Offline Reinforcement Learning: Towards Optimal Sample Complexity and Distributional Robustness

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Recent successes in reinforcement learning (RL)

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

RL holds great promise in the next era of artificial intelligence.
Background and problem formulation
Markov decision processes

- $S$: state space
- $A$: action space

$S_t$: state at time $t$

$A_t$: action at time $t$

$r_t = r(s_t, a_t)$: immediate reward

$p(s_{t+1} | s_t, a_t)$: transition probability

$\pi(\cdot | s_t)$: policy (or action selection rule)
Markov decision processes

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

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Markov decision processes

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- $r(s, a) \in [0, 1]$: immediate reward
- $\pi(\cdot | s)$: policy (or action selection rule)
- $P(\cdot | s, a)$: transition probabilities
Value function

Value/Q-function function of policy $\pi$:

$$\forall s \in S : \quad V^{\pi}(s) := \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t r_t \mid s_0 = s \right]$$

$$\forall (s, a) \in S \times A : \quad Q^{\pi}(s, a) := \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t r_t \mid s_0 = s, a_0 = a \right]$$
Value function

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- $\gamma \in [0, 1)$ is the discount factor; $\frac{1}{1-\gamma}$ is effective horizon
- Expectation is w.r.t. the sampled trajectory under $\pi$
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- $\gamma \in [0, 1)$ is the discount factor; $\frac{1}{1-\gamma}$ is effective horizon
- Expectation is w.r.t. the sampled trajectory under $\pi$
- Given initial state distribution $\rho$, let $V^\pi(\rho) = \mathbb{E}_{s \sim \rho} V^\pi(s)$.  

Searching for the optimal policy

**Goal:** find the optimal policy \( \pi^* \) that maximize \( V^\pi(\rho) \)

- optimal value / Q function: \( V^* := V^{\pi^*}, \ Q^* := Q^{\pi^*} \)
- optimal policy \( \pi^*(s) = \arg\max_{a \in A} Q^*(s, a) \)
Data source in RL

Observed: \{s^t, a^t, r^t\} \forall t \geq 0

Goal: estimate optimal value function \( V_{\bar{b}} \) based on sample trajectory

Key quantities of sample trajectory

- Minimum state-action occupancy probability
  \[ \mu_{\min} := \min \mu_{\bar{b}}(s, a) \]
- Mixing time: \( t_{\text{mix}} \)

Exploration

- Offline RL
- Online RL
- Generative model

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Data source in RL

Exploration

Sample trajectory and behavior policy

(s, a) \rightarrow P(\cdot|s, a) \rightarrow \text{generative model}

Observed: \{s_t, a_t, r_t\}_{t=0}^\infty

Markovian trajectory generated by behavior policy

Goal: estimate optimal value function \( V_\pi \) based on sample trajectory

Key quantities of sample trajectory

• minimum state-action occupancy probability
  \( \mu_{\min} = \min \mu_{\text{fib}}(s, a) \)
  stationary distribution

• mixing time: \( t_{\text{mix}} \)

Our focus: offline RL without exploration
Offline RL / Batch RL

- Sometimes we can not explore or generate new data
- But we have already stored tons of historical data

- medical records
- data of self-driving
- clicking times of ads
Offline RL / Batch RL

- Sometimes we can not explore or generate new data
- But we have already stored tons of historical data

medical records  data of self-driving  clicking times of ads

Can we learn a good policy based solely on historical data without active exploration?
Model-based offline RL is nearly minimax optimal
A simplified model of history data from behavior policy

Goal of online RL:
given history data \( D = (s_i; a_i; r_i; s_{0,i}) \) for \( N_i = 1 \), find an \( \varepsilon \)-optimal policy obeying \( V_b(s) \) in a sample-efficient manner.

No longer arbitrary!
A simplified model of history data from behavior policy

\[ s \sim \rho \rightarrow \pi^b(\cdot | s) \rightarrow (s, a) \rightarrow P(\cdot | s, a) \rightarrow s' \]

Initial distribution \rightarrow Behavior policy \rightarrow \text{Sample} \rightarrow Transition kernel \rightarrow \text{Sample}'}
A simplified model of history data from behavior policy

\[
D = \{(s_i, a_i, r_i, s'_i)\}_{i=1}^N.
\]

**Goal of offline RL:** given history data \( D \), find an \( \epsilon \)-optimal policy \( \hat{\pi} \) obeying

\[
V^*(\rho) - V^\hat{\pi}(\rho) \leq \epsilon
\]

--- in a sample-efficient manner ---
Challenges of offline RL

Partial coverage of state-action space:

samples cover all \((s, a)\) & all policies

uniform coverage over entire space
(sufficiently explored)
Challenges of offline RL

Partial coverage of state-action space:

- **Uniform coverage over entire space (sufficiently explored)**
  - Practically, samples cover all \((s, a)\) & all policies
  - Historical dataset \(\mathcal{D}\)
- **Partial coverage (inadequately explored)**
  - \(\pi_1\) & \(\pi_2\)
Challenges of offline RL

Partial coverage of state-action space:

\[ \text{Practically,} \quad \text{historical dataset } \mathcal{D} \]

\[ \quad \text{samples cover all } (s, a) \text{ & all policies} \]

uniform coverage over entire space (sufficiently explored)

partial coverage (inadequately explored)

Distribution shift:

\[ \text{distribution}(\mathcal{D}) \neq \text{target distribution under } \pi^* \]
How to quantify the distribution shift?

**Single-policy concentrability coefficient (Rashidineiadi et al.)**

\[
C^* := \max_{s,a} \frac{d^{\pi^*}(s, a)}{d^{\pi_b}(s, a)} \geq 1
\]

where \(d^\pi(s, a)\) is the state-action occupation density of policy \(\pi\).
How to quantify the distribution shift?

Single-policy concentrability coefficient (Rashidineiad et al.)

\[ C^* := \max_{s,a} \frac{d^{\pi^*}(s, a)}{d^{\pi^b}(s, a)} \geq 1 \]

where \( d^{\pi}(s, a) \) is the state-action occupation density of policy \( \pi \).

- captures distribution shift
- allows for partial coverage
How to quantify the distribution shift? — a refinement

**Single-policy clipped concentrability coefficient (Li et al., ’22)**

\[
C^\ast_{\text{clipped}} := \max_{s,a} \min \left\{ \frac{d^{\pi^*}(s,a)}{d^{\pi^b}(s,a)}, \frac{1}{S} \right\} \geq \frac{1}{S}
\]

where \( d^{\pi}(s,a) \) is the state-action occupation density of policy \( \pi \).
How to quantify the distribution shift? — a refinement

Single-policy clipped concentrability coefficient (Li et al., ’22)

\[ C_{\text{clipped}}^* := \max_{s,a} \frac{\min\{d^{\pi^*}(s,a), 1/S\}}{d^{\pi^b}(s,a)} \geq 1/S \]

where \( d^{\pi}(s,a) \) is the state-action occupation density of policy \( \pi \).

- captures distribution shift
- allows for partial coverage
- \( C_{\text{clipped}}^* \leq C^* \)
A “plug-in” model-based approach


Planning (e.g., value iteration) based on the empirical MDP $\hat{P}$:

$$\hat{Q}(s, a) \leftarrow r(s, a) + \gamma \langle \hat{P}(\cdot | s, a), \hat{V} \rangle,$$

$$\hat{V}(s) = \max_a \hat{Q}(s, a).$$

**Issue:** poor value estimates under partial and poor coverage.
Pessimism in the face of uncertainty

Penalize value estimate of $(s, a)$ pairs that were poorly visited

(Jin et al. '20, Rashidinejad et al. '21, Xie et al. '21)
Pessimism in the face of uncertainty

Penalize value estimate of \((s, a)\) pairs that were poorly visited

\[ \text{(Jin et al. '20, Rashidinejad et al. '21, Xie et al. '21)} \]

\[
\hat{Q}(s, a) \leftarrow \max \left\{ r(s, a) + \gamma \langle \hat{P}(\cdot | s, a), \hat{V} \rangle - b(s, a; \hat{V}), 0 \right\},
\]

where \( \hat{V}(s) = \max_a \hat{Q}(s, a). \)
A benchmark of prior arts

Sample complexity

- $\frac{SC^*}{(1 - \gamma)^5}$
- $\frac{SC^*}{(1 - \gamma)^3}$
- $\frac{SC^*}{1 - \gamma}$

Rashidinejad et al.
Yan et al.

$\frac{1}{\varepsilon^2}$

All prior results require a sample size of at least

Beck & Srikant '12

$|S||A|$
A benchmark of prior arts
A benchmark of prior arts

Can we close the gap with the minimax lower bound?
Theorem (Li, Shi, Chen, Chi, Wei ’22)

For any \( 0 < \epsilon \leq \frac{1}{1-\gamma} \), the policy \( \hat{\pi} \) returned by VI-LCB using a Bernstein-style penalty term achieves

\[
V^*(\rho) - V^{\hat{\pi}}(\rho) \leq \epsilon
\]

with high prob., with sample complexity at most

\[
\tilde{O} \left( \frac{SC^*_{\text{clipped}}}{(1 - \gamma)^3 \epsilon^2} \right).
\]
Sample complexity of model-based offline RL

**Theorem (Li, Shi, Chen, Chi, Wei ’22)**

For any $0 < \epsilon \leq \frac{1}{1 - \gamma}$, the policy $\hat{\pi}$ returned by VI-LCB using a Bernstein-style penalty term achieves

$$V^*(\rho) - V^{\hat{\pi}}(\rho) \leq \epsilon$$

with high prob., with sample complexity at most

$$\tilde{O}\left( \frac{SC^*_\text{clipped}}{(1 - \gamma)^3 \epsilon^2} \right).$$

- depends on distribution shift (as reflected by $C^\text{clipped}$)
- improves upon prior results by allowing $C^\text{clipped} \asymp 1/S$.
- full $\epsilon$-range (no burn-in cost)
Theorem (Li, Shi, Chen, Chi, Wei ’22)

For any $\gamma \in [2/3, 1)$, $S \geq 2$, $C^*_{\text{clipped}} \geq 8\gamma/S$, and $0 < \epsilon \leq \frac{1}{42(1-\gamma)}$, there exists some MDP and batch dataset such that no algorithm succeeds if the sample size is below

$$\tilde{\Omega}\left(\frac{SC^*_{\text{clipped}}}{(1 - \gamma)^3 \epsilon^2}\right).$$
Theorem (Li, Shi, Chen, Chi, Wei ’22)

For any $\gamma \in [2/3, 1)$, $S \geq 2$, $C_{\text{clipped}}^* \geq 8\gamma/S$, and $0 < \epsilon \leq \frac{1}{42(1-\gamma)}$, there exists some MDP and batch dataset such that no algorithm succeeds if the sample size is below

$$\tilde{\Omega}\left(\frac{SC_{\text{clipped}}^*}{(1-\gamma)^3\epsilon^2}\right).$$

- verifies the minimax optimality of the pessimistic model-based algorithm
Model-based RL is minimax optimal with no burn-in cost!
Offline RL meets distributional robustness
Safety and robustness in RL

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

Training environment ≠ Test environment
Safety and robustness in RL

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

Training environment ≠ Test environment

Can we learn optimal policies that are robust to model perturbations from historical data?
Distributionally robust MDP

Uncertainty set of the nominal transition kernel $P^o$:
$\mathcal{U}^\sigma(P^o) = \{ P : \KL(P \parallel P^o) \leq \sigma \}$

Robust value/Q function of policy $\pi$:

$\forall s \in S : \quad V^{\pi,\sigma}(s) := \inf_{P \in \mathcal{U}^\sigma(P^o)} \mathbb{E}_{\pi,P} \left[ \sum_{t=0}^{\infty} \gamma^t r_t \mid s_0 = s \right]$ 

$\forall (s, a) \in S \times A : \quad Q^{\pi,\sigma}(s, a) := \inf_{P \in \mathcal{U}^\sigma(P^o)} \mathbb{E}_{\pi,P} \left[ \sum_{t=0}^{\infty} \gamma^t r_t \mid s_0 = s, a_0 = a \right]$ 

The optimal robust policy $\pi^*$ maximizes $V^{\pi,\sigma}(\rho)$
Distributionally robust Bellman’s optimality equation

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

**Robust Bellman’s optimality equation:** the optimal robust policy \( \pi^* \) and optimal robust value \( V^{*,\sigma} \) satisfy

\[
Q^{*,\sigma}(s, a) = r(s, a) + \gamma \inf_{P_{s,a} \in \mathcal{U}^\sigma(P_{s,a}^o)} \langle P_{s,a}, V^{*,\sigma} \rangle,
\]

\[
V^{*,\sigma}(s) = \max_a Q^{*,\sigma}(s, a)
\]
Distributionally robust Bellman’s optimality equation

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

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

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

$$V^{*,\sigma}(s) = \max_a Q^{*,\sigma}(s, a)$$

Solvable by **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 $V(s) = \max_a Q(s, a)$.  

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Distributionally robust offline RL

\[(s, a) \sim d^b\]

\[P^0(\cdot | s, a)\]

\[s'\]

Not arbitrary!

Nominal Transition kernel
Goal of robust offline RL: given $D := \{(s_i, a_i, s'_i)\}_{i=1}^N$ from the nominal environment $P^0$, find an $\epsilon$-optimal robust policy $\widehat{\pi}$ obeying

$$V^{*,\sigma}(\rho) - V^{\widehat{\pi},\sigma}(\rho) \leq \epsilon$$

—in a sample-efficient manner
Prior art under full coverage

All prior results require a sample size of at least $|S||A|$ if we take $\mu = 1$. Can we improve the sample efficiency and allow partial coverage?
Prior art under full coverage

Questions: Can we improve the sample efficiency and allow partial coverage?
How to quantify the compounded distribution shift?

Robust single-policy concentrability coefficient

\[ C_{rob}^* := \max_{(s,a,P) \in S \times A \times \mathcal{U}(P^o)} \min \left\{ \frac{d^{\pi^*,P}(s,a), \frac{1}{\mathcal{S}}}{d^b(s,a)} \right\} \]

\[ = \left\| \frac{\text{occupancy distribution of } (\pi^*, \mathcal{U}(P^o))}{\text{occupancy distribution of } \mathcal{D}} \right\|_{\infty} \]

where \( d^{\pi,P} \) is the state-action occupation density of \( \pi \) under \( P \).
How to quantify the compounded distribution shift?

**Robust single-policy concentrability coefficient**

\[
C_{\text{rob}}^* := \max_{(s,a,P) \in \mathcal{S} \times \mathcal{A} \times \mathcal{U}(P^o)} \min \left\{ \frac{d_{\pi^*,P}(s,a)}{d_{\text{rob}}(s,a)} \frac{1}{f(s,a)} \right\}
\]

\[
= \left\| \frac{\text{occupancy distribution of } (\pi^*, \mathcal{U}(P^o))}{\text{occupancy distribution of } \mathcal{D}} \right\|_{\infty}
\]

where \(d_{\pi^*,P}\) is the state-action occupation density of \(\pi\) under \(P\).

- captures distributional shift due to behavior policy and environment.
- \(C_{\text{rob}}^* < A\) under full coverage.
Distributionally robust value iteration (DRVI) with LCB:

\[
\hat{Q}(s, a) \leftarrow \max \left\{ r(s, a) + \gamma \inf_{\mathcal{P} \in \mathcal{U}^\sigma(\hat{P}_{s,a})} \mathcal{P}\hat{V} - b(s, a; \hat{V}) , 0 \right\},
\]

where \( \hat{V}(s) = \max_a \hat{Q}(s, a) \).

**Key innovation:** design the penalty term to capture the variability in robust RL:

\[
\inf_{\mathcal{P} \in \mathcal{U}^\sigma(P_{s,a})} \mathcal{P}\hat{V} - \inf_{\mathcal{P} \in \mathcal{U}^\sigma(\hat{P}_{s,a})} \mathcal{P}\hat{V}
\]

No closed form w.r.t. \( P_{s,a} - \hat{P}_{s,a} \) due to \( \mathcal{U}^\sigma(\cdot) \).
Sample complexity of DRVI-LCB

**Theorem (Shi and Chi ’22)**

For any uncertainty level $\sigma > 0$ and small enough $\epsilon$, DRVI-LCB outputs an $\epsilon$-optimal policy with high prob., with sample complexity at most

$$\tilde{O}\left(\frac{SC^*_\text{rob}}{P^*_{\min}(1 - \gamma)^4 \sigma^2 \epsilon^2}\right),$$

where $P^*_{\min}$ is the smallest positive state transition probability of the nominal kernel visited by the optimal robust policy $\pi^*$. 
Sample complexity of DRVI-LCB

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where $P^*_\text{min}$ is the smallest positive state transition probability of the nominal kernel visited by the optimal robust policy $\pi^*$.

- scales linearly with respect to $S$
- reflects the impact of distribution shift of offline dataset ($C^*_\text{rob}$) and also model shift level ($\sigma$)
Theorem (Shi and Chi ’22)

Suppose that $\frac{1}{1-\gamma} \geq e^8$, $S \geq \log \left( \frac{1}{1-\gamma} \right)$, $C_{\text{rob}}^* \geq 8/S$, $\sigma \approx \log \frac{1}{1-\gamma}$ and $\epsilon \lesssim \frac{1}{(1-\gamma) \log \frac{1}{1-\gamma}}$, there exists some MDP and batch dataset such that no algorithm succeeds if the sample size is below

$$\tilde{\Omega} \left( \frac{SC_{\text{rob}}^*}{P_{\min}^* (1 - \gamma)^2 \sigma^2 \epsilon^2} \right).$$
Minimax lower bound

Theorem (Shi and Chi ’22)

Suppose that \( \frac{1}{1-\gamma} \geq e^8 \), \( S \geq \log \left( \frac{1}{1-\gamma} \right) \), \( C_{\text{rob}}^* \geq 8/S \), \( \sigma \approx \log \frac{1}{1-\gamma} \) and \( \epsilon \lesssim \frac{1}{(1-\gamma) \log \frac{1}{1-\gamma}} \), there exists some MDP and batch dataset such that no algorithm succeeds if the sample size is below

\[
\tilde{\Omega} \left( \frac{SC_{\text{rob}}^*}{P_{\min}(1 - \gamma)^2 \sigma^2 \epsilon^2} \right).
\]

- the first lower bound for robust MDP with KL divergence
- Establishes the near minimax-optimality of DRVI-LCB up to factors of \( 1/(1 - \gamma) \)
Compare to prior art under full coverage

Our DRVI-LCB method is near minimax-optimal!
Compare to prior art under full coverage

Our DRVI-LCB method is near minimax-optimal!
Numerical experiments

- DRVI-LCB: ours with pessimism
- DRVI: prior art
Numerical experiments

- DRVI-LCB: ours with pessimism
- DRVI: prior art

Pessimism improves the sample efficiency in robust offline RL!
Concluding remarks
Concluding remarks

Model-based offline RL algorithms with pessimism are near minimax-optimal in both nominal MDP and robust MDP!
• Settling the sample complexity of model-based offline reinforcement learning, arXiv:2204.05275.
• Pessimistic Q-Learning for Offline Reinforcement Learning: Towards Optimal Sample Complexity, ICML 2022.
• Distributionally Robust Model-Based Offline Reinforcement Learning with Near-Optimal Sample Complexity, arXiv:2208.05767.

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