Non-Asymptotic Analysis for Reinforcement Learning



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Non-asymptotic Analysis for Reinforcement Learning (Part 1)



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SIGMETRICS, June 2023

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Recent successes in reinforcement learning (RL)



RL holds great promise in the next era of artificial intelligence.

Recap: Supervised learning

Given i.i.d training data, the goal is to make prediction on unseen data:



— pic from internet

Reinforcement learning (RL)

In RL, an agent learns by interacting with an environment.

- no training data
- trial-and-error
- maximize total rewards
- delayed reward



"Recalculating ... recalculating ..."

Sample efficiency



Source: cbinsights.com

CBINSIGHTS

- prohibitively large state & action space
- collecting data samples can be expensive or time-consuming

Sample efficiency



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Challenge: design sample-efficient RL algorithms

Computational efficiency

Running RL algorithms might take a long time ...

- enormous state-action space
- nonconvexity



Computational efficiency

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Challenge: design computationally efficient RL algorithms

Theoretical foundation of RL



Theoretical foundation of RL



Understanding sample efficiency of RL requires a modern suite of non-asymptotic analysis tools

This tutorial



(large-scale) optimization

 $(\mathsf{high-dimensional}) \ \mathsf{statistics}$

Demystify sample- and computational efficiency of RL algorithms

This tutorial



(large-scale) optimization

 $(\mathsf{high-dimensional}) \ \mathsf{statistics}$

Demystify sample- and computational efficiency of RL algorithms

- Part 1. basics, and model-based RL
- Part 2. value-based RL

Part 3. policy optimization

We will illustrate these approaches for learning standard, robust, and multi-agent RL with simulator/online/offline data.

Outline (Part 1)

- Basics: Markov decision processes
- Basic dynamic programming algorithms
- Model-based RL ("plug-in" approach)

Basics: Markov decision processes

Markov decision process (MDP)



- S: state space
- \mathcal{A} : action space

Markov decision process (MDP)



- S: state space
- \mathcal{A} : action space
- $r(s,a) \in [0,1]$: immediate reward

Infinite-horizon Markov decision process



- S: state space
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- $\pi(\cdot|s)$: policy (or action selection rule)

Infinite-horizon Markov decision process



- S: state space
- \mathcal{A} : action space
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- $\pi(\cdot|s)$: policy (or action selection rule)
- $P(\cdot|s, a)$: unknown transition probabilities

Value function



Value of policy π : cumulative discounted reward

$$\forall s \in \mathcal{S}: \quad V^{\pi}(s) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} r(s_{t}, a_{t}) \, \middle| \, s_{0} = s\right]$$

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- $\gamma \in [0, 1)$: discount factor
 - \blacktriangleright take $\gamma \rightarrow 1$ to approximate long-horizon MDPs
 - effective horizon: $\frac{1}{1-\gamma}$

Q-function (action-value function)



Q-function of policy π :

$$\forall (s,a) \in \mathcal{S} \times \mathcal{A} : \quad Q^{\pi}(s,a) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} r_{t} \, \big| \, s_{0} = s, \mathbf{a}_{0} = \mathbf{a}\right]$$

• $(a_0, s_1, a_1, s_2, a_2, \cdots)$: induced by policy π

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• $(a_0, s_1, a_1, s_2, a_2, \cdots)$: induced by policy π

Finite-horizon MDPs



- *H*: horizon length
- S: state space with size S A: action space with size A
- $r_h(s_h, a_h) \in [0, 1]$: immediate reward in step h
- $\pi = {\pi_h}_{h=1}^H$: policy (or action selection rule)
- $P_h(\cdot \mid s, a)$: transition probabilities in step h

Finite-horizon MDPs



value function:
$$V_h^{\pi}(s) := \mathbb{E}\left[\sum_{t=h}^{H} r_h(s_h, a_h) \mid s_h = s\right]$$

Q-function: $Q_h^{\pi}(s, a) := \mathbb{E}\left[\sum_{t=h}^{H} r_h(s_h, a_h) \mid s_h = s, a_h = a\right]$



Optimal policy and optimal value



optimal policy π^\star : maximizing value function $\max_{\pi} V^{\pi}$

Proposition (Puterman'94)

For infinite horizon discounted MDP, there always exists a deterministic policy π^* , such that

$$V^{\pi^{\star}}(s) \ge V^{\pi}(s), \quad \forall s, \text{ and } \pi.$$

Optimal policy and optimal value



optimal policy π^* : maximizing value function $\max_{\pi} V^{\pi}$

• optimal value / Q function: $V^{\star} := V^{\pi^{\star}}$, $Q^{\star} := Q^{\pi^{\star}}$

Optimal policy and optimal value



optimal policy π^* : maximizing value function $\max_{\pi} V^{\pi}$

- optimal value / Q function: $V^{\star} := V^{\pi^{\star}}$, $Q^{\star} := Q^{\pi^{\star}}$
- How to find this π*?

Basic dynamic programming algorithms when MDP specification is known

Policy evaluation: Given MDP $\mathcal{M} = (\mathcal{S}, \mathcal{A}, r, P, \gamma)$ and policy $\pi : \mathcal{S} \mapsto \mathcal{A}$, how good is π ? (i.e., how to compute $V^{\pi}(s), \forall s$?)

Policy evaluation: Given MDP $\mathcal{M} = (\mathcal{S}, \mathcal{A}, r, P, \gamma)$ and policy $\pi : \mathcal{S} \mapsto \mathcal{A}$, how good is π ? (i.e., how to compute $V^{\pi}(s), \forall s$?)

Possible scheme:

- execute policy evaluation for each π
- find the optimal one

• $V^{\pi} \, / \, Q^{\pi}$: value / action-value function under policy π

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Bellman's consistency equation

$$V^{\pi}(s) = \mathbb{E}_{a \sim \pi(\cdot|s)} \left[Q^{\pi}(s, a) \right]$$
$$Q^{\pi}(s, a) = \underbrace{r(s, a)}_{\text{immediate reward}} + \gamma \underbrace{\mathbb{E}}_{s' \sim P(\cdot|s, a)} \left[\underbrace{V^{\pi}(s')}_{\text{next state's value}} \right]$$



Richard Bellman

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• one-step look-ahead



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- one-step look-ahead
- let P^π be the state-action transition matrix induced by π:

$$Q^{\pi} = r + \gamma P^{\pi} Q^{\pi} \implies Q^{\pi} = (I - \gamma P^{\pi})^{-1} r$$



Richard Bellman
Optimal policy π^* : Bellman's optimality principle

Bellman operator



• one-step look-ahead

Optimal policy π^* : Bellman's optimality principle

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• one-step look-ahead

Bellman equation: Q^* is *unique* solution to

$$\mathcal{T}(Q^{\star}) = Q^{\star}$$

 $\gamma\text{-contraction}$ of Bellman operator:

$$\|\mathcal{T}(Q_1) - \mathcal{T}(Q_2)\|_{\infty} \le \gamma \|Q_1 - Q_2\|_{\infty}$$



Richard Bellman

Two dynamic programming algorithms

Value iteration (VI) For t = 0, 1, ..., $Q^{(t+1)} = \mathcal{T}(Q^{(t)})$



Policy iteration (PI)

For t = 0, 1, ...,

policy evaluation: $Q^{(t)} = Q^{\pi^{(t)}}$ policy improvement: $\pi^{(t+1)}(s) = \operatorname*{argmax}_{a \in \mathcal{A}} Q^{(t)}(s, a)$



When the model is unknown



When the model is unknown ...



Need to learn optimal policy from samples w/o model specification

Three approaches



Model-based approach ("plug-in")

- 1. build an empirical estimate \widehat{P} for P
- 2. planning based on the empirical \widehat{P}

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Tutorial Part 2: Value-based approach

- learning w/o estimating the model explicitly

Tutorial Part 3: Policy-based approach

- optimization in the space of policies

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Model-based RL (a "plug-in" approach)

- 1. Sampling from a generative model (simulator)
- 2. Offline RL / batch RL
- 3. Robust RL

A generative model / simulator



• sampling: for each (s, a), collect N samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$

A generative model / simulator



- sampling: for each (s, a), collect N samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$
- construct $\widehat{\pi}$ based on samples (in total $|\mathcal{S}||\mathcal{A}| imes N$)

ℓ_{∞} -sample complexity: how many samples are required to learn an ε -optimal policy ? $\forall s: V^{\hat{\pi}}(s) \ge V^{\star}(s) - \varepsilon$

An incomplete list of works

- Kearns and Singh, 1999
- Kakade, 2003
- Kearns 3t al., 2002
- Azar et al., 2012
- Azar et al., 2013
- Sidford et al, 2018a, 2018b
- Wang, 2019
- Agarwal et al, 2019
- Wainwright, 2019a, 2019b
- Pananjady and Wainwright, 2019
- Yang and Wang, 2019
- Khamaru, 2020
- Mou et al., 2020
- Li et al., 2020
- Cui and Yang, 2021

• ...

Model estimation



Sampling: for each (s, a), collect N ind. samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$

Model estimation



Sampling: for each (s, a), collect N ind. samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$

Empirical estimates: $\widehat{P}(s'|s, a) = \underbrace{\frac{1}{N} \sum_{i=1}^{N} \mathbb{1}\{s'_{(i)} = s'\}}_{\text{empirical frequency}}$

Empirical MDP + planning

- Azar et al., 2013, Agarwal et al., 2019



Challenges in the sample-starved regime



• Can't recover P faithfully if sample size $\ll |\mathcal{S}|^2 |\mathcal{A}|!$

Challenges in the sample-starved regime



- Can't recover P faithfully if sample size $\ll |\mathcal{S}|^2 |\mathcal{A}|!$
- Can we trust our policy estimate when reliable model estimation is infeasible?

$\ell_\infty\text{-based}$ sample complexity

Theorem (Agarwal, Kakade, Yang '19)

For any $0 < \varepsilon \leq \frac{1}{\sqrt{1-\gamma}}$, the optimal policy $\widehat{\pi}^*$ of empirical MDP achieves $\|V^{\widehat{\pi}^*} - V^*\|_{\infty} \leq \varepsilon$

with high prob., with sample complexity at most

$$\widetilde{O}\left(\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^3\varepsilon^2}\right)$$

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• matches minimax lower bound: $\widetilde{\Omega}(\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^{3}\varepsilon^{2}})$ when $\varepsilon \leq \frac{1}{\sqrt{1-\gamma}}$ (equivalently, when sample size exceeds $\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^{2}}$) Azar et al., 2013

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- established upon leave-one-out analysis framework







Agarwal et al., 2019 still requires a burn-in sample size $\gtrsim \frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^2}$



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Question: is it possible to break this sample size barrier?

Perturbed model-based approach (Li et al. '20)





Find policy based on the empirical MDP with slightly perturbed rewards

Optimal $\ell_\infty\text{-based}$ sample complexity

Theorem (Li, Wei, Chi, Chen'20)

For any $0 < \varepsilon \leq \frac{1}{1-\gamma}$, the optimal policy $\widehat{\pi}_p^{\star}$ of perturbed empirical MDP achieves

$$\|V^{\widehat{\pi}_{\mathbf{p}}^{\star}} - V^{\star}\|_{\infty} \le \varepsilon$$

with high prob., with sample complexity at most

$$\widetilde{O}\left(\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^3\varepsilon^2}\right)$$

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- matches minimax lower bound: $\widetilde{\Omega}(\frac{|S||A|}{(1-\gamma)^{3}\varepsilon^{2}})$ Azar et al., 2013
- full ε -range: $\varepsilon \in \left(0, \frac{1}{1-\gamma}\right] \longrightarrow$ no burn-in cost
- established upon more refined leave-one-out analysis and a perturbation argument



Model-based RL (a "plug-in" approach)

- 1. Sampling from a generative model (simulator)
- 2. Offline RL / batch RL
- 3. Robust RL

- Collecting new data might be expensive or time-consuming
- But we have already stored tons of historical data



medical records



data of self-driving



clicking times of ads

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Question: Can we design algorithms based solely on historical data?

A historical dataset $\mathcal{D} = \{(s^{(i)}, a^{(i)}, s'^{(i)})\}$: N independent copies of

$$s \sim \rho^{\mathsf{b}}, \qquad a \sim \pi^{\mathsf{b}}(\cdot \,|\, s), \qquad s' \sim P(\cdot \,|\, s, a)$$

for some state distribution $\rho^{\rm b}$ and behavior policy $\pi^{\rm b}$

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Goal: given some test distribution ρ and accuracy level ε , find an ε -optimal policy $\hat{\pi}$ based on \mathcal{D} obeying

$$V^{\star}(\rho) - V^{\widehat{\pi}}(\rho) = \mathop{\mathbb{E}}_{s \sim \rho} \left[V^{\star}(s) \right] - \mathop{\mathbb{E}}_{s \sim \rho} \left[V^{\widehat{\pi}}(s) \right] \le \varepsilon$$

— in a sample-efficient manner

Challenges of offline RL

• Distribution shift:

 $\operatorname{distribution}(\mathcal{D}) \ \neq \ \operatorname{target} \ \operatorname{distribution} \ \operatorname{under} \ \pi^{\star}$

Challenges of offline RL

• Distribution shift:

distribution(\mathcal{D}) \neq target distribution under π^{\star}

Partial coverage of state-action space:


Challenges of offline RL

• Distribution shift:

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Partial coverage of state-action space:



How to quantify quality of historical dataset \mathcal{D} (induced by π^{b})?

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Single-policy concentrability coefficient

$$C^{\star} \coloneqq \max_{s,a} \frac{d^{\pi^{\star}}(s,a)}{d^{\pi^{\flat}}(s,a)}$$

where $d^{\pi}(s,a) = (1-\gamma) \sum_{t=0}^{\infty} \gamma^{t} \mathbb{P}((s^{t},a^{t}) = (s,a) \mid \pi)$

How to quantify quality of historical dataset \mathcal{D} (induced by π^{b})?

Single-policy concentrability coefficient

$$C^{\star} \coloneqq \max_{s,a} \frac{d^{\pi^{\star}}(s,a)}{d^{\pi^{\flat}}(s,a)} = \left\| \frac{\text{occupancy density of } \pi^{\star}}{\text{occupancy density of } \pi^{\flat}} \right\|_{\infty} \ge 1$$

where $d^{\pi}(s,a) = (1-\gamma) \sum_{t=0}^{\infty} \gamma^{t} \mathbb{P}((s^{t},a^{t}) = (s,a) \mid \pi)$

- captures distributional shift
- allows for partial coverage



— Jin et al. '20, Rashidinejad et al. '21, Xie et al. '21



upper confidence bounds

— promote exploration of under-explored (s, a)

— Jin et al. '20, Rashidinejad et al. '21, Xie et al. '21



— Jin et al. '20, Rashidinejad et al. '21, Xie et al. '21

A model-based offline algorithm: VI-LCB

- 1. build empirical model \widehat{P}
- 2. (value iteration) for $t \leq \tau_{\max}$:

$$\widehat{Q}_t(s,a) \leftarrow \left[r(s,a) + \gamma \left\langle \widehat{P}(\cdot \,|\, s,a), \widehat{V}_{t-1} \right\rangle \right]_+$$

for all (s,a), where $\widehat{V}_t(s) = \max_a \widehat{Q}_t(s,a)$

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compared w/ prior works

- no need of variance reduction
- variance-aware penalty

Minimax optimality of model-based offline RL

Theorem (Li, Shi, Chen, Chi, Wei'22)

For any $0 < \varepsilon \leq \frac{1}{1-\gamma}$, the policy $\widehat{\pi}$ returned by VI-LCB achieves

$$V^{\star}(\rho) - V^{\widehat{\pi}}(\rho) \le \varepsilon$$

with high prob., with sample complexity at most

$$\widetilde{O}\left(\frac{SC^{\star}}{(1-\gamma)^{3}\varepsilon^{2}}\right)$$

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- matches minimax lower bound: $\widetilde{\Omega}(\frac{SC^{\star}}{(1-\gamma)^{3}\varepsilon^{2}})$ Rashidinejad et al, 2021
- depends on distribution shift (as reflected by C^{*})
- full ε-range (no burn-in cost)



Model-based RL (a "plug-in" approach)

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- 2. Offline RL / batch RL
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Safety and robustness in RL

(Zhou et al., 2021; Panaganti and Kalathil, 2022; Yang et al., 2022;)



Training environment

 \neq



Test environment

Safety and robustness in RL

(Zhou et al., 2021; Panaganti and Kalathil, 2022; Yang et al., 2022;)



Training environment



Test environment

Sim2Real Gap: Can we learn optimal policies that are robust to model perturbations?

¥

Distributionally robust MDP



Uncertainty set of the norminal transition kernel P^o:

$$\mathcal{U}^{\sigma}(P^{o}) = \left\{ P : \ \rho(P, P^{o}) \le \sigma \right\}$$

Robust value/Q function of policy π :

$$\forall s \in \mathcal{S}: \qquad V^{\pi,\sigma}(s) := \inf_{\substack{P \in \mathcal{U}^{\sigma}(P^{o})}} \mathbb{E}_{\pi,P} \left[\sum_{t=0}^{\infty} \gamma^{t} r_{t} \mid s_{0} = s \right]$$
$$\forall (s,a) \in \mathcal{S} \times \mathcal{A}: \quad Q^{\pi,\sigma}(s,a) := \inf_{\substack{P \in \mathcal{U}^{\sigma}(P^{o})}} \mathbb{E}_{\pi,P} \left[\sum_{t=0}^{\infty} \gamma^{t} r_{t} \mid s_{0} = s, a_{0} = a \right]$$

The optimal robust policy π^* maximizes $V^{\pi,\sigma}(\rho)$

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Robust Bellman's optimality equation

(Iyengar. '05, Nilim and El Ghaoui. '05)

Robust Bellman's optimality equation: the optimal robust policy π^* and optimal robust value $V^{*,\sigma} := V^{\pi^*,\sigma}$ satisfy

$$Q^{\star,\sigma}(s,a) = r(s,a) + \gamma \inf_{\substack{P_{s,a} \in \mathcal{U}^{\sigma}(P_{s,a}^{o})}} \langle P_{s,a}, V^{\star,\sigma} \rangle,$$
$$V^{\star,\sigma}(s) = \max_{a} Q^{\star,\sigma}(s,a)$$

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$$V^{\star,\sigma}(s) = \max_{a} Q^{\star,\sigma}(s,a)$$

Robust value iteration:

$$Q(s,a) \leftarrow r(s,a) + \gamma \inf_{P_{s,a} \in \mathcal{U}^{\sigma}(P_{s,a}^{o})} \langle P_{s,a}, V \rangle,$$

where $V(s) = \max_a Q(s, a)$.

Learning distributionally robust MDPs



Learning distributionally robust MDPs



Goal of robust RL: given $\mathcal{D} := \{(s_i, a_i, s'_i)\}_{i=1}^N$ from the *nominal* environment P^0 , find an ε -optimal robust policy $\hat{\pi}$ obeying

$$V^{\star,\sigma}(\rho) - V^{\widehat{\pi},\sigma}(\rho) \le \varepsilon$$

— in a sample-efficient manner

A curious question



empirical MDP

A curious question



Robustness-statistical trade-off? Is there a statistical premium that one needs to pay in quest of additional robustness?

When the uncertainty set is TV



When the uncertainty set is TV



RMDPs are easier to learn than standard MDPs.

When the uncertainty set is χ^2 divergence



When the uncertainty set is χ^2 divergence



RMDPs can be harder to learn than standard MDPs.

Summary of this part

Model-based RL (a "plug-in" approach)

- Sampling from a generative model (simulator)
- Offline RL / batch RL
- Robust RL

Papers:

"Breaking the sample size barrier in model-based reinforcement learning with a generative model," G Li, Y Wei, Y Chi, Y Chen, *NeurIPS'20, Operators Research'23* "Settling the sample complexity of model-based offline reinforcement learning," G Li, L Shi, Y

Chen, Y Chi, Y Wei, 2022

"The curious price of distributional robustness in reinforcement learning with a generative model," L Shi, G Li, Y Wei, Y Chen, M Geist, Y Chi, 2023