, \Theta \varphi(s, a) \rangle k_\psi \\
\text{s.t.} \ \text{tr}((\Theta - \hat{\Theta}_t) M_t(\Theta - \hat{\Theta}_t)^\top) \leq \beta_t(\delta/2)^2.
\]

(27)

Applying the KKT conditions, we solve:

\[
\nabla_\Theta \ell(\Theta, \eta) = 0
\]

(28)

\[
\text{tr}((\Theta - \hat{\Theta}_t) M_t(\Theta - \hat{\Theta}_t)^\top) \leq \beta_t(\delta/2)^2
\]

(29)

with respect to \( \Theta \in \mathcal{L}(\mathcal{H}_\varphi, \mathcal{H}_\psi) \) and \( \eta \in \mathbb{R}, \eta \geq 0 \), where:

\[
\ell(\Theta, \eta) := \langle f, \Theta \varphi(s, a) \rangle k_\psi - \eta \left( \text{tr}((\Theta - \hat{\Theta}_t) M_t(\Theta - \hat{\Theta}_t)^\top) - \beta_t(\delta/2)^2 \right)
\]

(30)

Firstly, we have:

\[
\nabla_\Theta \ell(\Theta, \eta) = f \otimes \varphi(s, a) - 2\eta(\Theta - \hat{\Theta}_t) M_t = 0
\]

(31)

\[
\therefore \Theta = \hat{\Theta}_t + \frac{1}{2\eta} (f \otimes \varphi(s, a)) M_t^{-1}.
\]

(32)

Secondly, we note that, for this kind of quadratically constrained linear program, the maximum should lie at the border of the constrained set. Replacing the result above into the constraint, we obtain:

\[
\beta_t(\delta/2)^2 = \frac{1}{4\eta^2} \text{tr}((f \otimes \varphi(s, a)) M_t^{-1}(\varphi(s, a) \otimes f)) = \frac{1}{4\eta^2} \langle \varphi(s, a), M_t^{-1} \varphi(s, a) \rangle_{\mathcal{H}_\varphi} \langle f, f \rangle_{\mathcal{H}_\psi}
\]

(33)

\[
= \frac{1}{4\eta^2} ||\varphi(s, a)||_{M_t^{-1}}^2 ||f||_{\mathcal{H}_\psi}^2,
\]

so that:

\[
\eta = \frac{1}{2\beta_t(\delta/2)} ||\varphi(s, a)||_{M_t^{-1}} ||f||_{\mathcal{H}_\psi}.
\]

(34)

Combining the latter with Equation 32, the solution to Equation 25 is then given by:

\[
\Theta_\ast := \hat{\Theta}_t + \frac{\beta_t(\delta/2)}{||\varphi(s, a)||_{M_t^{-1}} ||f||_{\mathcal{H}_\psi}} (f \otimes \varphi(s, a)) M_t^{-1},
\]

(35)

which finally yields:

\[
\max_{\Theta_\ast \in \mathcal{C}_t} \mathbb{E}_P[f] = \langle f, \Theta_\ast \varphi(s, a) \rangle_{\mathcal{H}_\psi}
\]

\[
= \langle f, \hat{\Theta}_t \varphi(s, a) \rangle_{\mathcal{H}_\psi} + \beta_t(\delta/2) ||f||_{\mathcal{H}_\psi} ||\varphi(s, a)||_{M_t^{-1}}
\]

(36)

\[
= \langle f, \hat{\Theta}_t \varphi(s, a) \rangle_{\mathcal{H}_\psi} + \beta_t(\delta/2) \lambda^{-1/2} ||f||_{\mathcal{H}_\psi} \sigma_{\varphi, t}(s, a).
\]

Replacing \( f \) by \( V_{h+1} \) in the solution above and adding the reward function (cf. Equation 12), we recover Equation 13.
Appendix B. Proof of main results

B.1. Proof of Theorem 1

The proof of Theorem 1 is based on Lemma 1, which establishes a uniform concentration bound over the whole of $\mathcal{H}_\psi$ and for any given $f \in \mathcal{H}_\psi$. Using a particular choice of $f$ and taking a supremum over $q \in \mathcal{H}_\phi$ then allows us to establish a confidence set for the CME operator $\Theta_P$, as shown below.

Proof We take similar steps to Abbasi-Yadkori (2012, Corollary 3.15). Considering Lemma 1, for $f \in \mathcal{H}_\psi$, we first set $q := M_t(\hat{\Theta}_t - \Theta_P)^\top f \in \mathcal{H}_\phi$, yielding:

$$\forall t \geq 1, \quad \left\| (\hat{\Theta}_t - \Theta_P)^\top f \right\|_{M_t} \leq \left\| (\hat{\Theta}_t - \Theta_P)^\top f \right\|_{M_t} \beta_{f,t}(\delta),$$

(37)

since $\left\| M_t(\hat{\Theta}_t - \Theta_P)^\top f \right\|_{M_t} = \left\| (\hat{\Theta}_t - \Theta_P)^\top f \right\|_{M_t}$. Equation 37 holds for $\left\| (\hat{\Theta}_t - \Theta_P)^\top f \right\|_{M_t} = 0$ by default. So we can consider the non-zero case, dividing both sides by $\left\| (\hat{\Theta}_t - \Theta_P)^\top f \right\|_{M_t}$, which leads us to:

$$\forall t \geq 1, \quad \left\| (\hat{\Theta}_t - \Theta_P)^\top f \right\|_{M_t} \leq \beta_{f,t}(\delta).$$

(38)

The above holds with probability at least $1 - \delta$ for any given $f \in \mathcal{H}_\psi$. We may as well then consider the worst case, by taking a supremum over $\mathcal{H}_\psi$. Therefore, with probability as least $1 - \delta$, we have that:

$$\left\| (\hat{\Theta}_t - \Theta_P) M_t^{1/2} \right\| = \sup_{f \in \mathcal{H}_\psi : \| f \|_{\mathcal{H}_\psi} \leq 1} \left\| M_t^{1/2}(\hat{\Theta}_t - \Theta_P)^\top f \right\|_{\mathcal{H}_\psi}$$

$$\leq \sup_{f \in \mathcal{H}_\psi : \| f \|_{\mathcal{H}_\psi} \leq 1} \lambda^2 \left\| \Theta_P^\top f \right\|_{\mathcal{H}_\psi} + 2 \| f \|_{\infty} \sqrt{2 \log \left( \frac{\det(I + \lambda^{-1} K_{\phi,t})^{1/2}}{\delta} \right)}$$

(39)

$$\leq \sqrt{\lambda} \| \Theta_P \| + 2B_\psi \sqrt{2 \log \left( \frac{\det(I + \lambda^{-1} K_{\phi,t})^{1/2}}{\delta} \right)}, \quad \forall t \geq 1,$$

since $\| \Theta_P^\top f \| \leq \| \Theta_P \| \| f \|_{\mathcal{H}_\psi}$ and $\| f \|_{\infty} \leq B_\psi \| f \|_{\mathcal{H}_\psi}$. This concludes the proof.

B.2. Regret analysis of CME-RL

To prove the regret bound in Theorem 2, we establish a sequence of intermediate results to bound the performance gap between the optimal policy and the policy followed by CME-RL. In Lemma 2, we start with a control on the $Q$-function estimates $Q^t_h$, which in turn leads to the regret bound, as our policy is based on $Q^t_h$. The result implies that as long as the true transition distribution lies in the confidence set $C_t$, the $Q$-updates are optimistic estimates of the optimal $Q$-values and thus, allow us to pick an optimistic action while sufficiently exploring the state space.

Lemma 2 (Optimism) Let $P \in C_t$. Then, $Q^*_h(s, a) \leq Q^t_h(s, a)$ for all $h$, and $(s, a)$.

Proof We prove the lemma by induction on $h$. When $h = H$, the inequality holds by definition. Now we assume that the lemma holds for some $h' = h + 1$, where $1 \leq h < H$. This implies that
for all $s \in S$,

$$V^t_{h+1}(s) = \min \left\{ H, \max_{a \in A} Q^t_{h+1}(s, a) \right\} \geq \min \left\{ H, \max_{a \in A} Q^*_t(s, a) \right\} = V^*_t(s).$$

We then have, for all $(s, a) \in S \times A$, that

$$Q^t_h(s, a) = R(s, a) + \mathbb{E}_{X \sim P(\cdot|s, a)} \left[ V^t_{h+1}(X) \right]$$

where the third step follows from $\Theta \in C_t$. [1]

Let $g^t_h(s) := V^t_h(s) - V^*_h(s)$ denote the gap between the most optimistic value and the actual value obtained starting from state $s$ at the step $h$ of episode $t$.

**Lemma 3 (Gap between optimistic and actual values)** We have

$$g^t_h(s) \leq \sum_{h=1}^{H} Q^t_h(s^t_h, a^t_h) - \left( R(s^t_h, a^t_h) + \mathbb{E}_{X \sim P(\cdot|s^t_h, a^t_h)} \left[ V^t_{h+1}(X) \right] \right) + \sum_{h=1}^{H} m^t_h,$$

where $m^t_h := \mathbb{E}_{X \sim P(\cdot|s^t_h, a^t_h)} \left[ g^t_{h+1}(X) \right] - g^t_{h+1}(s^t_{h+1})$.

**Proof** Note that $a^t_h = \pi^t_h(s^t_h) = \arg\max_{a \in A} Q^t_h(s^t_h, a)$. Therefore

$$V^{\pi^t_h}(s^t_h) = R(s^t_h, a^t_h) + \mathbb{E}_{X \sim P(\cdot|s^t_h, a^t_h)} \left[ V^{\pi^t_h}_{h+1}(X) \right]$$

$$= R(s^t_h, a^t_h) + \mathbb{E}_{X \sim P(\cdot|s^t_h, a^t_h)} \left[ V^t_{h+1}(X) \right] - \mathbb{E}_{X \sim P(\cdot|s^t_h, a^t_h)} \left[ g^t_{h+1}(X) \right]$$

$$= R(s^t_h, a^t_h) + \mathbb{E}_{X \sim P(\cdot|s^t_h, a^t_h)} \left[ V^t_{h+1}(X) \right] - g^t_{h+1}(s^t_{h+1}) - m^t_h.$$”

We also have

$$V^t_h(s^t_h) = \min \left\{ H, \max_{a \in A} Q^t_h(s^t_h, a) \right\} \leq Q^t_h(s^t_h, a^t_h).$$

Therefore

$$g^t_h(s^t_h) \leq Q^t_h(s^t_h, a^t_h) - \left( R(s^t_h, a^t_h) + \mathbb{E}_{X \sim P(\cdot|s^t_h, a^t_h)} \left[ V^t_{h+1}(X) \right] \right) + g^t_{h+1}(s^t_{h+1}) + m^t_h.$$”

Since, by definition $g^t_{h+1}(s) = 0$ for all $s \in S$, a simple recursion over all $h \in [H]$ yields

$$g^t_h(s^t_h) \leq \sum_{h=1}^{H} Q^t_h(s^t_h, a^t_h) - \left( R(s^t_h, a^t_h) + \mathbb{E}_{X \sim P(\cdot|s^t_h, a^t_h)} \left[ V^t_{h+1}(X) \right] \right) + \sum_{h=1}^{H} m^t_h,$$

which completes the proof. [1]

**Lemma 4 (Cumulative regret expressed through $Q$-estimates)** Let $\Theta \in C_t$ for all $t \geq 1$. Then for any $\delta \in (0, 1]$, the following holds with probability at least $1 - \delta/2$:

$$\mathcal{R}(N) \leq \sum_{t \in T, h \leq H} Q^t_h(s^t_h, a^t_h) - \left( R(s^t_h, a^t_h) + \mathbb{E}_{X \sim P(\cdot|s^t_h, a^t_h)} \left[ V^t_{h+1}(X) \right] \right) + 2H \sqrt{2N \log(2/\delta)}.$$”

**Proof** If $\Theta \in C_t$ for all $t$, we have from Lemma 2 that

$$\forall t \geq 1, \quad V^t_h(s^t_h) = \min \left\{ H, \max_{a \in A} Q^t_h(s^t_h, a) \right\} \geq \min \left\{ H, \max_{a \in A} Q^*_t(s^t_h, a) \right\} = V^*_t(s^t_h).$$
Therefore the cumulative regret after \( N = TH \) steps is given by
\[
\mathcal{R}(N) = \sum_{t=1}^{T} \left[ V^*_t(s^*_t) - V^\pi_t(s_1^t) \right] \leq \sum_{t=1}^{T} \left( V_t^t(s_1^t) - V_t^\pi_t(s_1^t) \right) = \sum_{t=1}^{T} g_t(s_1^t).
\]

We then have from Lemma 3 that
\[
\mathcal{R}(N) \leq \sum_{t \leq T, h \leq H} Q_h(s_t^h, a_t^h) - \left( R(s_t^h, a_t^h) + \mathbb{E}_{X \sim \mathcal{P}(s_t^h, a_t^h)} \left[ V_{h+1}^t(X) \right] \right) + \sum_{t \leq T, h \leq H} m_h^t.
\]

We now define \( \mathcal{F}_h^t \) as the filtration induced by the sequence \( \mathcal{D}_t \cup \{ (s_h^t, a_h^t) \} \), where \( \mathcal{D}_t \) denotes the replay buffer at the beginning of episode \( t \). Then \( (m_h^t)_{t,h} \) is a martingale difference sequence adapted to \( \mathcal{F}_h^t \) with each term bounded by \( 2H \). Hence, by Azuma-Hoeffding inequality, with probability at least \( 1 - \delta/2 \), we have
\[
\sum_{t \leq T, h \leq H} m_h^t \leq 2H \sqrt{2TH \log(2/\delta)} = 2H \sqrt{2N \log(2/\delta)},
\]
which proves the result.

\[\square\]

**Lemma 5 (Concentration of mean embedding estimates)** For \( \Theta_P \in C_t \), we have:
\[
\forall t \geq 1, \quad \left\| \check{g}_t(s,a) - \hat{g}_t(s,a) \right\|_{\mathcal{H}_\varphi} \leq \lambda^{-1/2} \beta_t(\delta/2) \sigma_{\varphi,t}(s,a), \quad \forall (s,a) \in S \times A,
\]

**Proof** For \( \Theta_P \in C_t \), uniformly over all \( t \in \mathbb{N} \), the mean embeddings satisfy

\[
\left\| \check{g}_t(s,a) - \hat{g}_t(s,a) \right\|_{\mathcal{H}_\varphi} \leq \left\| (\Theta_P - \hat{\Theta}_t) \varphi(s,a) \right\|_{\mathcal{H}_\varphi} \leq \left\| (\Theta_P - \hat{\Theta}_t) (\hat{C}_{\varphi,t} + \lambda I)^{-1/2} \left\| (\hat{C}_{\varphi,t} + \lambda I)^{-1/2} \varphi(s,a) \right\|_{\mathcal{H}_\varphi} \leq \beta_t(\delta/2) \lambda^{-1/2} \sigma_{\varphi,t}(s,a),
\]

which concludes the proof.

\[\square\]

**Lemma 6 (Error in Q-estimates)** Let \( \Theta_P \in C_t \). Then, for all \( h \leq H \) and \( (s,a) \in S \times A \), we have
\[
Q_h^t(s,a) - \left( R(s,a) + \mathbb{E}_{X \sim \mathcal{P}(s,a)} \left[ V_{h+1}^t(X) \right] \right) \leq 2B_V \beta_1(\delta/2) \lambda^{-1/2} \sigma_{\varphi,t}(s,a).
\]

**Proof** By Assumption 1, \( V_{h+1}^t \in \mathcal{H}_\varphi \). Hence the Q-estimates (Equation 13) can rewritten as
\[
Q_h^t(s,a) = R(s,a) + \left( V_{h+1}^t, \hat{\varphi}_t(s,a) \right)_{\mathcal{H}_\varphi} + B_V \beta_1(\delta/2) \lambda^{-1/2} \sigma_{\varphi,t}(s,a).
\]

Therefore, we have
\[
Q_h^t(s,a) - \left( R(s,a) + \mathbb{E}_{X \sim \mathcal{P}(s,a)} \left[ V_{h+1}^t(X) \right] \right) = \left( V_{h+1}^t, \hat{\varphi}_t(s,a) - \check{\varphi}_t(s,a) \right)_{\mathcal{H}_\varphi} + B_V \beta_1(\delta/2) \lambda^{-1/2} \sigma_{\varphi,t}(s,a) \leq 2B_V \beta_1(\delta/2) \lambda^{-1/2} \sigma_{\varphi,t}(s,a),
\]

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where the last step holds since $\|V_{h+1}^t\|_{H_{\psi}} \leq B_V$ and $\Theta_P \in C_t$. 

**Lemma 7 (Sum of predictive variances)** Let $\sup_{s,a} \sqrt{\mathbf{E}(h,(s,a),(s,a))} \leq B_{\psi}$. Then

$$\sum_{t \leq T, h \leq H} \lambda^{-1} \sigma_{\varphi,t}^2(s_h^t, a_h^t) \leq (1 + \lambda^{-1} B_{\psi}^2 H) \log \det(I + \lambda^{-1} K_{\psi,T+1}).$$

**Proof** Let us first denote $M_t = \tilde{C}_{\varphi,t} + \lambda I$. We then have from Equation 9 that

$$\lambda^{-1} \sigma_{\varphi,t}^2(s, a) = \langle \varphi(s, a), M_t^{-1} \varphi(s, a) \rangle_{\mathcal{H}_{\psi}} = \text{tr} \left( M_t^{-1} \varphi(s, a) \otimes \varphi(s, a) \right).$$

We also note that $M_t \geq \lambda I$ and $\varphi(s, a) \otimes \varphi(s, a) \leq B_{\psi}^2 I$. Therefore $M_t^{-1} \varphi(s, a) \otimes \varphi(s, a) \leq \lambda^{-1} B_{\psi}^2 I$. Now, since $M_{t+1} = M_t + \sum_{h \leq H} \varphi(s_h^t, a_h^t) \otimes \varphi(s_h^t, a_h^t)$, we have

$$M_t^{-1} = \left( I + M_t^{-1} \sum_{h \leq H} \varphi(s_h^t, a_h^t) \otimes \varphi(s_h^t, a_h^t) \right) M_{t+1}^{-1} \leq (1 + \lambda^{-1} B_{\psi}^2 H) M_{t+1}^{-1}.$$

We then have

$$\sum_{t \leq T, h \leq H} \lambda^{-1} \sigma_{\varphi,t}^2(s_h^t, a_h^t) \leq (1 + \lambda^{-1} B_{\psi}^2 H) \sum_{t \leq T} \text{tr} \left( M_{t+1}^{-1} (M_{t+1} - M_t) \right) = (1 + \lambda^{-1} B_{\psi}^2 H) \sum_{t \leq T} \log \frac{\det(M_{t+1})}{\det(M_t)} = (1 + \lambda^{-1} B_{\psi}^2 H) \log \frac{\det(M_{t+1})}{\det(\lambda I)} = (1 + \lambda^{-1} B_{\psi}^2 H) \log \det(I + \lambda^{-1} M_{T+1}) = (1 + \lambda^{-1} B_{\psi}^2 H) \log \det(I + \lambda^{-1} K_{\psi,T+1}).$$

Here, in the second step we have used that for two positive definite operators $A$ and $B$ such that $A - B$ is positive semi-definite, $\text{tr}(A^{-1}(A - B)) \leq \log \frac{\det(A)}{\det(B)}$. The last step follows from Sylvester’s determinant identity.

Based on the results in the previous section, we can finally derive a proof for **Theorem 2**.

**B.2.1. PROOF OF THEOREM 2**

We have from Lemma 4 and 6 that if $\Theta_P \in C_t$ for all $t$, then with probability at least $1 - \delta/2$, the cumulative regret

$$\mathcal{R}(N) \leq \sum_{t \leq T, h \leq H} 2B_V \beta_t(\delta/2) \lambda^{-1/2} \sigma_{\varphi,t}(s_h^t, a_h^t) + 2H \sqrt{2N \log(2/\delta)} \leq 2B_V \beta_T(\delta/2) \sum_{t \leq T, h \leq H} \lambda^{-1/2} \sigma_{\varphi,t}(s_h^t, a_h^t) + 2H \sqrt{2N \log(2/\delta)} \leq 2B_V \alpha_{N,\delta} \sqrt{TH} \sum_{t \leq T, h \leq H} \lambda^{-1} \sigma_{\varphi,t}^2(s_h^t, a_h^t) + 2H \sqrt{2N \log(2/\delta)} \leq 2B_V \alpha_{N,\delta} \sqrt{2(1 + \lambda^{-1} B_{\psi}^2 H)N \gamma_N} + 2H \sqrt{2N \log(2/\delta)}.$$
The second step follows from the fact that $\beta_t(\delta)$ with $t$, the third step is due to Cauchy-Schwartz’s inequality and the fact that $\beta_T(\delta/2) \leq \alpha_{N,T}$, and the final step follows from Lemma 7. The proof now can be completed using Theorem 1 and taking a union bound.

**B.3. Regret analysis of CME-RL under model misspecification**

To prove the regret bound in Theorem 3, we follow the similar arguments used in proving Theorem 2, but with necessary modifications taking the effect of the misspecification error $\zeta$ into account. We first derive the following result.

**Lemma 8 (Error in approximate Q-values)** Let $\Theta_T \in C_t$. Then, for all $h \in [H]$ and $(s, a) \in S \times A$, we have that:

$$Q^t_h(s, a) - (R(s, a) + \mathbb{E}_{X \sim P(\cdot|s, a)} [V^t_{h+1}(X)]) \leq 2 \left( B_V + \zeta \left\| \mathcal{M}_{\psi} \right\|_{\mathcal{H}_\psi} \right) \lambda^{-1} \beta_t(\delta/2) \sigma_{\varphi, t}(s, a) + 2\zeta.$$  

**Proof** Note that the $Q$-estimates (Equation 15) can rewritten as:

$$Q^t_h(s, a) := R(s, a) + \alpha_t(s, a) ^ T v^t_{h+1} + \left( B_V + \zeta \left\| \mathcal{M}_{\psi} \right\|_{\mathcal{H}_\psi} \right) \lambda^{-1} \beta_t(\delta/2) \sigma_{\varphi, t}(s, a),$$

By Assumption 3, there exists a function $V^t_{h+1} \in \mathcal{H}_\psi$ such that $\|V^t_{h+1} - \hat{V}^t_{h+1}\|_\infty \leq \zeta$. We now define the vector $\hat{v}^t_{h+1} := \left[ \hat{V}^t_{h+1}(s^T_{h+1}) \right]_{\tau < t, t' \leq H}$ and introduce the shorthand notation $\mathbb{E}_{P(\cdot|s, a)}[f] := \mathbb{E}_{X \sim P(\cdot|s, a)}[f(X)]$. We then have:

$$\left\| \alpha_t(s, a) ^ T v^t_{h+1} - \mathbb{E}_{X \sim P(\cdot|s, a)} [V^t_{h+1}(X)] \right\|_\infty$$

$$= \left\| \alpha_t(s, a) ^ T v^t_{h+1} - \alpha_t(s, a) ^ T (v^t_{h+1} - \hat{v}^t_{h+1}) - \mathbb{E}_{P(\cdot|s, a)} [\hat{V}^t_{h+1}] + \mathbb{E}_{P(\cdot|s, a)} [V^t_{h+1} - \hat{V}^t_{h+1}] \right\|_\infty$$

$$\leq \left\| \alpha_t(s, a) ^ T (v^t_{h+1} - \hat{v}^t_{h+1}) \right\|_\infty + \left\| \alpha_t(s, a) \right\| \left\| V^t_{h+1} - \hat{V}^t_{h+1} \right\|_\infty + \left\| \hat{V}^t_{h+1} \right\|_\infty$$

$$\leq \left\| \alpha_t(s, a) ^ T v^t_{h+1} - \mathbb{E}_{P(\cdot|s, a)} [\hat{V}^t_{h+1}] \right\|_\infty + \zeta \left( 1 + \left\| \alpha_t(s, a) \right\|_1 \right),$$

which follows by an application of Hölder’s inequality. Now, as $\Theta_T \in C_t$ and $\left\| \hat{V}^t_{h+1} \right\|_\mathcal{H}_\psi \leq B_V$, the following also holds:

$$\left\| \alpha_t(s, a) ^ T v^t_{h+1} - \mathbb{E}_{P(\cdot|s, a)} [\hat{V}^t_{h+1}] \right\|_\infty = \left\| \left[ \hat{V}^t_{h+1}, \hat{\theta}_t(s, a) - \vartheta_P(s, a) \right] \right\|_\mathcal{H}_\psi$$

$$\leq \left\| \hat{V}^t_{h+1} \right\|_\mathcal{H}_\psi \left( 1 + \left\| \alpha_t(s, a) \right\|_1 \right) \lambda^{-1} \beta_t(\delta/2) \sigma_{\varphi, t}(s, a).$$

By Assumption 4, the constant function $1 : S \to \mathbb{R}$ is an element of $\mathcal{H}_\psi$. For stationary (radial) kernels $k_\varphi$, we have $\left\| \alpha_t(s, a) \right\|_\mathcal{H}_\psi \geq 0, \forall \tau \leq t, h \leq H$. Now, as $\Theta_T \in C_t$, we have:

$$\left\| \alpha_t(s, a) \right\|_1 = \left\langle \hat{\vartheta}^{(s, a)}_t, 1 \right\rangle_{\mathcal{H}_\psi}$$

$$= \left\langle \hat{\vartheta}^{(s, a)}_t, 1 \right\rangle_{\mathcal{H}_\psi} + \left\langle \vartheta^{(s, a)}_t - \vartheta^{(s, a)}_P, 1 \right\rangle_{\mathcal{H}_\psi}$$

$$\leq \mathbb{E}_{X \sim P(\cdot|s, a)}[1(X)] + \left\| \vartheta^{(s, a)}_P - \vartheta^{(s, a)}_P \right\|_{\mathcal{H}_\psi}$$

$$= 1 + \left\| \mathcal{M}_{\psi} \right\|_{\mathcal{H}_\psi} \lambda^{-1} \beta_t(\delta/2) \sigma_{\varphi, t}(s, a).$$
Combining Equation 42 and Equation 43 with Equation 41 yields:
\[
\begin{align*}
\alpha_t(s, a) &\dagger v_{h+1}^t - \mathbb{E}_{X \sim P(s|s,a)(X)}[V_{h+1}^t] \\
&\leq B_\nu \lambda^{-1/2} \beta_t(\delta/2) \sigma_{\varphi,t}(s, a) + \zeta \left( 2 + \|1\|_{\mathcal{H}_\varphi} \lambda^{1/2} \beta_t(\delta/2) \sigma_{\varphi,t}(s, a) \right) \\
&\leq \left( B_\nu + \zeta \|1\|_{\mathcal{H}_\varphi} \right) \lambda^{-1/2} \beta_t(\delta/2) \sigma_{\varphi,t}(s, a) + 2\zeta.
\end{align*}
\]
(44)

Finally, the result follows by noting that
\[
\begin{align*}
Q^*_h(s, a) - \mathbb{E}_{X \sim P(s|s,a)}[V_{h+1}^t(X)] &\leq \alpha_t(s, a) \dagger v_{h+1}^t - \mathbb{E}_{X \sim P(s|s,a)}[V_{h+1}^t] + \left( B_\nu + \zeta \|1\|_{\mathcal{H}_\varphi} \right) \lambda^{-1/2} \beta_t(\delta/2) \sigma_{\varphi,t}(s, a) \\
&\leq 2 \left( B_\nu + \zeta \|1\|_{\mathcal{H}_\varphi} \right) \lambda^{-1/2} \beta_t(\delta/2) \sigma_{\varphi,t}(s, a) + 2\zeta,
\end{align*}
\]
which concludes the proof.

With the result above, we can derive an upper bound on the optimal value $Q^*_h$ as follows.

**Lemma 9** Let $\Theta_P \in \mathcal{C}_t$. Then
\[
\forall h \in [H], \forall (s, a) \in \mathcal{S} \times \mathcal{A}, \quad Q^*_h(s, a) \leq Q^*_h(s, a) + 2(H - h)\zeta.
\]

**Proof** We prove the lemma by induction on $h$. When $h = H$, the inequality holds by definition.

Now we assume that the lemma holds for some $h' = h + 1$, where $1 \leq h < H$. This implies that:
\[
\forall s \in \mathcal{S}, \quad V_{h+1}^t(s) = \min \left\{ H_t, \max_{a \in \mathcal{A}} Q^*_h(s, a) \right\} \geq \min \left\{ H_t, \max_{a \in \mathcal{A}} Q^*_h(s, a) \right\} - 2(H - h - 1)\zeta = V_{h+1}^t(s) - 2(H - h - 1)\zeta.
\]

We then have, for all $(s, a) \in \mathcal{S} \times \mathcal{A}$, that
\[
Q^*_h(s, a) = R(s, a) + \mathbb{E}_{X \sim P(s|s,a)}[V_{h+1}^t(X)] \leq R(s, a) + \mathbb{E}_{X \sim P(s|s,a)}[V_{h+1}^t(X)] + 2(H - h - 1)\zeta.
\]
Using Equation 44 in the proof of Lemma 8, we now see that
\[
\mathbb{E}_{X \sim P(s|s,a)}[V_{h+1}^t(X)] \leq \alpha_t(s, a) \dagger v_{h+1}^t + \left( B_\nu + \zeta \|1\|_{\mathcal{H}_\varphi} \right) \lambda^{-1/2} \beta_t(\delta/2) \sigma_{\varphi,t}(s, a) + 2\zeta
\]
which holds as $\Theta_P \in \mathcal{C}_t$. We then have from Equation 45 that
\[
Q^*_h(s, a) \leq R(s, a) + \alpha_t(s, a) \dagger v_{h+1}^t + \left( B_\nu + \zeta \|1\|_{\mathcal{H}_\varphi} \right) \lambda^{-1/2} \beta_t(\delta/2) \sigma_{\varphi,t}(s, a) + 2(H - h)\zeta = Q^*_h(s, a) + 2(H - h)\zeta,
\]
which follows from the definition of $Q$-estimates.

Given Lemma 8 and Lemma 9, we can finally prove Theorem 3.

**B.3.1. PROOF OF THEOREM 3**

If $\Theta_P \in \mathcal{C}_t$ for all $t \geq 1$, we have from Lemma 9 that $V^*_{t+1}(s_1) \leq V^*_t(s_1) + 2(H - 1)\zeta$. Then following similar steps as in the proof of Theorem 2 and Lemma 4, with probability at least $1 - \delta/2$,
we have the following:
\[
\mathcal{R}(N) \leq \sum_{t \leq T, h \leq H} Q_h^t(s_h^t, a_h^t) - \left( R(s_h^t, a_h^t) + \mathbb{E}_{X \sim P_t(s_h^t, a_h^t)} [V_t^{t+1}(X)] \right) \\
+ 2H \sqrt{2N \log(2/\delta)} + 2\zeta T(H - 1)
\]
\[
\leq 2 \left( B_V + \zeta \|1\|_{\mathcal{H}_\psi} \right) \sum_{t \leq T, h \leq H} \lambda^{-1/2} \beta_t(\delta/2) \sigma_{\varphi,t}(s_h^t, a_h^t) + 2\zeta TH \\
+ 2H \sqrt{2N \log(2/\delta)} + 2\zeta T(H - 1)
\]
\[
\leq 2 \left( B_V + \zeta \|1\|_{\mathcal{H}_\psi} \right) \beta_T(\delta/2) \sum_{t \leq T, h \leq H} \lambda^{-1/2} \sigma_{\varphi,t}(s_h^t, a_h^t) + 4\zeta TH + 2H \sqrt{2N \log(2/\delta)}
\]
\[
\leq 2 \left( B_V + \zeta \|1\|_{\mathcal{H}_\psi} \right) \alpha_{N,\delta} \sqrt{TH} \sum_{t \leq T, h \leq H} \lambda^{-1} \sigma_{\varphi,t}^2(s_h^t, a_h^t) + 4\zeta TH + 2H \sqrt{2N \log(2/\delta)}
\]
\[
\leq 2 \left( B_V + \zeta \|1\|_{\mathcal{H}_\psi} \right) \alpha_{N,\delta} \sqrt{2(1 + \lambda^{-1} B_{\varphi}^2 H)} N \gamma_N + 4\zeta N + 2H \sqrt{2N \log(2/\delta)}.
\]

The second step follows from Lemma 8, the third step from monotonicity of \( \beta_t(\delta) \) with \( t \), the fourth step is due to Cauchy-Schwartz’s inequality and the fact that \( \beta_T(\delta/2) \leq \alpha_{N,\delta} \), and the final step follows from Lemma 7. The proof now can be completed using Theorem 1 and taking a union bound.