Kernel-Based Function Approximation for Average Reward Reinforcement Learning: An Optimist No-Regret Algorithm

Sattar Vakili (MediaTek Research)

 $\mathbf{Julia\ Olkhovskaya}\ (\mathrm{TU\ Delft})$



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Overview

- Regression
- 2 Bandits / Bayesian optimization
- 3 MDP
- 4 KUCB-RL Algorithm
- 6 Confidence Intervals
- 6 Performance Grantees

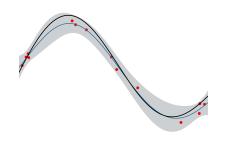
Provided a dataset of t observation:

$$\left\{ (z_j, Y(z_j)) \right\}_{j=1}^t, Y(z_j) = f(z_j) + \varepsilon_j$$



Predictor:

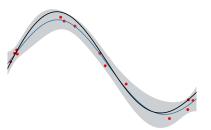
$$\hat{f}(z) = \boldsymbol{\kappa}_t^{\top}(z)(\mathbf{K}_t + \rho I)^{-1}\mathbf{y}_t$$



- $\kappa_t(z) = [\kappa(z_1, z), \kappa(z_2, z), \cdots, \kappa(z_t, z)]$
- $\mathbf{K}_t = [\kappa(z_i, z_j)]_{i,j=1}^t$
- $\mathbf{y}_t = [Y(z_1), Y(z_2), \cdots, Y(z_t)]$

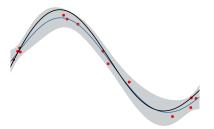
Uncertainty estimator:

$$(\sigma_t(z))^2 = \kappa(z, z) - \kappa_t^{\top}(z)(\mathbf{K}_t + \rho I)^{-1}\kappa_t(z)$$



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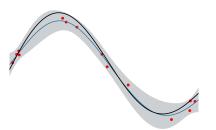
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Closed from expressions for prediction and uncertainty quantification!

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Closed from expressions for prediction and uncertainty quantification!

Confidence interval
$$|f(z) - \hat{f}_t(z)| \leq \beta(\delta)\sigma_t(z)$$
, w.p. $1 - \delta$

Bayesian and Frequentist Interpretations

Bayesian: Posterior mean (maximum likelihood estimation) assuming a prior centered Gaussian process distribution $\mathcal{GP}(\mathbf{0}, \kappa)$ and Gaussian noise

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Frequntist: Regularized Least Squares Error Estimation

$$\hat{f} = \operatorname{arg min}_{g \in \mathcal{H}_{\kappa}} \sum_{j=1}^{t} (Y(z_j) - g(z_j))^2 + \lambda ||g||_{\mathcal{H}_{\kappa}}^2$$

Reproducing Kernel Hilbert Space

RKHS:

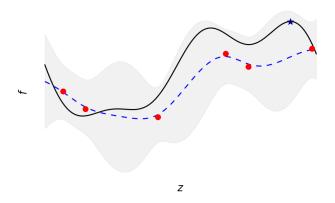
$$\mathcal{H}_{\kappa} = \left\{ f(\cdot) = \sum_{m=1}^{\infty} w_m \phi_m(\cdot) \right\}$$

- Inner product $\langle f, g \rangle_{\mathcal{H}_{\kappa}} = \boldsymbol{w}_f^{\top} \boldsymbol{w}_g$
- $\bullet \|f\|_{\mathcal{H}_{\kappa}} = \|\mathbf{w}\|$
- $\phi_m = \sqrt{\lambda_m} \varphi_m$ form an orthonormal basis

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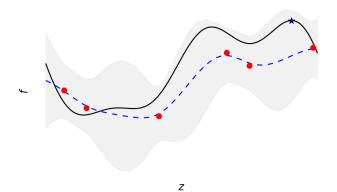
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Bandits (Bayesian Optimization)



Procedure: Sequentially select points z_1, z_2, \dots, z_T

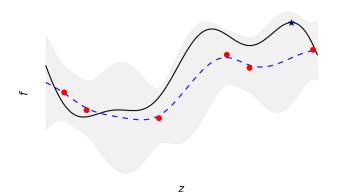
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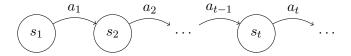
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Optimistic Algorithm: $z_t = \arg \max_z \left(\hat{f}_{t-1}(z) + \beta(\delta) \sigma_{t-1}(z) \right)$

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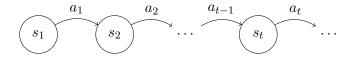
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Markov Decision Process



Procedure: Observe $s_t \sim P(\cdot|s_{t-1}, a_{t-1})$, select $a_t = \pi(s_t)$

Markov Decision Process

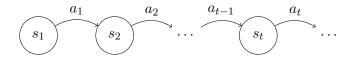


Procedure: Observe $s_t \sim P(\cdot|s_{t-1}, a_{t-1})$, select $a_t = \pi(s_t)$

Performance measure: Regret $(T) = \sum_{t=1}^{T} (J^* - r(s_t, a_t)).$

$$J^* = \max_{\pi} \lim \inf_{T \to \infty} \frac{1}{T} \left[\sum_{t=1}^{T} r(s_t, a_t) \right]$$
$$a_t = \pi(s_t), s_{t+1} \sim P(\cdot | s_t, a_t)$$

Markov Decision Process



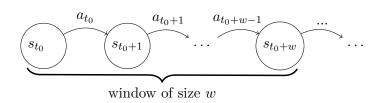
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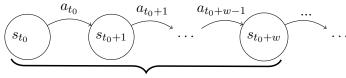
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Weekly Communicating MDP

Value Function



Value Function



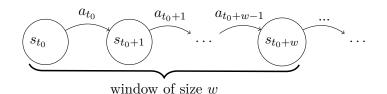
window of size w

▶ The value of a policy π over a window w

$$v_w^{\pi}(s) = \mathbb{E}\left[\sum_{t=t_0}^{t_0+w-1} r(s_t, a_t)\right]$$

$$s = s_{t_0}, \ a_t = \pi(s_t), \ s_{t+1} \sim P(\cdot|s_t, a_t)$$

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Dynamic Programming

Dynamic Programming



Dynamic Programming

$$Pv](s,a) := \mathbb{E}_{s' \sim P(\cdot|s,a)}[v(s')]$$

$$= \int_{s' \in \mathcal{S}} v(s') P(s'|s,a) ds'$$

- $\mathbf{v}_{t_0+w} \leftarrow \mathbf{0}$
- ▶ Recursively $t = t_0 + w 1, t_0 + w 2, \dots, t_0$:

$$q_t(s, a) = r(s, a) + [Pv_{t+1}](s, a)$$

 $v_t(s) = \max_{a} q_t(s, a)$

Dynamic Programming

$$\begin{aligned}
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 $\blacktriangleright \pi_t^{\star,w}(s) = \arg\max_a q_t(s,a)$

Unknown Model: RL

r and P are unknown in RL

$$f_t = [Pv_{t+1}]$$

$$UCB = \hat{f}_t + \beta(\delta)\sigma_t$$

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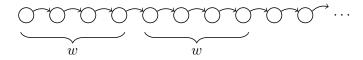
$$q_t(s, a) = r(s, a) + Pv_{t+1}(s, a)$$

$$q_t(s, a) = r(s, a) + UCB(Pv_{t+1})$$

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KUCB-RL Algorithm



- \triangleright Fix a window size w
- ▶ For each window $t \in [t_0, t_0 + w 1]$, compute q_t and v_t , recursively, starting from $v_{t_0+w} = \mathbf{0}$
- ▶ Unroll the policy $a_t = \arg \max_a q_t(s_t, a)$ over this window

This is equivalent to solving a w-step look ahead MDP

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 \blacktriangleright How to create confidence intervals for f = [Pv]

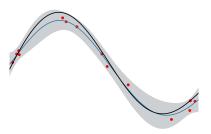
$$\left|\hat{f}_t(s,a) - [Pv](s,a)\right| \le \beta(\delta)\sigma_t(s,a).$$

 \blacktriangleright How to create confidence intervals for f = [Pv]

$$\left| \hat{f}_t(s, a) - [Pv](s, a) \right| \le \beta(\delta)\sigma_t(s, a).$$

▶ For a fixed $f \in \mathcal{H}_{\kappa}$ with non-adaptive inputs z_1, \ldots, z_t ,

$$\beta(\delta) \approx ||f||_{\mathcal{H}_{\kappa}} + \frac{w}{\sqrt{\rho}} \sqrt{d \log(\frac{t}{\delta})}$$



Challenge 1: Inputs $(s_1, a_1), \ldots, (s_t, a_t)$ are adaptive!

Solution: Self-normalized concentration inequalities for vector-valued martingales extended to kernel setting (Abbasi-Yadkori 2013; Whitehouse et al. 2023):

$$\beta(\delta) \approx ||f||_{\mathcal{H}_{\kappa}} + \frac{w}{\sqrt{\rho}} \sqrt{\gamma(t; \rho) + \log(\frac{1}{\delta})}$$

► Maximum information gain:

$$\gamma(t; \rho) = \sup_{\{z_i\}_{i=1}^t \subset \mathcal{Z}} \frac{1}{2} \log \det \left(I + \frac{K_t}{\rho} \right)$$

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Solution: Optimistic closure assumption

▶ For all $v \in \mathcal{V}$ and some $\kappa' : \mathcal{S} \times \mathcal{S} \to \mathbb{R}$, $\|v\|_{\mathcal{H}_{\kappa'}} \leq C_v = \mathcal{O}(w)$

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- ▶ Proof idea:
 - Write v in terms of the feature space of κ'
 - For *M* largest eigenvalues use standard confidence intervals (Whitehouse et al. 2023)
 - The rest is bounded using the eigendecay

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Theorem: Regret bound w.p. $1 - \delta$

$$\mathcal{R}(T) = \mathcal{O}\left(\underbrace{\frac{T}{w}}_{\text{w-step look ahead}} + \underbrace{\beta(\delta)\sum_{t=1}^{T} \sigma_{w \lfloor \frac{t-1}{w} \rfloor}(s_t, a_t))}_{\text{Uncertainties in values}}\right)$$

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$$\mathcal{R}(T) = \mathcal{O}\left(\frac{T}{w} + \left(w + \frac{w}{\sqrt{\rho}}\sqrt{\gamma(T;\rho) + \log\left(\frac{T}{\delta}\right)}\right)\sqrt{\rho T \gamma(T;\rho) + \rho^2 w^2 \gamma(T;\rho) \gamma(T/w;\rho)}\right)$$

Result

Matérn ν kernel (Neural tangent kernel)

$$\mathcal{R}(T) = \tilde{\mathcal{O}}(T^{\frac{3\nu + 4d}{4\nu + 4d}})$$

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- $ightharpoonup \mathcal{R}(T) = o(T)$, the algorithm converges to the optimal stationary policy $\implies no\text{-regret!}$
- ▶ For comparison, the regret bound for UCB algorithm in BO:

$$\mathcal{R}(T) = \tilde{\mathcal{O}}(T^{\frac{\nu+2d}{2\nu+2d}})$$
 (Whitehouse et al. 2023)

Discussion and Technical Challenges

 \triangleright The policy is updated every w step: delay in using samples

$$\sum_{t=1}^{T} \sigma_{w \lfloor \frac{t-1}{w} \rfloor}(s_t, a_t)) \leq \sqrt{\rho T \gamma(T; \rho) + \rho^2 w^2 \gamma(T; \rho) \gamma(T/w; \rho)}$$

Elliptical potential lemma (Srinivas et al. 2010).

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- ▶ The algorithm follows a *w*-step look ahead policy: this seems to be the main factor contributing to the difference with BO $\mathcal{O}(\frac{T}{w} + ...)$
- ► Confidence interval is not applied to prefixed functions (as in BO)

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The first no-regret performance guarantee for an algorithm in the infinite-horizon average-reward RL setting with kernel-based modeling

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Open problem: Is our bound improvable? What is the minimum rate of regret growth with T?

References I

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- N. Srinivas, A. Krause, S. Kakade, and M. Seeger. Gaussian process optimization in the bandit setting: No regret and experimental design. In ICML 2010 -Proceedings, 27th International Conference on Machine Learning, pages 1015–1022, July 2010.
- J. Whitehouse, A. Ramdas, and S. Z. Wu. On the sublinear regret of gp-ucb. Advances in Neural Information Processing Systems, 36, 2023.