

Sample Complexity of Reinforcement Learning with a Generative Oracle

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Mainly based on the note:

`http://www.liziniu.org/docs/rl-generative-model.pdf`

Outline

Background & Literature Review

Model-free Methods

- Phased Value Iteration

- Variance-reduced Value Iteration

- Q-Learning

- Speedy-Q-Learning

- Variance-reduced Q-Learning

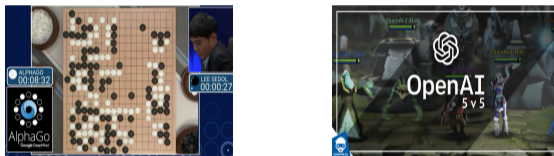
Model-based Methods

- Model-based Value Iteration

Summary

Emerging Applications with Reinforcement Learning

- ▶ Recently, there are successful applications with (deep) reinforcement learning (RL).



Figures from Internet.

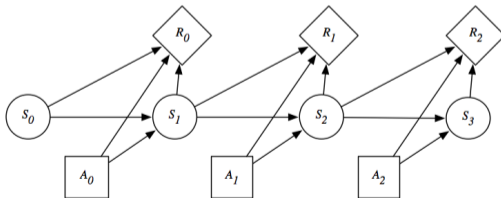
- ▶ Existing methods might not be optimal due to lack of theory and full of bag of tricks.
- ▶ To design more effective methods, we need the mathematical framework of [Markov Decision Process](#) [Puterman, 1994, Sutton and Barto, 2018].

Markov Decision Process

- ▶ Consider an infinite-horizon Markov Decision Process $\mathcal{M}^* = (\mathcal{S}, \mathcal{A}, P, R, \gamma, d_0)$ [Puterman, 1994, Sutton and Barto, 2018].
 - \mathcal{S} and \mathcal{A} are the (finite) state and action space, respectively.
 - P determines the transition probability of s_{t+1} conditioned on s_t and a_t .
 - R is the (bounded) reward function, which assigns a reward $r(s, a)$ for state-action pair (s, a) .
 - $\gamma \in [0, 1)$ is a discount factor, balancing the importance of future rewards.
 - d_0 specifies the initial state distribution.

Markov Decision Process

- ▶ The decision process is characterized as follows:
 - At the beginning of the epoch, the environment resets to some initial state s_0 according to d_0 ;
 - The agent observes the state s_0 and selects an action a_0 to perform;
 - The environment transits to s_1 according to P and sends a reward signal r_0 to the agent.
 - This process repeats until some terminal signal is released, after which the environment resets to some initial state again.



Markov Decision Process

- ▶ The above action selection procedure can be described as a policy $\pi : \mathcal{S} \mapsto \Delta(\mathcal{A})$, which maps the state space to a probability simplex over the action space.
- ▶ The goal of an intelligent agent is to maximize its payoff by searching the optimal policy π^* with maximal cumulative rewards.

$$\pi^* = \arg \max_{\pi} \mathbb{E}_{\pi} \left[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \right].$$

- ▶ Though the above decision-making procedure seems endless, the effective planning horizon is $1/(1 - \gamma)$.

$$\mathbb{E}_{\pi} \left[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \right] \leq \frac{R_{\max}}{1 - \gamma},$$

where R_{\max} is the maximal reward, which is assumed to be 1 without loss of generality.

Value Function

- ▶ The (state) value function (or V -function) for an infinite-horizon MDP is defined as:

$$V^\pi(s) = \mathbb{E} \left[\sum_{k=0}^{\infty} \gamma^k r(s_k, a_k) \mid s_0 = s, a_k \sim \pi(\cdot | s), k \geq 0 \right].$$

- ▶ Similarly, the (state-action) value function (or Q -function) is defined as:

$$Q^\pi(s, a) = \mathbb{E} \left[\sum_{k=0}^{\infty} \gamma^k r(s_k, a_k) \mid s_0 = s, a_0 = a, a_{k+1} \sim \pi(\cdot | s), k \geq 0 \right]$$

- ▶ The policy value is defined as the expected long-term return:

$$V(\pi) = \mathbb{E}_{s_0 \sim \rho(s)} [V^\pi(s_0)].$$

Bellman Optimality Equation

- ▶ The Bellman Optimality Equation for V -function and Q -function is defined as:

$$\begin{cases} V(s) &= \max_{a \in \mathcal{A}} [r(s, a) + \gamma \mathbb{E}_{s' \sim p(\cdot | s, a)} [V(s')]] & (V\text{-function}) \\ Q(s, a) &= r(s, a) + \gamma \mathbb{E}_{s' \sim p(\cdot | s, a)} [\max_{a' \in \mathcal{A}} Q(s', a')] & (Q\text{-function}) \end{cases} \quad (1)$$

- ▶ Define the optimal (state/state-action) value function as:

$$V^*(s) = \max_{\pi} V^{\pi}(s), \quad Q^*(s, a) = \max_{\pi} Q^{\pi}(s, a) \quad \forall (s, a) \in \mathcal{S} \times \mathcal{A}.$$

Bellman Operator for V -function

- ▶ The (population-based) Bellman operator \mathcal{T} for V -function is a mapping from $\mathbb{R}^{|S|}$ to itself:

$$\mathcal{T}(V)(s) \equiv \max_{a \in \mathcal{A}} [r(s, a) + \gamma \mathbb{E}_{s' \sim p(\cdot | s, a)} [V(s')]].$$

- ▶ It can be proved V^* is the unique solution to Equation (1) [Puterman, 1994].

$$V^* = \mathcal{T}(V^*).$$

- ▶ Thus, repeatedly applying Bellman operator from any point converges to the optimal state value function.

Bellman Operator for Q -function

- ▶ Similarly, the (population-based) Bellman operator \mathcal{T} for Q -function is a mapping from $\mathbb{R}^{|\mathcal{S}| \times \mathcal{A}}$ to itself:

$$\mathcal{T}(Q)(s, a) \equiv r(s, a) + \gamma \mathbb{E}_{s' \sim p(\cdot | s, a)} \left[\max_{a' \in \mathcal{A}} Q(s', a') \right].$$

- ▶ Similarly, Q^* is the unique solution to Equation (1) [Puterman, 1994].

$$Q^* = \mathcal{T}(Q^*).$$

- ▶ Again, repeatedly applying Bellman operator from any point converges to the optimal state-action value function.

Properties of Bellman Operator

- ▶ (γ -contractive) For any two value function V_1 and V_2 , we have

$$\|\mathcal{T}(V_1) - \mathcal{T}(V_2)\|_\infty \leq \gamma \|V_1 - V_2\|_\infty.$$

- Corollary: $\|\mathcal{T}(V) - V^*\|_\infty \leq \gamma \|V - V^*\|_\infty.$

- ▶ (Order-reserving) For any two V_1 and V_2 satisfying that $V_1 \leq V_2$ (\leq holds elementwise), we have

$$\mathcal{T}(V_1) \leq \mathcal{T}(V_2).$$

- ▶ The above properties also hold for Q -function.

Methods to Markov Decision Process

- ▶ Contraction-based Method
 - Value-based: (Q or V) value iteration.
 - Policy-based: policy iteration; policy gradient.
- ▶ Not-Contraction-based method
 - Linear programming [Puterman, 1994] (notes on this will be released later).

Main Algorithm of Value Iteration

Algorithm 1 Value Iteration

Input: initial value V_0 and iteration number L .

1: Initialize an auxiliary variable $Z \in \mathbb{R}^{|\mathcal{S}|}$.

2: **for** $\ell = 1, 2, \dots, L$ **do**

3: **for** each state $s \in \mathcal{S}$ **do**

4: % Performing population-based Bellman update.

5: $Z(s) = \max_{a \in \mathcal{A}} [r(s, a) + \gamma \mathbb{E}_{s' \sim p(\cdot|s,a)} [V_{\ell-1}(s')]]$.

6: **end for**

7: Set $V_\ell = Z$.

8: **end for**

Output: V_L .

Theoretical Guarantee for Value Iteration

Theorem 1 (Linear Convergence of Value Iteration).

With the parameter

$$L = \left\lceil \frac{1}{1-\gamma} \log \frac{1}{\epsilon} \right\rceil,$$

Value Iteration (see Algorithm 1) can find a sub-optimal value function V_L such that $\|V_L - V^*\|_\infty \leq \epsilon$ from any initial solution V_0 , where $\epsilon \in (0, \frac{1}{1-\gamma}]$ is the error tolerance.

Task of Reinforcement Learning

- ▶ Setting of Reinforcement Learning [Sutton and Barto, 2018]:
 - Transition probability P is unknown.
 - Reward function R is unknown (option).
 - Interaction with the environment is allowed.
- ▶ Goal: **quickly** find an ϵ -optimal policy π .
 - This can also be achieved by learning an $\epsilon/(1 - \gamma)$ -optimal Q -function, upon which we derive a greedy policy $\pi(s) = \arg \max_a Q(s, a)$ [Bertsekas and Tsitsiklis, 1996].

$$0 \leq V(\pi^*) - V(\pi) \leq \epsilon.$$

Setting of RL: Online Learning

- ▶ In addition to previous conditions, the environment/simulator can only start from some initial states.
- ▶ Interactions come from in the way of stream-data, a.k.a., online learning.
- ▶ The learner needs to balance the trade-off of exploration and exploitation.
- ▶ Not the focus of this presentation.

Setting of RL: Generative Oracle

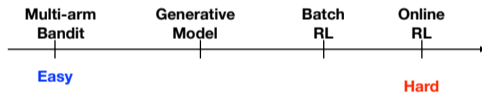
- ▶ **Generative Oracle** \mathcal{M} : we can directly reset it to any state s_t , after which we can take an action a_t and observe the next state $s_{t+1} \sim p(\cdot | s_t, a_t)$ and the reward $r(s_t, a_t)$.
 - Compared to the pure MDP problem, we still do not know P in advance.
 - Compared to the online RL problem, we can go to any s_t without the planning from an initial state s_0 .
 - In particular, we have access to the whole state space and action space (i.e., **no exploration issue**).
- ▶ Example: a perfect simulator (e.g., some video game simulators), where we can load (reset) the state s_t from RAM.
- ▶ The main focus of this presentation.

Setting of RL: Offline Learning

- ▶ The learner cannot interact with the environment, but is provided with some fixed dataset.
- ▶ The learner needs to make safe improvement from this insufficient dataset.
- ▶ Not the focus of this presentation.

Setting Comparison

- ▶ Difficulty comparison with different settings:



Lower Bound with a Generative Oracle

Definition 2 ((ϵ, δ)-correct algorithm).

Let V be the output of some RL algorithm \mathbb{A} . We say that \mathbb{A} is (ϵ, δ)-correct on the class of MDPs $\mathbb{M} = \{\mathcal{M}_1, \dots, \mathcal{M}_m\}$ if $\|V_{\mathcal{M}}^* - V\|_{\infty} \leq \epsilon$ with probability at least $1 - \delta$ for each $\mathcal{M} \in \mathbb{M}$.

Theorem 3 (Lower bound with generative oracle [Azar et al., 2013]).

There exist some constants $\epsilon_0, \delta_0, c_1, c_2$ and a class MDPs \mathbb{M} , such that for all $\epsilon \in (0, \epsilon_0)$, $\delta \in (0, \delta_0)$, and every (ϵ, δ)-correct RL algorithm on the class of MDPs \mathbb{M} , the total number of state-transition samples needs to be at least

$$T = \left\lceil \frac{|\mathcal{S}| \times |\mathcal{A}|}{c_1 \epsilon^2 (1 - \gamma)^3} \log \left(\frac{|\mathcal{S}| \times |\mathcal{A}|}{c_2 \delta} \right) \right\rceil.$$

Comment on Lower Bound

- ▶ Define $T_{\mathcal{M}}(\mathbb{A})$ as the number of samples of algorithm \mathbb{A} to get an ϵ -accurate solution on MDP \mathcal{M} with probability at least $1 - \delta$.
- ▶ Understanding the lower bound and upper bound:

$$\underbrace{T_{\mathcal{M}}(\mathbb{A})}_{\text{(actual performance)}} \leq \underbrace{\sup_{\mathcal{M}} T_{\mathcal{M}}(\mathbb{A})}_{\text{(upper bound)}},$$
$$\underbrace{\inf_{\mathbb{A}} \sup_{\mathcal{M}} T_{\mathcal{M}}(\mathbb{A})}_{\text{(lower bound)}} \leq \underbrace{\sup_{\mathcal{M}} T_{\mathcal{M}}(\mathbb{A})}_{\text{(upper bound)}}.$$

- ▶ An algorithm \mathbb{A} is said to be minimax-optimal if its upper bound matches the lower bound (constant and logarithmic terms can be ignored).

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Phased Value Iteration

- ▶ A simple method with a generative oracle is to replace the population-based Bellman operator \mathcal{T} with sample-average-approximation, see Algorithm 2 [Kearns and Singh, 1999].

Algorithm 2 Phased Value Iteration

Input: initial value V_0 , iteration number L , and sample size n .

- 1: Initialize $\hat{V}_0 = V_0$ and a policy $\hat{\pi}_0 \in \mathbb{R}^{|\mathcal{S}|}$.
- 2: Initialize an auxiliary variable $Z \in \mathbb{R}^{|\mathcal{S}| \times |\mathcal{A}|}$.
- 3: **for** $\ell = 1, 2, \dots, L$ **do**
- 4: **for** each state $s \in \mathcal{S}$ **do**
- 5: **for** each $a \in \mathcal{A}$ **do**
- 6: % Sample-average-approximation to \mathcal{T} .
- 7: Sample n next states $\{s'_i\}_{i=1}^n$ by calling \mathcal{M} .
- 8: Set $Z(s, a) = r(s, a) + \gamma \sum_{i=1}^n \frac{1}{n} \hat{V}_{\ell-1}(s'_i)$.
- 9: **end for**
- 10: Set $\hat{V}_\ell(s) = \max_{a \in \mathcal{A}} Z(s, a)$ and $\hat{\pi}_\ell(s) = \arg \max_{a \in \mathcal{A}} Z(s, a)$.
- 11: **end for**
- 12: **end for**

Output: $(\hat{V}_L, \hat{\pi}_L)$.

Theoretical Guarantee for Phased Value Iteration

Theorem 4 (Sample Complexity of Phased Value Iteration).

Given a generative oracle \mathcal{M} , with the parameters:

$$L = \left\lceil \frac{1}{1-\gamma} \log \frac{2}{(1-\gamma)\epsilon} \right\rceil, \quad n = \frac{4}{\epsilon^2(1-\gamma)^4} \log \left(\frac{2 \times |\mathcal{S}| \times |\mathcal{A}| \times T}{\delta} \right), \quad V_0 = 0,$$

Phased Value Iteration (see Algorithm 2) ensures that $\|V^* - \hat{V}_L\|_\infty \leq \epsilon$ with probability at least $1 - \delta$, and the number of total samples used is

$$\mathcal{O} \left(\frac{|\mathcal{S}| \times |\mathcal{A}|}{\epsilon^2(1-\gamma)^5} \log \left(\frac{1}{\delta} \right) \right).$$

Proof Idea of Theorem 4

- ▶ Suppose we can choose a large sample number n to ensure that sampling-based $\hat{\mathcal{T}}$ is accurate such that for any state s , we have

$$\left| \sum_{i=1}^n \frac{1}{n} \hat{V}_t(s'_i) - \mathbb{E}_{s' \sim p(\cdot|s,a)} [\hat{V}_t(s')] \right| \leq \epsilon_n.$$

- ▶ Based on the assumption, we can prove that the “flaw” of $\hat{\mathcal{T}}$ is:

$$\|V_\ell - \hat{V}_\ell\|_\infty \leq \gamma \|V_{\ell-1} - \hat{V}_{\ell-1}\|_\infty + \gamma \epsilon_n \stackrel{V_{\ell-1} = \hat{V}_{\ell-1}}{=} \gamma \epsilon_n.$$

- V_ℓ : the ℓ -th iterator of Value Iteration.
- \hat{V}_ℓ : the ℓ -th iterator of Phased Value Iteration.

For any state $s \in \mathcal{S}$,

$$\begin{aligned}
& \left| V_\ell(s) - \hat{V}_\ell(s) \right| \\
&= \left| \max_{a \in \mathcal{A}} \left\{ r(s, a) + \gamma \mathbb{E}_{s' \sim p(\cdot|s, a)} [V_{\ell-1}(s')] \right\} - \max_{a \in \mathcal{A}} \left\{ r(s, a) + \gamma \mathbb{E}_{s' \sim \hat{p}(\cdot|s, a)} [\hat{V}_{\ell-1}(s')] \right\} \right| \\
&\stackrel{(i)}{\leq} \max_{a \in \mathcal{A}} \left| \left\{ r(s, a) + \gamma \mathbb{E}_{s' \sim p(\cdot|s, a)} [V_{\ell-1}(s')] \right\} - \left\{ r(s, a) + \gamma \mathbb{E}_{s' \sim \hat{p}(\cdot|s, a)} [\hat{V}_{\ell-1}(s')] \right\} \right| \tag{2} \\
&= \gamma \max_{a \in \mathcal{A}} \left| \mathbb{E}_{s' \sim p(\cdot|s, a)} [V_{\ell-1}(s')] - \mathbb{E}_{s' \sim \hat{p}(\cdot|s, a)} [\hat{V}_{\ell-1}(s')] \right| \\
&\stackrel{(ii)}{\leq} \gamma \max_{a \in \mathcal{A}} \left| \mathbb{E}_{s' \sim p(\cdot|s, a)} [V_{\ell-1}(s')] - \mathbb{E}_{s' \sim p(\cdot|s, a)} [\hat{V}_{\ell-1}(s')] \right| + \gamma \epsilon_n \\
&\leq \gamma \max_{s' \in \mathcal{S}} \left| V_{\ell-1}(s') - \hat{V}_{\ell-1}(s') \right| + \gamma \epsilon_n,
\end{aligned}$$

- ▶ Recall that the optimality gap shrinks with a linear speed:

$$\|V_\ell - \hat{V}_\ell\|_\infty \leq \gamma \|V_{\ell-1} - \hat{V}_{\ell-1}\|_\infty + \gamma \epsilon_n. \quad (3)$$

- ▶ Repeatedly applying the above inequality, we get the optimality gap:

$$\begin{aligned} \|V_\ell - \hat{V}_\ell\|_\infty &\leq \gamma^\ell \|V_0 - \hat{V}_0\|_\infty + \sum_{i=1}^{\ell} \gamma^i \epsilon_n \\ &\leq \frac{1}{1 - \gamma} \epsilon_n, \end{aligned}$$

where we assume that $V_0 = \hat{V}_0$ and ϵ_n is an iteration-independent term.

- ▶ By triangle inequality, suppose the sampling-based Bellman update is accurate such that

$$\frac{1}{1-\gamma}\epsilon_n \leq \frac{1}{2}\epsilon \implies \epsilon_n \leq \frac{1-\gamma}{2}\epsilon,$$

then we have:

$$\|\hat{V}_\ell - V^*\|_\infty \leq \underbrace{\|V_\ell - \hat{V}_\ell\|_\infty}_{\frac{1}{2}\epsilon} + \underbrace{\|V_\ell - V^*\|_\infty}_{\frac{1}{2}\epsilon} \leq \epsilon.$$

- ▶ By Hoeffding's inequality, we require that the sample size $n \sim \mathcal{O}\left(\frac{1}{(1-\gamma)^4\epsilon^2}\right)$.
- ▶ It remains to note that the total iteration number $L \sim \mathcal{O}\left(\frac{1}{1-\gamma}\right)$.

Comment on Phased Value Iteration

- ▶ (Uniform Convergence) Phased Value Iteration requires fresh data to update each value function iterator.
 - The accuracy is uniform over iterations, which has the same order with the final accuracy.
- ▶ (Error Bound of Induced Policy) The induced greedy policy $\hat{\pi}_L$ suffers much from the inaccuracy of \hat{V}_L , that is,

$$\left\| V^{\hat{\pi}_L} - V^{\pi^*} \right\|_{\infty} \leq \mathcal{O}\left(\frac{1}{\epsilon^2(1-\gamma)^7}\right).$$

- (Lemma [Bertsekas and Tsitsiklis, 1996]) For any value function \hat{V} such that $\|\hat{V} - V^*\|_{\infty} \leq \epsilon$, suppose that $\hat{\pi}$ is the induced greedy policy by \hat{V} , then

$$\|V^{\hat{\pi}} - V^{\pi^*}\|_{\infty} \leq \frac{2\gamma}{1-\gamma}\epsilon.$$

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Phased Value Iteration: Stochastic Approximation

- ▶ Phased Value Iteration (actually all methods with a generative oracle) is a stochastic approximation (SA) method to solve the Bellman equation.

$$V = \mathcal{T}(V) \implies V_{t+1} = 0 \cdot V_t + \widehat{\mathcal{T}}(V_t).$$

- ▶ By stochastic approximation, there is always sampling-noise in the update, which precludes convergence to the fixed point.
- ▶ The same issue also holds for the stochastic gradient descent (SGD) [Johnson and Zhang, 2013].

$$\nabla F(x) = 0 \implies x_{t+1} = x_t - \eta_t \nabla f_i(x_t).$$

Improve Phased Value Iteration with SA

- ▶ Technically, reducing the variance of noise is to control the estimate of value range when applying Hoeffding's inequality.

$$\mathbb{E}[X^2] = \text{Var}[X] + \mathbb{E}^2[X].$$

- ▶ Though naively annealing the stepsize could reduce the variance, which is not the optimal method (this also is true for SGD [Johnson and Zhang, 2013]).

Variance-reduced Value Iteration

- ▶ We consider the control variate method:

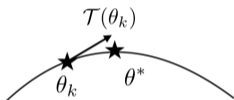
$$V := \tilde{\mathcal{T}}(\tilde{V}) + \hat{\mathcal{T}}(V) - \hat{\mathcal{T}}(\tilde{V}) \quad (4)$$

$$\implies \tilde{\mathcal{T}}(\tilde{V}) + \hat{\mathcal{T}}(V) - \hat{\mathcal{T}}(\tilde{V}) \quad (V \approx \tilde{V}) \quad (5)$$

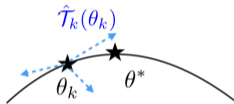
$$\implies \mathcal{T}(V) \quad (\tilde{\mathcal{T}} \approx \mathcal{T}) \quad (6)$$

- ▶ We introduce an auxiliary iterator \tilde{V} and (sampling-based) Bellman operator $\tilde{\mathcal{T}}$ to eliminate the sampling noise.
 - \tilde{V} could be the previous iterator.
 - Each iteration, using the samples to update both V and \tilde{V} .
 - $\tilde{\mathcal{T}}(\tilde{V})$ does not change over iterations within the loop.

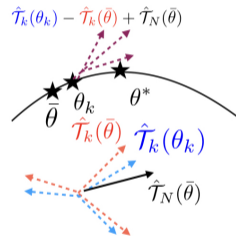
Illustration of Variance-reduced Value Iteration



Expected Bellman Update



Q-learning



Variance-Reduced Q-learning

Why Variance-reduced?

- ▶ Rearrange the estimator formula:

$$\begin{aligned} V &:= \tilde{\mathcal{T}}(\tilde{V}) + \hat{\mathcal{T}}(V) - \hat{\mathcal{T}}(\tilde{V}) \\ &:= \underbrace{\tilde{\mathcal{T}}(\tilde{V})}_{\text{one-pass}} + \underbrace{\hat{\mathcal{T}}(V - \tilde{V})}_{\text{many-pass}}. \end{aligned}$$

- ▶ The first term only requires samples before the iteration, whose value range estimate cannot be improved.
- ▶ The second term requires samples within the iteration, whose value range estimate is reduced (since $V \approx \tilde{V}$).

Main-Algorithm of Variance-reduced Value Iteration

Algorithm 3 Sublinear Randomized Value Iteration: `SublinearRandomizedVI(ϵ, δ)`

Input: desired precision ϵ and failure probability $\delta \in (0, 1)$.

1: Set $K = \left\lceil \log_2 \left(\frac{1}{\epsilon(1-\gamma)} \right) \right\rceil$, and $L = \left\lceil \frac{1}{1-\gamma} \log \left(\frac{4}{1-\gamma} \right) \right\rceil$

2: Set $V_0 = \vec{0}$ and $\epsilon_0 = \frac{1}{1-\gamma}$.

3: **for** each iteration $k = 1, 2, \dots, K$ **do**

4: Set $\epsilon_k = \frac{1}{2} \epsilon_{k-1} = \frac{1}{2^k(1-\gamma)}$.

% Iteratively shrink the estimate range

5: $(V_k, \pi_k) = \text{SampledRandomizedVI}(V_{k-1}, L, (1-\gamma)\epsilon_k/(4\gamma), \delta/K)$. *% Variance-reduced update*

6: **end for**

Output: (V_K, π_K) .

Sub-Algorithm of Variance-reduced Value Iteration

Algorithm 4 Sampled Randomized Value Iteration: $\text{SampledRandomizedVI}(V_0, L, \epsilon, \delta)$

Input: initial value V_0 and number of iterations $L > 0$

Input: target accuracy $\epsilon > 0$ and failure probability $\delta \in (0, 1)$

1: % Estimate the control variate

2: Sample n samples to obtain approximate offsets: $\mathcal{X} \in \mathbb{R}^{|\mathcal{S}| \times |\mathcal{A}|}$ with $|\mathcal{X}(s, a) - \mathbb{E}_{s' \sim p(\cdot|s,a)}[V_0(s')]| \leq \epsilon$ for all (s, a) .

$$n = \left\lceil \frac{2\|V_0\|_\infty^2}{\epsilon^2} \log \left(\frac{2L}{\delta} \right) \right\rceil.$$

3: % Single Epoch of Variance-reduced update

4: **for** each round $\ell = 1, 2, \dots, L$ **do**

5: $(V_\ell, \pi_\ell) = \text{ApxVal}(V_{\ell-1}, V_0, \mathcal{X}, \epsilon, \delta/(2L))$.

6: **end for**

Output: (V_L, π_L) .

Sub-Algorithm of Variance-reduced Value Iteration

Algorithm 5 Approximate Value Operator: $\text{ApxVal}(V, \tilde{V}, \mathcal{X}, \epsilon, \delta)$

Input: current value $V \in \mathbb{R}^{|\mathcal{S}|}$, and reference-point $\tilde{V} \in \mathbb{R}^{|\mathcal{S}|}$.

Input: precomputed offset $\mathcal{X} \in \mathbb{R}^{|\mathcal{S}| \times |\mathcal{A}|}$ such that $|\mathcal{X}(s, a) - \mathbb{E}_{s' \sim p(\cdot | s, a)}[\tilde{V}(s')]| \leq \epsilon$ for all (s, a) .

Input: desired accuracy $\epsilon \in (0, 1)$ and failure probability $\delta \in (0, 1)$.

1: Set $n = \left\lceil \frac{2\|V - \tilde{V}\|_\infty^2}{\epsilon^2} \log\left(\frac{2}{\delta}\right) \right\rceil$.

2: Initialize variables $Z_t \in \mathbb{R}^{|\mathcal{S}| \times |\mathcal{A}|}$, $\bar{V} \in \mathbb{R}^{|\mathcal{S}|}$ and $\pi \in \mathbb{R}^{|\mathcal{S}|}$.

3: **for** each state $s \in \mathcal{S}$ **do**

4: **for** each action $a \in \mathcal{A}$ **do**

5: Sample n next states $\{s'_i\}_{i=1}^n$ by calling \mathcal{M} .

6: % Variance-reduced update, see Equation (4)

7: Set $Z(s, a) = r(s, a) + \gamma \left(\mathcal{X}(s, a) + \sum_{i=1}^n \frac{1}{n} [V(s'_i) - \tilde{V}(s'_i)] \right)$.

8: **end for**

9: Set $\bar{V}(s) = \max_{a \in \mathcal{A}} Z(s, a)$, and $\pi(s) = \arg \max_{a \in \mathcal{A}} Z(s, a)$.

10: **end for**

Output: (\bar{V}, π) .

Theoretical Guarantee of Variance-reduced Value Iteration

Theorem 5 (Sample Complexity of Sublinear Randomized Value Iteration [Sidford et al., 2018]).

In invocation of Sublinear Randomized Value Iteration (see Algorithm 3) requires

$$\tilde{O} \left(|\mathcal{S}| \times |\mathcal{A}| \left(\frac{1}{\epsilon^2(1-\gamma)^4} + \frac{1}{(1-\gamma)^3} \right) \log \left(\frac{1}{\delta} \right) \right)$$

samples to obtain an ϵ -optimal value function with probability at least $1 - \delta$, where $\epsilon \in (0, \frac{1}{1-\gamma}]$.

Comment on Variance-reduced Value Iteration

- ▶ There are two terms governing the sample complexity and the dominate term is task-dependent.

$$\tilde{O}\left(\underbrace{\frac{1}{\epsilon^2(1-\gamma)^4}}_{\rightarrow \hat{T}} + \underbrace{\frac{1}{(1-\gamma)^3}}_{\rightarrow \tilde{T}}\right).$$

- ▶ To obtain an ϵ -optimal policy, the sample complexity becomes [Bertsekas and Tsitsiklis, 1996]

$$\tilde{O}\left(\frac{1}{\epsilon^2(1-\gamma)^6} + \frac{1}{(1-\gamma)^3}\right) \implies \tilde{O}\left(\frac{1}{\epsilon^2(1-\gamma)^6}\right).$$

- Only improve $1/(1-\gamma)$ over Phased Value Iteration (see Algorithm 2).

Proof Idea of Theorem 5

- ▶ `ApxVal` is almost same with the direct sample-average-approximation expect that the offset term is ϵ -optimal.
- ▶ With the same reasoning, the quality of `ApxVal` is reserved.

Lemma 6 (Quality of Approximate Value Operator).

With probability at least $1 - \delta$, the output of Approximate Value Operator (see Algorithm 5) satisfies that

$$\|\bar{V} - \mathcal{T}(V)\|_{\infty} \leq 2\gamma\epsilon.$$

Proof Idea of Theorem 5

- ▶ Based on Lemma 6, we can show that the quality of `SampledRandomizedVI` (i.e., the variance-reduced Bellman operator) is also maintained:

$$\begin{aligned}\|V_\ell - V^*\|_\infty &\leq \|V_\ell - V_\ell^\sharp\|_\infty + \|V_\ell^\sharp - V^*\|_\infty \\ &= \|V_\ell - \mathcal{T}(V_{\ell-1}) + \mathcal{T}(V_{\ell-1}) - V_\ell^\sharp\|_\infty + \|V_\ell^\sharp - V^*\|_\infty \\ &\leq 2\gamma\epsilon + \gamma \|V_{\ell-1} - V_{\ell-1}^\sharp\|_\infty + \gamma^\ell \|V_0 - V^*\|_\infty \\ &\leq \frac{2\gamma\epsilon}{1-\gamma} + \gamma^\ell \|V_0 - V^*\|_\infty,\end{aligned}\tag{7}$$

where V_ℓ^\sharp is the ℓ -th iterator of exact Value Iteration and we assume that $V_0 = V_0^\sharp$.

Proof Idea of Theorem 5

- ▶ By choosing a large enough iteration number L , e.g.,

$$L \geq \left\lceil \frac{1}{1-\gamma} \log \left(\frac{\|V_0 - V^*\|_\infty}{2\gamma\epsilon} \right) \right\rceil \implies \gamma^L \|V_0 - V^*\|_\infty \leq \frac{2\gamma\epsilon}{1-\gamma}.$$

- ▶ Therefore, we have

$$\|V_\ell - V^*\|_\infty \leq \frac{2\gamma\epsilon}{1-\gamma} + \gamma^L \|V_0 - V^*\|_\infty \leq \frac{4\gamma\epsilon}{1-\gamma}. \quad (8)$$

- ▶ The sample complexity is computed in the next page.

Proof Idea of Theorem 5

- ▶ Sample complexity is consist of two terms: control-variate and the variance-reduced update.
- ▶ To obtain an ϵ -optimal control variate, we directly use Hoeffding's inequality:

$$n = \left\lceil \frac{2\|V_0\|_\infty^2}{\epsilon^2} \log\left(\frac{2L}{\delta}\right) \right\rceil \implies n \sim \tilde{O}\left(\frac{1}{(1-\gamma)^2\epsilon^2}\right).$$

- ▶ To analyze the variance-reduced update, we need to upper bound the estimation range $\|V_\ell - V_0\|_\infty$.
- ▶ Importantly, the estimation range is reduced compared with the ordinary one $\|V_\ell\|_\infty$ in Phased Value Iteration.

Proof Idea of Theorem 5

- ▶ The estimation range $\|V_\ell - V_0\|_\infty$ is reduced over epochs.

$$\begin{aligned}\|V_\ell - V_0\|_\infty^2 &\leq \|V_\ell - V^* + V^* - V_0\|_\infty^2 \\ &\leq (\|V_\ell - V^*\|_\infty + \|V^* - V_0\|_\infty)^2 \\ &\stackrel{(i)}{\leq} 2\|V_\ell - V^*\|_\infty^2 + 2\|V^* - V_0\|_\infty^2 \\ &\stackrel{(ii)}{\leq} 2\left(\frac{2\gamma\epsilon}{1-\gamma} + \|V_0 - V^*\|_\infty\right)^2 + 2\|V^* - V_0\|_\infty^2 \\ &\leq \frac{8\epsilon^2}{(1-\gamma)^2} + 8\|V_0 - V^*\|_\infty^2,\end{aligned}\tag{9}$$

- ▶ To conclude, the sample complexity of `SublinearRandomizedVI` is bounded by

$$\mathcal{O}\left(|\mathcal{S}| \times |\mathcal{A}| \left[\frac{1}{(1-\gamma)^2\epsilon^2} + L \left(\frac{\|V_0 - V^*\|_\infty^2}{\epsilon^2} + \frac{1}{(1-\gamma)^2} \right) \right] \log\left(\frac{|\mathcal{S}| \times |\mathcal{A}| \times L}{\delta}\right)\right)\tag{10}$$

Proof Idea of Theorem 5

- ▶ By choosing $\epsilon_k = 0.5\epsilon_{k-1}$ in SublinearRandomizedVI, we infer that $\|V_k - V^*\|_\infty \leq \epsilon_k$ holds over epochs.

$$\mathcal{O} \left(|\mathcal{S}| \times |\mathcal{A}| \left[\frac{1}{(1-\gamma)^2 \epsilon^2} + L \left(\frac{\|V_0 - V^*\|_\infty^2}{\epsilon^2} + \frac{1}{(1-\gamma)^2} \right) \right] \log \left(\frac{|\mathcal{S}| \times |\mathcal{A}| \times L}{\delta} \right) \right)$$

- ▶ By substituting $\epsilon := (1-\gamma)\epsilon$ in Equation (10) (due to the accuracy in Equation (8)), we note that the number of epochs K is a $1/(1-\gamma)$ independent term.
- ▶ Thus, the total sample complexity becomes:

$$\begin{aligned} &\implies \tilde{\mathcal{O}} \left(\frac{1}{(1-\gamma)^4 \epsilon^2} + \frac{L}{(1-\gamma)^2} \right) \\ &\implies \tilde{\mathcal{O}} \left(\frac{1}{(1-\gamma)^4 \epsilon^2} + \frac{1}{(1-\gamma)^3} \right). \end{aligned}$$

Variance-reduced Value Iteration (Refined)

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Model-based Value Iteration

- ▶ On the other hand, the learner can first construct a virtual MDP $\hat{\mathcal{M}}$ with collected samples, and then performs (population) Bellman operator on this recovered MDP $\hat{\mathcal{M}}$.
- ▶ In this way, the learner does not need the iterative learning in Phased Value Iteration (see Algorithm 2), which requires new samples each iteration.

Model-based Value Iteration

Algorithm 6 Model-based Value Iteration

Input: n .

- 1: Collect n next states for each state-action pair by calling the generative model \mathcal{M} .
- 2: Construct a virtual MDP with \hat{P} :

$$\hat{P}(s'|s, a) = \frac{\# \text{ times } (s, a) \mapsto s'}{n}.$$

- 3: $\hat{V}^* \leftarrow$ Run Value Iteration (see Algorithm 1) on the virtual MDP.

Output: \hat{V}^* .

Theoretical Guarantee for Model-based Value Iteration

Theorem 7 (Sample Complexity of Model-based Value Iteration (Corase Analysis)).

Given a generative model \mathcal{M} , with the parameter:

$$n = \left\lceil \frac{1}{\epsilon^2(1-\gamma)^4} \log \left(\frac{2 \times |\mathcal{S}| \times |\mathcal{A}|}{\delta} \right) \right\rceil,$$

Model-based Value Iteration (see Algorithm 6) can find a sub-optimal value function V_T such that $\|V_T - V^*\|_\infty \leq \epsilon$ from any initial solution V_0 , where $\epsilon \in (0, \frac{1}{1-\gamma}]$ is the error tolerance with probability at least $1 - \delta$, and the number of total samples used is

$$\mathcal{O} \left(\frac{|\mathcal{S}| \times |\mathcal{A}|}{\epsilon^2(1-\gamma)^4} \log \left(\frac{|\mathcal{S}| \times |\mathcal{A}|}{\delta} \right) \right).$$

Proof Idea of Theorem 7

- ▶ Error decomposition:

$$\begin{aligned}\|V^* - \hat{V}^*\|_\infty &= \|\mathcal{T}(V^*) - \hat{\mathcal{T}}(\hat{V}^*)\|_\infty \\ &= \|\mathcal{T}(V^*) - \mathcal{T}(\hat{V}^*) + \mathcal{T}(\hat{V}^*) - \hat{\mathcal{T}}(\hat{V}^*)\|_\infty \\ &\leq \gamma \|V^* - \hat{V}^*\|_\infty + \epsilon_n,\end{aligned}$$

where we assume that the estimation error $\|\mathcal{T}(\hat{V}^*) - \hat{\mathcal{T}}(\hat{V}^*)\|_\infty \leq \epsilon_n$.

- ▶ Rearranging yields the bound:

$$\|V^* - \hat{V}^*\|_\infty \leq \frac{\gamma}{1 - \gamma} \epsilon_n. \tag{11}$$

Proof Idea of Theorem 7

- ▶ Model-based Value Iteration only requires the sample-average-approximation is accurate for \hat{V}^* .
- ▶ By substituting $\epsilon_n := \epsilon/(1 - \gamma)$ in Equation (11), applying Hoeffding's inequality, we have

$$n \sim \mathcal{O}\left(\frac{1}{(1 - \gamma)^4 \epsilon^2}\right) \implies \left\|V^* - \hat{V}^*\right\|_{\infty} \leq \epsilon.$$

Comment on Model-based Value Iteration

- ▶ Model-based Value Iteration only requires $\hat{\mathcal{T}}$ to be accurate for \hat{V}^* .
 - On the contrast, Phased Value Iteration requires $\hat{\mathcal{T}}$ to be accurate for each iterator \hat{V}_t .
- ▶ In this way, Model-based Value Iteration improves $\mathcal{O}(\frac{1}{1-\gamma})$ complexity compared to Phased Value Iteration.
- ▶ The above analysis for Model-based Value Iteration is coarse.
 - We independently bound the estimation error for each (s, a) pair then use a union bound.
 - For a single value function, the sequential structure of Bellman equation could provide a tighter bound to estimate the variance.

Refined Sample Complexity of Model-based Value Iteration

Theorem 8 (Refined Sample Complexity of Model-based Value Iteration [Azar et al., 2013]).

Given a generative oracle \mathcal{M} , with the parameter:

$$n = \mathcal{O} \left(\frac{1}{\epsilon^2(1-\gamma)^3} \log \left(\frac{2 \times |\mathcal{S}| \times |\mathcal{A}|}{\delta} \right) \right),$$

Model-based Value Iteration (see Algorithm 6) can find a sub-optimal value function V_T such that $\|V_T - V^\|_\infty \leq \epsilon$ from any initial solution V_0 , where $\epsilon \in (0, \frac{1}{1-\gamma}]$ is the error tolerance with probability at least $1 - \delta$, and the number of total samples used is*

$$\mathcal{O} \left(\frac{|\mathcal{S}| \times |\mathcal{A}|}{\epsilon^2(1-\gamma)^3} \log \left(\frac{|\mathcal{S}| \times |\mathcal{A}|}{\delta} \right) \right).$$

Proof Idea of Theorem 8

- ▶ We start with the general form of the error decomposition.
- ▶ Note that $\hat{V}^* \geq \hat{V}^{\pi^*}$, we have

$$\begin{aligned} V^* - \hat{V}^* &\leq V^* - \hat{V}^{\pi^*} \\ &= \left(\mathbb{I} - \gamma P^{\pi^*}\right)^{-1} r^{\pi^*} - \left(\mathbb{I} - \gamma \hat{P}^{\pi^*}\right)^{-1} r^{\pi^*} \quad \left(r^{\pi^*}(s) = r(s, \pi^*(s))\right) \\ &= \left(\mathbb{I} - \gamma \hat{P}^{\pi^*}\right)^{-1} \left[\left(\mathbb{I} - \gamma \hat{P}^{\pi^*}\right) - \left(\mathbb{I} - \gamma P^{\pi^*}\right) \right] \left(\mathbb{I} - \gamma P^{\pi^*}\right)^{-1} r^{\pi^*} \\ &= \gamma \left(\mathbb{I} - \gamma \hat{P}^{\pi^*}\right)^{-1} \left[P^{\pi^*} - \hat{P}^{\pi^*} \right] \left(\mathbb{I} - \gamma P^{\pi^*}\right)^{-1} r^{\pi^*} \\ &= \underbrace{\gamma \left(\mathbb{I} - \gamma \hat{P}^{\pi^*}\right)^{-1}}_{\text{precondition}} \underbrace{\left[P^{\pi^*} - \hat{P}^{\pi^*} \right]}_{\text{estimation}} V^*, \end{aligned}$$

where \leq holds elementwise.

Proof Idea of Theorem 8

- ▶ Similarly, we have the elementwise-error bound:

$$\begin{cases} V^* - \hat{V}^* \leq \gamma \left(\mathbb{I} - \gamma \hat{P}^{\pi^*} \right)^{-1} \left[P^{\pi^*} - \hat{P}^{\pi^*} \right] V^* \\ V^* - \hat{V}^* \geq \gamma \left(\mathbb{I} - \gamma \hat{P}^{\hat{\pi}^*} \right)^{-1} \left[P^{\pi^*} - \hat{P}^{\hat{\pi}^*} \right] V^*. \end{cases}$$

- ▶ To apply Bernstein's inequality, we need to consider the variance of estimation.

$$\sigma_{V^\pi}^2(s, a) = \gamma^2 \mathbb{V}_{s' \sim p(\cdot|s, a)} [V^\pi(s')], \quad \text{and} \quad \hat{\sigma}_{V^*}^2(s, a) = \gamma^2 \mathbb{V}_{s' \sim \hat{p}(\cdot|s, a)} [V^\pi(s')].$$

- ▶ Furthermore, we need to unify the RHS to get a single variance bound (see the next page).

Proof Idea of Theorem 8

Lemma 9 (Elementwise bounds on σ_{V^*}).

With probability at least $1 - \delta$, the following relations hold separately:

$$\begin{aligned}\sigma_{V^*} &\leq \hat{\sigma}_{\hat{V}^{\pi^*}} + b_v \vec{1}, \\ \sigma_{V^*} &\leq \hat{\sigma}_{\hat{V}^{\hat{\pi}^*}} + b_v \vec{1},\end{aligned}$$

where b_v is defined as

$$b_v = \left(\frac{18\gamma^4 \log\left(\frac{3|\mathcal{S}| \times |\mathcal{A}|}{\delta}\right)}{n(1-\gamma)^4} \right)^{1/4} + \sqrt{\frac{4\gamma^2 \log\left(\frac{6|\mathcal{S}| \times |\mathcal{A}|}{\delta}\right)}{n(1-\gamma)^4}}$$

Proof Idea of Theorem 8

► With Lemma 9, we can bound the estimation error.

Lemma 10 (Elementwise bounds on $(P^{\pi^*} - \hat{P}^{\pi^*})V^*$).

Define the following constants:

$$c_{pv} = 2 \log \left(\frac{2|\mathcal{S}| \times |\mathcal{A}|}{\delta} \right)$$
$$b_{pv} = \left(\frac{5 \log \left(\frac{6|\mathcal{S}| \times |\mathcal{A}|}{\delta} \right)}{n} \left(\frac{\gamma}{1-\gamma} \right)^{4/3} \right)^{3/4} + \frac{4 \log \left(\frac{12|\mathcal{S}| \times |\mathcal{A}|}{\delta} \right)}{n(1-\gamma)^2}.$$

With probability at least $1 - \delta$, we have

$$-\sqrt{\frac{c_{pv} \hat{\sigma}_{\hat{V}^{\pi^*}}^2}{n}} - b_{pv} \vec{1} \leq \gamma \left(P^{\pi^*} - \hat{P}^{\pi^*} \right) V^* \leq \sqrt{\frac{c_{pv} \hat{\sigma}_{\hat{V}^{\pi^*}}^2}{n}} + b_{pv} \vec{1}$$

Proof Idea of Theorem 8

- ▶ Finally, we need to consider the multiplication by the precondition matrix and the variance.

$$\left(\mathbb{I} - \gamma \hat{P}^{\pi^*}\right)^{-1} \left[P^{\pi^*} - \hat{P}^{\pi^*}\right] V^* \approx \left(\mathbb{I} - \gamma \hat{P}^{\pi^*}\right)^{-1} \hat{\sigma}_{\hat{V}^{\pi^*}}.$$

- ▶ A naive bound with Cauchy-Schwarz inequality is $\mathcal{O}\left(\frac{1}{(1-\gamma)^2}\right)$.
 - Together with $\sqrt{\frac{1}{n}}$ in Lemma 10, this yields the sample complexity of $\mathcal{O}\left(\frac{1}{(1-\gamma)^4}\right)$.
- ▶ However, we will show that the sequential structure of MDP yields a tighter bound of $\mathcal{O}\left(\frac{1}{(1-\gamma)^{1.5}}\right)$.

Proof Idea of Theorem 8

- ▶ Consider the “total variance”:

$$\Sigma^\pi(s, a) = \mathbb{E} \left[\left\{ \sum_{t \geq 0} \gamma^t r(s_t, a_t) - Q^\pi(s, a) \right\}^2 \mid s_0 = s, a_0 = a \right].$$

- ▶ We show that “total variance” satisfies the following Bellman equation.

Lemma 11 (Bellman-like variance).

Σ^π satisfies the following Bellman equation:

$$\Sigma^\pi = \sigma_{V^\pi}^2 + \gamma^2 P^\pi \Sigma^\pi.$$

Proof Idea of Theorem 8

- ▶ With Lemma 11, we get a tighter bound:

$$\begin{aligned}\left\|(\mathbb{I} - \gamma^2 P^\pi)^{-1} \sigma_{V^\pi}^2\right\|_\infty &= \|\Sigma^\pi\|_\infty \leq \frac{1}{(1-\gamma)^2} \\ \left\|(\mathbb{I} - \gamma P^\pi)^{-1} \sigma_{V^\pi}\right\|_\infty &\leq 2\left\|\sqrt{\frac{1}{1-\gamma}} \Sigma^\pi\right\|_\infty \leq \frac{2}{(1-\gamma)^{1.5}}.\end{aligned}$$

- ▶ In this way, we prove that the total sample complexity is $\mathcal{O}\left(\frac{1}{(1-\gamma)^3 \epsilon^2}\right)$.

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Summary

Summary

- ▶ Model-free methods have the following properties:
 - they iteratively collect samples and update the value function.
 - variance-reduction plays an important role.
- ▶ Model-based methods have the following properties:
 - they collect enough samples once and solve the optimal value function.
 - it's easy to achieve the minimax-optimal bound for both policy/(value function).
- ▶ It's non-trivial to obtain an ϵ -optimal policy from an imperfect value function.

Prior Art

Sample Complexity to obtain an ϵ -optimal policy

algorithm	sample size range	sample complexity	ϵ -range
empirical QVI Azar et al. '13	$\left[\frac{ \mathcal{S} ^2 \mathcal{A} }{(1-\gamma)^2}, \infty \right)$	$\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^3 \epsilon^2}$	$\left(0, \frac{1}{\sqrt{(1-\gamma) \mathcal{S} }} \right]$
sublinear randomized VI Sidford et al. '18a	$\left[\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^2}, \infty \right)$	$\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^4 \epsilon^2}$	$\left(0, \frac{1}{1-\gamma} \right]$
variance-reduced QVI Sidford et al. '18b	$\left[\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^3}, \infty \right)$	$\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^3 \epsilon^2}$	$(0, 1]$
randomized primal-dual Wang '17	$\left[\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^2}, \infty \right)$	$\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^4 \epsilon^2}$	$\left(0, \frac{1}{1-\gamma} \right]$
empirical MDP + planning Agarwal et al. '19	$\left[\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^2}, \infty \right)$	$\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^3 \epsilon^2}$	$\left(0, \frac{1}{\sqrt{1-\gamma}} \right]$

Table from <http://www.stat.cmu.edu/~ytwei/documents/slides/model-based-rl-slides.pdf>.

Open Problem

- ▶ Q1: breaking the sample barrier for model-free methods with a generative oracle.
- ▶ Q2: online model-free learning with variance-reduction.

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