Provable Model-based Nonlinear Bandit and RL: Shelve Optimism, Embrace Virtual Curvature

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Toward a Theory for Deep RL

Existing RL theory cannot apply to Neural Nets

• None of these give polynomial sample complexities for even one-layer NNs.

| | B-Rank | B-Complete | W-Rank | Bilinear Class (this work) |
|--|-----------------------------------|--------------|--------------|----------------------------|
| Tabular MDP | \checkmark | \checkmark | \checkmark | \checkmark |
| Reactive POMDP [Krishnamurthy et al., 2016] | \checkmark | × | \checkmark | ✓ |
| Block MDP [Du et al., 2019a] | \checkmark | × | \checkmark | \checkmark |
| Flambe / Feature Selection [Agarwal et al., 2020b] | \checkmark | × | \checkmark | \checkmark |
| Reactive PSR [Littman and Sutton, 2002] | \checkmark | × | \checkmark | \checkmark |
| Linear Bellman Complete [Munos, 2005] | X | \checkmark | × | \checkmark |
| Linear MDPs [Yang and Wang, 2019, Jin et al., 2020] | √! | \checkmark | √! | \checkmark |
| Linear Mixture Model [Modi et al., 2020b] | X | × | X | \checkmark |
| Linear Quadratic Regulator | X | \checkmark | X | \checkmark |
| Kernelized Nonlinear Regulator [Kakade et al., 2020] | X | × | × | \checkmark |
| Q^* "irrelevant" State Aggregation [Li, 2009] | \checkmark | × | X | \checkmark |
| Linear Q^*/V^* (this work) | X | X | X | \checkmark |
| RKHS Linear MDP (this work) | X | X | X | \checkmark |
| RKHS Linear Mixture MDP (this work) | X | × | X | \checkmark |
| Low Occupancy Complexity (this work) | × | × | X | \checkmark |
| Q^{\star} State-action Aggregation [Dong et al., 2020] | X | × | X | × |
| Deterministic linear Q^* [Wen and Van Roy, 2013] | × | × | X | × |
| Linear Q^* [Weisz et al., 2020] | Sample efficiency is not possible | | | |

Du, Simon S., et al. "Bilinear Classes: A Structural Framework for Provable Generalization in RL."

Neural Net Bandit: A Simplification

- Reward function $\eta(\theta, a)$
 - $\theta \in \Theta$: model parameter
 - $a \in \mathcal{A}$: continuous action
- Linear bandit: $\eta(\theta, a) = \theta^{\top} a$
- Neural net bandit: $\eta(\theta, a) = NN_{\theta}(a)$
- Realizable and deterministic reward setting:
 - Agent observes ground-truth reward $\eta(\theta^{\star}, a)$ after playing action a
- Goal: finding the best action

$$a^{\star} = \operatorname{argmax}_{a \in \mathcal{A}} \eta(\theta^{\star}, a)$$

Neural Net Bandit is **Statistically** Hard!

• Θ, \mathcal{A} : unit ℓ_2 -ball in \mathbb{R}^d

• $\eta(\theta, a) = \operatorname{relu}(\theta^{\top}a - 0.9), \quad a^* = \operatorname{argmax}_{\substack{||a||_2 \le 1}} \operatorname{relu}(\theta^{*\top}a - 0.9) = \theta^*$



Neural Net Bandit is **Statistically** Hard!



$$\eta((\theta,\beta),a) = \theta^{\mathsf{T}}a + 20 \cdot \operatorname{relu}(\beta^{\mathsf{T}}a - 0.9)$$

needle in a haystack!

A New Paradigm for Bandit/RL

1. Convergences to local maxima for general instances



2. Analysis of the landscape of the true reward $\eta(\theta^{\star}, \cdot)$

Main Results

• Theorem (informal): Under Lipschitz assumptions on η , our algorithm (ViOlin) converges to a ϵ -approximate local maxima in $\tilde{O}(R(\Theta)\epsilon^{-8})$.

measures hardness of online learning w.r.t. model class

• Similar results for nonlinear RL (with many more assumptions and stochastic policies.)

Reviewing the Analysis of UCB

1. Optimization (high virtual reward):

by optimism, $\eta(\theta_t, a_t) = \max_{\theta, a} \eta(\theta, a) \ge \eta(\theta^*, a^*)$

2. Extrapolation (in average):

$$\sum_{t=1}^{T} \left(\eta(\theta_t, a_t) - \eta(\theta^*, a_t) \right)^2 \le \sqrt{\dim_E(\Theta) \cdot T}$$

Eluder dimension

- 1+2 $\Rightarrow \eta(\theta^{\star}, a_t) \rightarrow \eta(\theta^{\star}, a^{\star})$
- Step 2 fails for neural net models because $\dim_E(\Theta) \approx \exp(d)$

This result was independently proven in Li, Gene, Pritish Kamath, Dylan J. Foster, and Nathan Srebro. "Eluder Dimension and Generalized Rank."

Re-Prioritizing the Two Steps

1. Extrapolation by online learning (OL) oracles:

$$\mathbb{E}\left[\sum_{t=1}^{T} \left(\eta(\theta_t, a_t) - \eta(\theta^*, a_t)\right)^2\right] \le \tilde{O}\left(\sqrt{R(\Theta)T}\right)$$

OL oracle outputs a distribution of θ_t

Sequential Rademacher Complexity [Rakhlin-Sridharan-Tewari'15]

- For finite hypothesis Θ , $R(\Theta) = \log|\Theta|$
- For neural nets:

 $R(\Theta) = poly(d)$ vs. Eluder dim = exp(d)

Re-Prioritizing the Two Steps

1. Extrapolation by online learning (OL) oracles

$$\mathbb{E}\left[\sum_{t=1}^{T} \left(\eta(\theta_t, a_t) - \eta(\theta^*, a_t)\right)^2\right] \le \sqrt{R(\Theta)T \text{ polylog}(T)}$$

2. High virtual reward:

best attempt:
$$a_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \mathbb{E}[\eta(\theta_t, a)]$$

 $\eta(\theta^*, \cdot)$
 $getting stuck \otimes$
 $(\operatorname{lack of optimism})$
 $\eta(\theta_{t+1}, \cdot)$
 a_t
 a_{t-1}
 a_t

Embrace Virtual Curvature

- Need the online learner to work harder to guarantee an increasing virtual reward
- Estimating the curvature: learn θ_t such that
 - 1. $\eta(\theta_t, a_t) \approx \eta(\theta^*, a_t)$
 - 2. $\nabla_a \eta(\theta_t, a_t) \approx \nabla_a \eta(\theta^*, a_t)$
 - 3. $\nabla_a^2 \eta(\theta_t, a_t) \approx \nabla_a^2 \eta(\theta^*, a_t)$



Algorithm and Theorem

$$\ell_{t}(\theta) = \left(\eta(\theta, a_{t}) - \eta(\theta^{\star}, a_{t})\right)^{2} + \left(\eta(\theta, a_{t-1}) - \eta(\theta^{\star}, a_{t-1})\right)^{2} + \langle \nabla \eta(\theta, a_{t-1}) - \nabla \eta(\theta^{\star}, a_{t-1}), u_{t} \rangle^{2}$$

$$(Computed by finite difference)$$

- ViOlin (Virtual Ascent with Online Model Learner)
- 1. Sample $u_t \sim \mathcal{N}(0, I)$
- 2. Use OL to minimize losses ℓ_t and get a distribution of θ_t
- 3. Take $a_t = \operatorname{argmax}_a \mathbb{E}_{\theta_t}[\eta(\theta_t, a)]$
- Theorem (informal): Under Lipschitz assumptions on η , ViOlin converges to a ϵ -approximate local maxima in $\tilde{O}(R(\Theta)\epsilon^{-8})$.

Instantiations

- Linear bandit with structured model family: $\eta(\theta, a) = \theta^{T} a$
 - Θ is finite: poly(log $|\Theta|$) sample complexity
 - Θ contains *s*-sparse vectors: poly(*s*, log *d*) sample complexity
 - local maximum are global because $\eta(\theta^{\star}, \cdot)$ is concave.
 - only hold for deterministic reward
- Neural net bandit: $\eta(W, a) = w_2^{\mathsf{T}} \sigma(W_1 a)$
 - assume O(1) norms bounds on $||w_2||_1$, $||W_1||_{\infty \to \infty}$
 - $R(W) \leq \tilde{O}(1)$
 - sample complexity for local max = $\tilde{O}(1)$
 - Local maximum are global for input-concave neural nets

Summary

- Global convergence for nonlinear models is statistically intractable
- ViOlin: convergence to a local maximum with sample complexity that only depends on the model class
- Similar results for nonlinear RL (with many more assumptions and stochastic policies.)

Thank you for your attention $\ensuremath{\mathfrak{O}}$