Statistical and Information-Theoretic Considerations in Fitted Q-Iteration

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References

- Main Materials
  - CS598 Statistical Reinforcement Learning:
    Notes on Fitted Q-Iteration (Jiang, 2018)
- Advanced Materials
  - Information-Theoretic Considerations in Batch Reinforcement Learning (Chen and Jiang, 2019)
  - Diagnosing Bottlenecks in Deep Q-learning Algorithms (Fu et al., 2019)
  - Off-Policy Deep Reinforcement Learning without Exploration (Fujimoto et al., 2019)

Background: State Abstraction $\Rightarrow$ Generalization

An abstraction ϕ is … if … $\forall\, s^{(1)}, s^{(2)}$ where $\phi(s^{(1)}) = \phi(s^{(2)})$

- π^*-irrelevant: $\exists\, \pi_M{}^*$ s.t. $\pi_M{}^*(s^{(1)}) = \pi_M{}^*(s^{(2)})$
- Q^*-irrelevant: $\forall\, a$, $Q_M{}^*(s^{(1)}, a) = Q_M{}^*(s^{(2)}, a)$
- Model-irrelevant: $\forall\, a \in A$, $R(s^{(1)}, a) = R(s^{(2)}, a)$
  (bisimulation) $\forall\, a \in A,\ x' \in \phi(S)$, $P(x' \mid s^{(1)}, a) = P(x' \mid s^{(2)}, a)$

$$\boxed{\sum_{s' \in \phi^{-1}(x')} P(s' | s^{(1)}, a)}$$

Theorem: Model-irrelevance $\Rightarrow$ Q^*-irrelevance $\Rightarrow$ π^*-irrelevance

Fitted Q-Iteration (FQI)

Let $D = \{(s, a, r, s')\}$ denote a dataset of past transitions.
The value function is updated iteratively,

$$Q_{t+1} = \arg\min_{Q \in \mathcal{Q}} L_D(Q; Q_t) \approx \mathcal{T} Q_t$$

where $L_D(\cdot; \cdot)$ is the empirical Bellman error evaluated by dataset D.

$$L_D(Q; Q_t) = \frac{1}{|D|} \sum_{(s,a,r,s') \in D} \left(r + \gamma \max_{a' \in \mathcal{A}} Q_t(s', a') - Q(s, a) \right)^2$$

FQI is equivalent to value iteration while $\mathcal{Q} = \mathbb{R}^{\mathcal{S} \times \mathcal{A}}$.

Why do we need target values?

Given a function class $\mathcal{Q}$. Assume realizability $Q^* \in \mathcal{Q}$.
Consider an alternative algorithm:

$$Q^\dagger \leftarrow \arg\min_{Q \in \mathcal{Q}} \frac{1}{|D|} \sum_{(s,a,r,s') \in D} \left(r + \gamma \max_{a' \in \mathcal{A}} Q(s', a') - Q(s, a) \right)^2$$

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Does this modification help to simply our algorithmic framework?

Unfortunately, $Q^* \neq Q^\dagger$ in some cases.

A Problematic Alternative Objective

Assume we have infinite data across all state-action pairs.

$$
\begin{aligned}
&\mathop{\mathbb{E}}_{(s,a,r,s')\sim D}\left[\left(r+\gamma\max_{a'\in\mathcal{A}}Q(s',a')-Q(s,a)\right)^2\right] \\
&= \mathop{\mathbb{E}}_{(s,a)\sim D}\left[\left(\mathop{\mathbb{E}}_{(r,s')\sim D_{s,a}}\left[r+\gamma\max_{a'\in\mathcal{A}}Q(s',a')\right]-Q(s,a)\right)^2\right] && (1) \\
&\quad+\mathop{\mathbb{E}}_{(s,a)\sim D}\left[\mathop{\mathrm{Var}}_{r,s'}\left[r+\gamma\max_{a'\in\mathcal{A}}Q(s',a')\right]\right] && (2)
\end{aligned}
$$

The term (1) is what we want, i.e., $\|(\mathcal{T}Q)(s,a)-Q(s,a)\|_{2,D}$.
The term (2) incorrectly penalizes the variance w.r.t. random transitions.

Workaround #1: Double Sampling Trick

Adopting two independent samples of r and s' (indexed by A and B).

$$\left(\mathbb{E}_{(r,s')\sim D_{s,a}} \left[r + \gamma \max_{a'\in\mathcal{A}} Q(s',a') \right] - Q(s,a) \right)^2$$

$$= \mathbb{E}_{\substack{(r_A,s'_A)\sim D_{s,a}\\(r_B,s'_B)\sim D_{s,a}}} \left[\left(r_A + \gamma \max_{a'\in\mathcal{A}} Q(s'_A,a') - Q(s,a) \right) \left(r_B + \gamma \max_{a'\in\mathcal{A}} Q(s'_B,a') - Q(s,a) \right) \right]$$

It requires a strong assumption on simulator.

Workaround #2: Estimating the Second Term

Adopting another function class $\mathcal{G}$ to estimate the second term.

$$
\begin{aligned}
&\mathop{\mathbb{E}}_{(s,a)\sim D}\left[\mathop{\mathrm{Var}}_{r,s'}\left[r+\gamma\max_{a'\in\mathcal{A}} Q(s',a')\right]\right] \\
&= \mathop{\mathbb{E}}_{(s,a,r,s')\sim D}\left[\left(r+\gamma\max_{a'\in\mathcal{A}} Q(s',a') - (\mathcal{T}Q)(s,a)\right)^2\right] \\
&\approx \inf_{g\in\mathcal{G}} \mathop{\mathbb{E}}_{(s,a,r,s')\sim D}\left[\left(r+\gamma\max_{a'\in\mathcal{A}} Q(s',a') - g(s,a)\right)^2\right] \qquad (3)
\end{aligned}
$$

Subtracting the term (3) from the original objective (Antos et al., 2008; Dai et al., 2018).

Return to Fitted Q-Iteration

Q and g can be optimized iteratively.

$$
\begin{aligned}
Q_t = \arg\min_{Q \in \mathcal{Q}} & \mathop{\mathbb{E}}_{(s,a,r,s') \sim D} \left[\left(r + \gamma \max_{a' \in \mathcal{A}} Q(s', a') - Q(s, a) \right)^2 \right] \\
& - \cancel{\inf_{g \in \mathcal{G}}} \mathop{\mathbb{E}}_{(s,a,r,s') \sim D} \left[\left(r + \gamma \max_{a' \in \mathcal{A}} Q(s', a') - g_{t-1}(s, a) \right)^2 \right] \\
g_t = \arg\min_{g \in \mathcal{G}} & \mathop{\mathbb{E}}_{(s,a,r,s') \sim D} \left[\left(r + \gamma \max_{a' \in \mathcal{A}} Q_t(s', a') - g(s, a) \right)^2 \right] \qquad (4)
\end{aligned}
$$

Notice that $g_t = \mathcal{T} Q_t$ is the optimal solution of Eq. (4).
Another kind of target values: g_t is a backup of $\mathcal{T} Q_t$.

Return to Fitted Q-Iteration

More clearly, let $\hat{Q}$ denote a frozen copy of value function.

$$
\begin{aligned}
&\mathop{\mathbb{E}}_{(s,a,r,s')\sim D}\left[\left(r + \gamma \max_{a'\in\mathcal{A}} \hat{Q}(s',a') - Q(s,a)\right)^2\right] \\
&= \mathop{\mathbb{E}}_{(s,a)\sim D}\left[\left(\mathop{\mathbb{E}}_{(r,s')\sim D_{s,a}}\left[r + \gamma \max_{a'\in\mathcal{A}} \hat{Q}(s',a')\right] - Q(s,a)\right)^2\right] \\
&\quad + \mathop{\mathbb{E}}_{(s,a)\sim D}\left[\operatorname*{Var}_{r,s'}\left[r + \gamma \max_{a'\in\mathcal{A}} \hat{Q}(s',a')\right]\right] \qquad (5)
\end{aligned}
$$

The term (5) is independent from the selection of Q.

Convergence?

Bellman operator $\mathcal{T}$ is γ-contraction

$$\forall (Q_1, Q_2) \in \mathcal{Q}^2, \quad \|\mathcal{T}Q_1 - \mathcal{T}Q_2\|_\infty \leq \gamma \|Q_1 - Q_2\|_\infty$$

which provides convergence guarantee for value iteration.
How about Fitted Q-Iteration?

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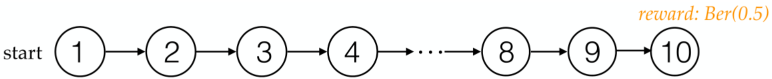
How about Fitted Q-Iteration?

Lots of counterexamples have been proposed (Baird, 1995; Gordon, 1995; Tsitsiklis and Van Roy, 1996).

A Simple Example (Finite Horizon, $\gamma = 1$)



- Dataset $D = \{(s, r, s')\}$ looks like (action omitted):
  $\{(①, 0, ②), (②, 0, ③), \ldots, (⑩, 1, end), \ldots, (⑩, 0, end)\}$

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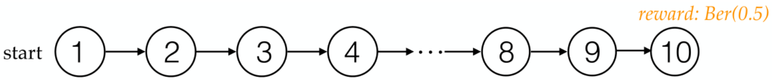

FQI Iter #1: Data: (⑩, 1, *end*), …, (⑩, 0, *end*) ⇨ 0.501

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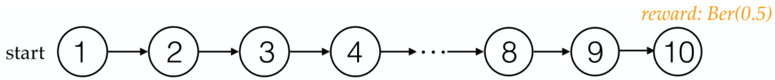

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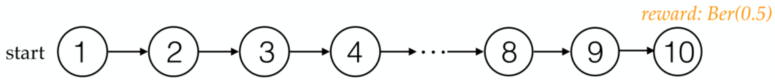

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…

Iter #10: 0.501 0.501 0.501 0.501 … 0.501 0.501 0.501

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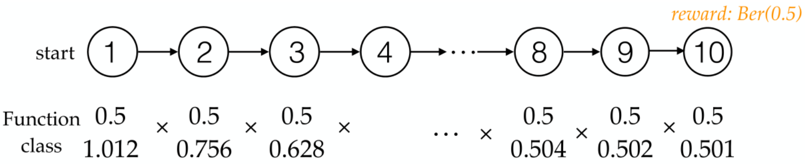
How Things Goes Wrong



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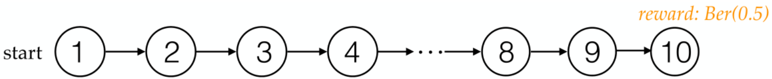

Function class $\begin{matrix}0.5\\1.012\end{matrix} \times \begin{matrix}0.5\\0.756\end{matrix} \times \begin{matrix}0.5\\0.628\end{matrix} \times \cdots \times \begin{matrix}0.5\\0.504\end{matrix} \times \begin{matrix}0.5\\0.502\end{matrix} \times \begin{matrix}0.5\\0.501\end{matrix}$

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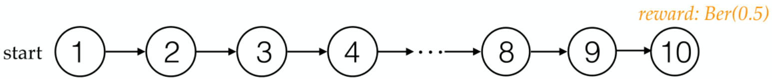

Function class	0.5 / 1.012	×	0.5 / 0.756	×	0.5 / 0.628	×	…	×	0.5 / 0.504	×	0.5 / 0.502	× 0.5 / 0.501

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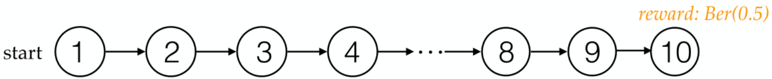

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⋯

Iter #10: 1.012 0.756 0.628 ⋯ 0.502 0.501

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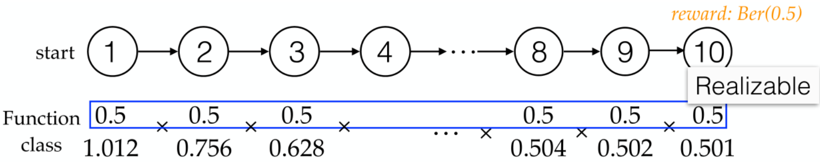

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…

!!!

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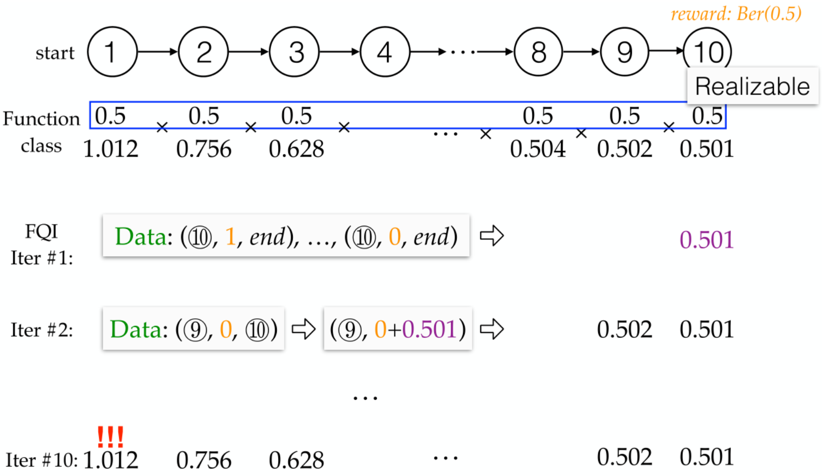
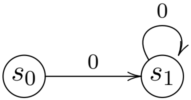
What is the cause of divergence?

Empirical Error? Projection Error?



Another Simple Example with Linear Function Approximation

An MDP with two state s_0, s_1 and features $f(s_0) = 1, f(s_1) = 2$.
Linear Function Approximation $V(s_i) = \theta f(s_i)$.



FQI diverges in this MDP if $\gamma > \frac{5}{6}$ (Tsitsiklis and Van Roy, 1996).

$$
\begin{aligned}
\theta_k &= \arg\min_{\theta} \left[(\theta f(s_0) - \gamma \theta_{k-1} f(s_1))^2 + (\theta f(s_1) - \gamma \theta_{k-1} f(s_1))^2 \right] \\
&= \arg\min_{\theta} \left[(\theta - 2\gamma\theta_{k-1})^2 + (2\theta - 2\gamma\theta_{k-1})^2 \right] \\
&= \frac{6}{5} \gamma \theta_{k-1}
\end{aligned}
$$

Representation Condition of Function Class

Realizability

The optimal value function Q is realizable, i.e. $Q^* \in \mathcal{Q}$.

Completeness

$\mathcal{Q}$ is closed under $\mathcal{T}$, i.e. $\forall Q \in \mathcal{Q}$, $\mathcal{T}Q \in \mathcal{Q}$.
In an approximated view, the violation is measured by

$$\epsilon_{\mathcal{T}} = \sup_{Q \in \mathcal{Q}} \inf_{\hat{Q} \in \mathcal{Q}} \|\hat{Q} - \mathcal{T}Q\|_2^2$$

If $\mathcal{Q}$ is finite, $\epsilon_{\mathcal{T}} = 0$ implies *Realizability*.
If $\epsilon_{\mathcal{T}} = 0$ and data is adequate, FQI is equivalent to value iteration.

One Last Assumption: Data

With *Realizability* and *Completeness* assumptions, FQI works pretty well while data is adequate.

How about the situation with finite samples?

Sample Complexity in Supervised Learning

- $D \in \Delta(\mathcal{X} \times \{0,1\})$ denotes a data distribution, $S \sim D^m$ is a set of samples.
- $\mathcal{H}$ is a finite set of functions mapping from $\mathcal{X}$ to $\mathcal{Y}$.
- $R(h)$ and $\hat{R}(h)$ denote the overall error and the empirical error of $h \in \mathcal{H}$.

$$R(h) = \mathop{\mathbb{P}}_{(x,y)\sim D}[h(x) \neq y] \qquad \hat{R}(h) = \frac{1}{m}\sum_{(x,y)\in S} \mathbb{I}[h(x) \neq y]$$

Learning Bound

For a finite hypothesis class $\mathcal{H}$, $\forall \delta > 0$, with probability $1-\delta$, $\forall h \in \mathcal{H}$,

$$R(h) \leq \hat{R}(h) + \sqrt{\frac{\log|\mathcal{H}| + \log\frac{2}{\delta}}{2m}}$$

To make $R(h) \leq \hat{R}(h) + \epsilon$, we need $m = O\left(\frac{\log|\mathcal{H}| + \log\frac{1}{\delta}}{\epsilon^2}\right)$.

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- e.g., VC dimension, growth function, covering number.

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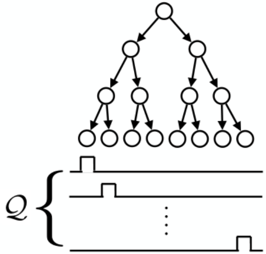
Is it possible to guarantee $\mathrm{Poly}(|\mathcal{A}|, H, \log |\mathcal{Q}|, \frac{1}{\epsilon}, \frac{1}{\delta})$ sample complexity in FQI?

Is it possible to guarantee Poly$(|\mathcal{A}|, H, \log|\mathcal{Q}|, \frac{1}{\epsilon}, \frac{1}{\delta})$ sample complexity?

Notice that unbounded numbers of states are allowed.
Construct a depth-H complete tree to emulate a multi-arm bandit with $|\mathcal{A}|^H$ arms.

Let $\mathcal{Q}$ contain all possible optimal functions.
Then $O(\log|\mathcal{Q}|) = O(H\log|\mathcal{A}|)$ is tractable.

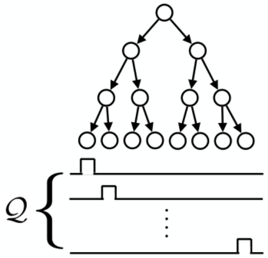
However, the lower bound of sample complexity of this MDP is $\Omega(|\mathcal{A}|^H)$.



Issues on Data Distribution

What causes the exponential sample complexity

- All paths are symmetric.
- Training data should be uniform.



How to define the term "uniform"?
What kind of data distribution is uniform?

Additional Assumption on Data Distribution

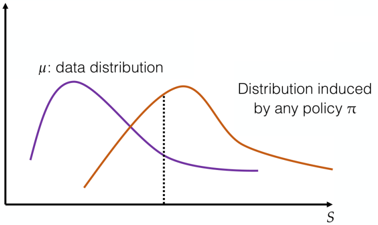
Concentratability

Let $\mu(s)$ denote the data distribution of states, i.e. $D_s \sim \mu$.
There exists a constant $C < \infty$,

$$\forall \nu, \forall s \in \mathcal{S}, \quad \frac{\nu(s)}{\mu(s)} \leq C$$

where ν is generated by a policy π (can be non-stationary and stochastic).

- Sample complexity can have polynomial dependence on C. (Munos, 2003)
- Implicitly assume C is small.



An Ideal Data Distribution

Construct a dataset

- $s \sim \mu$, $a \sim \mathrm{Unif}(\mathcal{A})$, $r \sim R(\cdot|s,a)$, $s' \sim P(\cdot|s,a)$
- A uniform bound on norms, $\forall \nu$, $\forall \pi$,

$$\|\cdot\|_{2,\nu\times\pi} \leq \sqrt{C|\mathcal{A}|}\|\cdot\|_{2,\mu\times\mathrm{Unif}(\mathcal{A})}$$

Under *Completeness* assumption

- To achieve $V^* - V^\pi \leq \epsilon \cdot \frac{R_{\max}}{1-\gamma}$, we need

$$|D| = O\left(\frac{C|\mathcal{A}|\log\frac{|\mathcal{Q}|}{\delta}}{\epsilon^2(1-\gamma)^4}\right)$$

- An error bound with approximated *Completeness* ($\epsilon_{\mathcal{T}} \neq 0$) refers to Chen and Jiang (2019).

The Magnitude of Concentratability Constant C

How large can the constant C be?

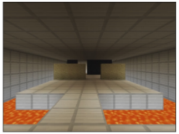
- In the worst case, $C = O(|\mathcal{S}|)$.
- We have not gotten rid of the dependence on state space.

In some specific classes of problems, C is small.

MDPs with Rich Observation (ROMDP)

- a finite hidden state space $\mathcal{Z}$
- an arbitrarily large observation space $\mathcal{S}$
- hidden state dynamics $\Gamma : \mathcal{Z} \times \mathcal{A} \to \mathcal{Z}$
- emission process $\Psi : \mathcal{Z} \to \Delta(\mathcal{S})$
- $\forall z_1 \neq z_2, \forall s \in \mathcal{S}, \ \Psi(s|z_1) \cdot \Psi(s|z_2) = 0.$
  In other words, this MDP is Markovian w.r.t. $\mathcal{S}$.

hidden state



Markovian high-dimensional observation

Result: In ROMDPs, $C = O(|\mathcal{Z}|)$.

Rethinking Learning State Representation

In ROMDPs, the sample complexity to achieve $V^* - V^\pi \leq \epsilon \cdot \frac{R_{\max}}{1-\gamma}$ is

$$|D| = O\left(\frac{|\mathcal{Z}||\mathcal{A}| \log \frac{|\mathcal{Q}|}{\delta}}{\epsilon^2 (1-\gamma)^4}\right)$$

In an information-theoretic view, the algorithm can learn to generalize by itself.

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Rethink: Is it principal to learn a state abstraction explicitly?

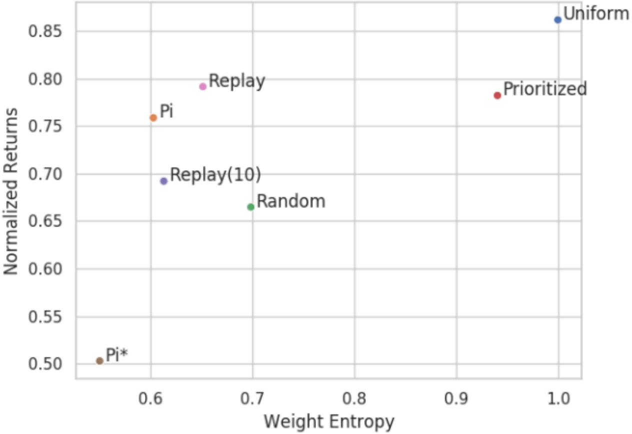
- Deep Q-Learning = FQI + Online Exploration
- Potentially pruning function class $\mathcal{Q}$
- Optimization matters in terms of $\epsilon_{\mathcal{T}}$

Reviewing Prioritized Experience Replay

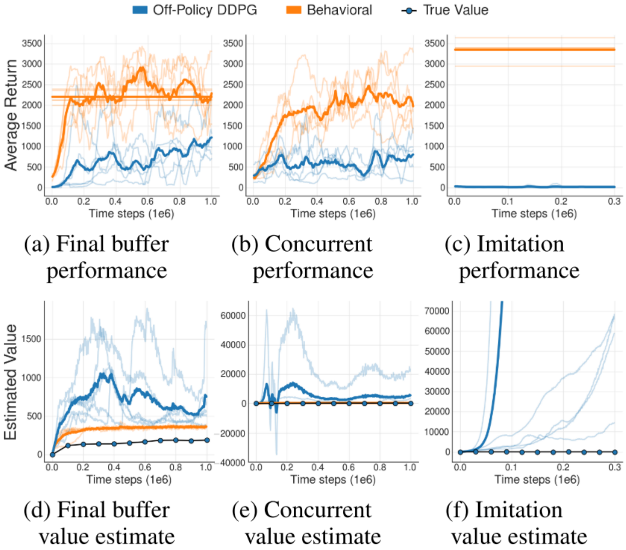
Prioritized Experience Replay (PER)

- manipulating data distribution
- using heuristics to reduce C
- prioritizing by Bellman error (Schaul et al., 2016)
- prioritizing by energy cost (Zhao and Tresp, 2018)

Experiments from Fu et al. (2019)



Experiments from Fujimoto et al. (2019)



Summary

- Assumptions to make FQI provably work
  - Realizability
  - Completeness
  - Concentratability
- Sample complexity of FQI under certain assumptions
- Connecting with empirical results

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