# Online Reinforcement Learning: PAC Exploration in Discounted MDPs

Mohammad Sadegh Talebi m.shahi@di.ku.dk Department of Computer Science



#### MDP Classification Based on Horizon

Three classes of MDPs based on the horizon N:

- Discounted MDPs
- Finite-horizon MDPs
- Average-reward MDPs



#### From MDPs to RI

- In RL, we consider the same interaction model as in MDPs, but assume that P and R are unknown.
- The agent wishes to maximize her collected (discounted) rewards
- An optimal policy, or a near-optimal one, must be learnt but the available information is the history of experience

$$h_t = (s_1, a_1, r_1, \dots, s_{t-1}, a_{t-1}, r_{t-1}, s_t)$$



#### RL Problems Based on N

A classification of RL problems based on (task) horizon N:

- Discounted MDPs ⇒ Discounted RL problems
- Average-reward MDPs
   Average-reward RL problems



#### Discounted RL

• The agent interacts with a discounted MDP

$$M = (\mathcal{S}, \mathcal{A}, \underbrace{P, R}_{\mathsf{unknown}}, \gamma)$$

- The interaction proceeds for an arbitrary number of time steps without any reset.
- The initial state is chosen by Nature.
- Objective: to learn a policy solving

$$\max_{\pi \in \Pi^{SD}} V^{\pi}(s) = \mathbb{E}^{\pi} \left[ \sum_{t=1}^{\infty} \gamma^{t-1} r_t \middle| s_1 = s \right]$$

for any initial state  $s \in \mathcal{S}$ .



# **RL Settings**

#### Common taxonomies of RL settings:

#### Off-policy vs. On-policy

- In off-policy, data is collected using some behavior policy (logging policy).
   Hence, the learned policy does not influence data collection.
- Whereas in on-policy, actions are taken according to the learned policy.

#### • Offline (Batch) vs. Online

- Offline RL works with pre-collected data using some behavior policy, whereas in online RL data is collected along the way.
- Both aim to find a near-optimal policy using as few samples as possible.
- They look at different performance metrics.
- Offline RL closely resembles supervised ML.

Offline-vs-online taxonomy appears more relevant in practice as well as the recent literature.



# RL: Design Approaches

Three main approaches to algorithm design in RL:

- Model-Based: Consists in maintaining an approximate MDP model through estimating R and P, and deriving a value function from the approximate MDP.
  - Examples: UCB1, UCRL2.
- Model-Free: Directly learns a value function (without estimating R and P), and derives a policy from it.
  - Examples: TD, variants of Q-Learning, DQN.
- Policy Search: Directly searches in the space of policies.
  - Example: Policy Gradient, PPO.

More recent terminology: Model-based vs. Valued-based vs. Policy-based



# Online Discounted RL: Setting and Performance Metrics



#### Recap

Online Discounted RL. An agent interacts with a discounted MDP  $M = (\mathcal{S}, \mathcal{A}, P, R, \gamma)$  for some (potentially unbounded) rounds without any reset

At each time step  $t = 1, 2, \ldots$ :

- The agent observes the current state  $s_t$  and takes an action  $a_t \in \mathcal{A}$
- M decides a reward  $r_t \sim R(s_t, a_t)$  and a next state  $s_{t+1} \sim P(\cdot | s_t, a_t)$
- The agent receives  $r_t$  (any time in step t before start of t+1)

M is unknown (beyond S and A), and the goal is to maximize  $\sum_{t=1}^{\infty} \gamma^{t-1} r_t$  (in expectation) using collected experience (history):

$$h_t = (s_1, a_1, r_1, \dots, s_{t-1}, a_{t-1}, r_{t-1}, s_t)$$

Need to balance exploration and exploitation.



#### Online RL: Performance Metrics

- Many offline algorithms can be made online with some tricks (e.g., QL).
- But will they explore well?

For online RL, we need performance metrics to measure the quality of exploration-exploitation tradeoff.



#### Online RL: Performance Measures

The performance of a learning algorithm  $\mathbb{A}$  can be measured through:

- Convergence: Whether A converges to an optimal (or near-optimal) policy.
- PAC Sample Complexity: The number of steps where the value of the current policy output by A is not near-optimal with high-probability.
- ullet Regret: The amount of reward lost due to choosing sub-optimal actions by  ${\mathbb A}$ . In fact these metrics measure how exploration-exploitation tradeoff is implemented.

More precise definitions to follow.



# Sample Complexity of Exploration

Consider an RL algorithm  $\mathbb{A}$ , and  $h_t = (s_1, a_1, r_1, \dots, s_{t-1}, a_{t-1}, r_{t-1}, s_t)$  a history of  $\mathbb{A}$ , with  $a_t \sim \pi_t(\cdot|s_t)$ . I.e.,  $\pi_t$  is the learned policy at time t.

A notion of sample complexity introduced by (Kakade, 2003):

#### Sample Complexity of Exploration

For input  $\varepsilon > 0$ , time step t is bad if  $\pi_t$  is not  $\varepsilon$ -optimal for the current state  $s_t$ :

$$V^{\pi_t}(s_t) < V^{\star}(s_t) - \varepsilon \implies t \text{ is } \varepsilon\text{-bad}$$

The sample complexity of exploration of  $\mathbb{A}$  is the total number of  $\varepsilon$ -bad time steps over the entire trajectory:

$$\sum_{t=1}^{\infty} \mathbb{I}\left\{V^{\pi_t}(s_t) < V^{\star}(s_t) - \varepsilon\right\}$$

- It measures the number of mistakes along the whole trajectory.
- Sample complexity can be used as a relevant performance measure in discounted RL problems.



# PAC-MDP Algorithms

We are interested in RL algorithms, whose sample complexities are controlled by some functions that are not too large as a function of relevant parameters  $S,A,\varepsilon,\delta$  and  $\gamma.$ 

#### PAC-MDP Algorithm

An algorithm  $\mathbb A$  is called  $(\varepsilon, \delta)$ -PAC-MDP if for any  $\varepsilon$  and  $\delta$ , the sample complexity of  $\mathbb A$  is upper bounded w.p.  $\geq 1-\delta$  by some polynomial in

$$S,\,A,\,rac{1}{arepsilon},\,rac{1}{\delta},\,\, ext{and}\,\,rac{1}{1-\gamma}.$$

PAC-MDP 

Probably Approximately Correct in MDPs



# **OFU Principle**

#### Optimism in the Face of Uncertainty (OFU)

- A well-known principle in balancing exploration-exploitation in bandits and online RL dating back to (Lai & Robbins, 1985).
- Also known as the Optimism principle

**The OFU Principle:** In an uncertain world, suppose that the environment is the best possible (in terms of rewards)!

- ullet If the chosen action is optimal  $\Longrightarrow$  no penalty
- If sub-optimal ⇒ reducing uncertainty



# Optimism in the Face of Uncertainty (OFU)

In bandits, OFU prescribes replacing unknown mean rewards by their corresponding high-probability UCBs. the most prominent example is the UCB algorithm.

In MDPs, different implementations exist depending on the approach

- In model-based: Select the best candidate environment (among all plausible models/MDPs), i.e. the one leading to the highest possible value function.
- In model-free: When updating the Q-function, be optimistic. Initialize all
  Q-values to their highest possible value and use "reward + exploration bonus"
  instead of "reward" alone.

This lecture: two OFU-based PAC-MDP algorithms (UCB-QL, MBIE).



# Q-Learning (Revisited)

QL (Q-Learning) for online RL (via OFU):

• Initialization:

$$Q_0(s,a) = rac{R_{ ext{max}}}{1-\gamma}$$
 (optimistic intialization)

Value Update:

$$Q_{t+1}(s,a) = \begin{cases} Q_t(s,a) + \alpha_t \Big( r_t + \gamma \max_{b \in \mathcal{A}} Q_t(s_{t+1},b) - Q_t(s,a) \Big) & (s,a) = (s_t,a_t) \\ Q_t(s,a) & \text{else.} \end{cases}$$

 $\bullet$   $\mbox{\bf Action Selection:}$  trust your current  $Q_t$  but use a bit of exploration. Hence, take

$$a_t \sim \pi_t(\cdot|s_t; Q_t)$$

where  $\pi_t(\cdot|s_t;Q_t)$  depends on  $Q_t$  but uses some exploration too.



# Q-Learning (Revisited)

Examples of  $\pi_t(Q_t)$  with (built-in) exploration device:

• E.g.,  $\varepsilon$ -greedy policy (for some  $\varepsilon > 0$ )

$$\pi_{\varepsilon\text{-greedy}}(s) = \begin{cases} \operatorname{argmax}_a Q_t(s, a) & \text{w.p. } 1 - \varepsilon \\ \text{sample uniformly at random from } \mathcal{A} & \text{w.p. } \varepsilon \end{cases}$$

• E.g., Boltzmann's policy (a.k.a. softmax):

at state 
$$s$$
, select action  $a \in \mathcal{A}$  w.p. 
$$\frac{e^{\eta Q_t(s,a)}}{\sum_{b \in \mathcal{A}} e^{\eta Q_t(s,b)}}$$

where  $\eta > 0$  is a parameter controlling exploration.

These balance exploration-exploitation. But what can be said about the quality of exploration-exploitation?

Such QL variants converge to  $\pi^*$  (and play it often). Yet, not sufficient to make QL PAC-MDP.



# PAC-MDP Algorithms Exist

#### Some PAC-MDP algorithms:

- Kakade (2003) defined the notion of sample complexity of exploration.
- Some model-based algorithms include:
  - Rmax (Brafman & Tennenholtz, 2002), one of the earliest PAC-MDP algorithms.
  - MBIE (Strehl & Littman, 2008), UCRLγ (Lattimore & Hutter, 2014),
- Delayed Q-Learning (Strehl et al., 2006) is the first model-free PAC-MDP algorithm.
- UCB-QL (Dong et al., 2020) is a recent model-free PAC-MDP algorithm.

This lecture: UCB-QL and MBIE, and worst-case lower bound.



UCB-QL: UCB + Q-Learning



UCB-QL

UCB-QL is a recent model-free PAC-MDP algorithm presented and analyzed in (Dong et al., 2020).

We present UCB-QL and investigates its theoretical and empirical sample complexity.

- It is model-free and maintains Q functions.
- It has a Q-update resembling the one in QL -hence the name.
- Its main departure from QL (and its variants for off-policy RL) is use of UCB-type exploration to maintain optimism –hence the name (again).



# Recap: UCB

Recall UCB in a K-armed bandit (coinciding with an MDP with a single state and K actions):

$$a_t \in \arg\max_{a \in [K]} \mathtt{UCB}_t(a) := \left(\widehat{\mu}_t(a) + \sqrt{\frac{3 \log(t)}{2N_t(a)}}\right)$$

A proposal for QL-type update + exploration:

$$Q_{t+1}(s_t, a_t) = (1 - \alpha_t)Q_t(s_t, a_t) + \alpha_t \left(r_t + \Box \sqrt{\frac{\log(t)}{N_t(s_t, a_t)}} + \gamma \max_{a' \in \mathcal{A}} Q_t(s_{t+1}, a')\right)$$

- The term □ must capture the range of Q-values.
- A sound proposal, but needs some considerations.



#### UCB-QL

UCB-QL maintains two Q-functions:

- Optimistic Q-function  $Q \in \mathbb{R}^{S \times A}$
- Historical minimum Q-function  $\widehat{Q} \in \mathbb{R}^{S \times A}$ .

The update is performed on Q but actions are taken greedily w.r.t.  $\widehat{Q}$ . More precisely, at each t

• We update Q using "reward + bonus"  $r_t + b(N_t(s_t, a_t))$ :

$$\begin{split} Q(s_t, a_t) \leftarrow Q(s_t, a_t) \\ &+ \alpha_{N_t(s_t, a_t)} \Big[ r_t + \underbrace{b \big( N_t(s_t, a_t) \big)}_{\text{bonus}} + \gamma \max_{a} \widehat{Q}(s_{t+1}, a) - Q(s_t, a_t) \Big] \end{split}$$

where for some large enough parameter H (see next slides), we define

$$\alpha_k = \frac{H+1}{H+k}, \quad b(k) = \frac{1}{1-\gamma} \sqrt{\frac{32H}{k} \log \frac{SA(k+1)(k+2)}{\delta}}$$



Then we update  $\widehat{Q}$ :  $\widehat{Q}(s_t, a_t) \leftarrow \min \left\{ \widehat{Q}(s_t, a_t), Q(s_t, a_t) 
ight\}$ 

#### UCB-QL

- input:  $\varepsilon, \delta$
- initialization: For all (s, a),

$$-N(s,a)=1$$

$$-\hat{Q}(s,a) = Q(s,a) = \frac{R_{\text{max}}}{1-\gamma}$$

- for t = 1, 2, ...
  - Take  $a_t \in \operatorname{argmax}_a \widehat{Q}(s_t, a)$
  - Receive  $r_t \sim R(s_t, a_t)$  and  $s_{t+1} \sim P(\cdot | s_t, a_t)$
  - Update Q:

$$Q(s_t, a_t) \leftarrow (1 - \alpha_k)Q(s_t, a_t) + \alpha_k \left[ r_t + b(k) + \gamma \max_{a} \widehat{Q}(s_{t+1}, a) \right]$$

where 
$$k = N(s_t, a_t)$$
.

- Update  $\widehat{Q}$ :  $\widehat{Q}(s_t, a_t) \leftarrow \min \left\{ \widehat{Q}(s_t, a_t), Q(s_t, a_t) \right\}$
- $-N(s_t,a_t) \leftarrow N(s_t,a_t) + 1.$

See next slide for H, b(k), and  $\alpha_k$ .



#### UCB-QL: Parameters

Recall  $k = N_t(s, a)$ . Choose

$$\alpha_k = \frac{H+1}{H+k}$$

$$b(k) = \frac{1}{1-\gamma} \sqrt{\frac{32H}{k} \log \frac{SAk^2}{\delta}}$$

for some fictitious horizon number  $H := H(\gamma, \varepsilon)$ .

One can set H to the effective horizon:

$$H = H_{\text{eff}} := \frac{-1}{1 - \gamma} \log(\varepsilon (1 - \gamma))$$

Then

$$H = H_{\text{eff}} \implies b(k) = b(N_t(s, a)) = \widetilde{\mathcal{O}}\left(\sqrt{\frac{H_{\text{eff}}^3}{N_t(s, a)}}\right) = \widetilde{\mathcal{O}}\left(\frac{1}{(1 - \gamma)^{3/2}\sqrt{N_t(s, a)}}\right)$$



### UCB-QL: Sample Complexity

Sample complexity of UCB–QL in any discounted MDP with S states and A actions (i.e., worst-case bound):

#### Theorem (Sample Complexity of UCB-QL)

For any  $\varepsilon \! > \! 0$ ,  $\delta \! \in \! (0,1)$ , the sample complexity of UCB-QL is bounded by

$$\widetilde{\mathcal{O}}\bigg(\frac{SA}{\varepsilon^2(1-\gamma)^7}\log\frac{1}{\delta}\bigg), \quad \textit{w.p.} \ \geq 1-\delta,$$

where  $\widetilde{\mathcal{O}}(\cdot)$  hides poly-logarithmic terms in  $SA, \varepsilon^{-1}$ , and  $\frac{1}{1-\gamma}$ .

⇒ UCB-QL is PAC-MDP. More precisely:

$$\mathbb{P}\bigg\{\sum_{t=1}^{\infty} \underbrace{\mathbb{I}\big\{V^{\star}(s_t) - V^{\pi_t}(s_t) > \varepsilon\big\}}_{t \text{ is } \varepsilon\text{-bad}} > \widetilde{O}\left(\frac{SA}{\varepsilon^2(1-\gamma)^7}\log\frac{1}{\delta}\right)\bigg\} < \delta,$$



#### UCB-QL: Proof Idea

The (complicated) proof lies on the following facts:

• Implementing optimism:  $\widehat{Q}_t \geq Q^\star$  for all t w.h.p. In particular,

$$egin{aligned} \widehat{Q}_t(s_t,a_t) &\geq \widehat{Q}_t(s_t,\pi^\star(s_t)) & \text{ (by algorithm design)} \ &\geq Q^\star(s_t,\pi^\star(s_t)) & \text{ (by optimism)} \ &= V^\star(s_t) & \text{ (by definition of } Q^\star) \end{aligned}$$

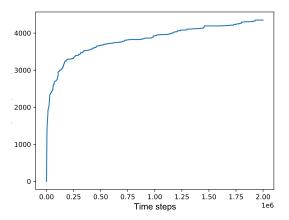
ullet So to count arepsilon-bad steps, one can upper bound steps where

$$\widehat{Q}_t(s_t, a_t) - Q^*(s_t, a_t) > \varepsilon$$

ullet Carefully chosen H and  $lpha_k$  guarantee that  $\widehat{Q}_t$  is not overly optimistic.



# Numerical Experiments



The number of  $\varepsilon$ -steps for a single run of UCB-QL in 5-state RiverSwim ( $\gamma=0.9,\ \varepsilon=0.1,\ \delta=0.05$ ).



# MBIE: Model-Based Interval Estimation



#### OFU: Model-Based

MBIE (Strehl & Littman, 2008) is a model-based PAC-MDP algorithm designed based on OFU.

Model-based recipe for the optimism principle (OFU):

- Step 1: Maintains a set of plausible MDPs (models) (i.e., consistent with history  $h_t$ ). This can be done by defining high-probability confidence sets for R and P, and forming a corresponding set of MDPs.
- Step 2: Choose an optimistic model (among all models) and an optimistic policy leading to the highest value.



# Step 1: Confidence Sets - Empirical MDP

For any t > 1, define

•  $N_t(s, a, s')$ : number of visits, up to t, to (s, a) followed by a visit to s'

$$N_t(s, a, s') = \sum_{i=1}^{t-1} \mathbb{I}\{s_i = s, a_i = a, s_{i+1} = s'\}$$

•  $N_t(s,a)$ : number of visits, up to t, to (s,a)

$$N_t(s, a) = \sum_{s' \in \mathcal{S}} N_t(s, a, s')$$

#### Empirical Estimator for P:

$$\forall s' \in \mathcal{S}: \quad \widehat{P}_t(s'|s,a) = \begin{cases} \frac{N_t(s,a,s')}{N_t(s,a)} & \text{if } N_t(s,a) > 0\\ \frac{1}{S} & \text{otherwise} \end{cases}$$

#### Empirical Estimator for R:



$$\widehat{R}_t(s, a) = \frac{1}{N_t(s, a)} \sum_{i=1}^{t-1} r_i \mathbb{I}\{s_i = s, a_i = a\}$$

# **Empirical MDP**

The empirical MDP:

$$\widehat{M}_t = (\mathcal{S}, \mathcal{A}, \widehat{P}_t, \widehat{R}_t, \gamma)$$

Why not only using  $\widehat{M}_t$ . I.e., finding the optimal policy in  $\widehat{\pi}_t^{\star}$  and taking  $a_t = \widehat{\pi}_t^{\star}(s_t)$  each step.

 $\rightarrow$  No exploration-exploitation tradeoff. Will not lead to a PAC-MDP algorithm.



# Step 1: Confidence Sets

 $\delta \in (0,1)$  is given.

#### Confidence Set for R:

• Define a confidence set for R(s,a) as

$$C_{s,a} = \left\{ \lambda \in [0,1] : |\widehat{R}_t(s,a) - \lambda| \le \beta_{N_t(s,a)} \right\}$$

for some suitable function  $\beta_{N_t(s,a)}$ .

For example, using Hoeffding's inequality (combined with Laplace's methods):

$$\beta_n = \sqrt{\frac{1}{2n}(1+\frac{1}{n})\log\frac{SA\sqrt{n+1}}{\delta}}, \quad n \in \mathbb{N}.$$

$$\mathbb{P}\Big(\forall t \ge 1, \, \forall (s, a) : \, R(s, a) \in C_{s, a}\Big) \ge 1 - \delta$$



# Recap: Confidence Sets

Consider a distribution p over a set  $\mathcal{X}$ .

- p is unknown.
- Consider n i.i.d. samples from p:  $X_1, \ldots, X_n \sim_{\text{i.i.d.}} p$ .
- Empirical estimate of p:

$$\widehat{p}_n(x) := \frac{1}{n} \sum_{i=1}^n \mathbb{I}\{X_i = x\} \qquad \forall x \in \mathcal{X}.$$

Weissman's inequality (for deterministic n)

For  $\delta \in (0,1)$ ,

$$\mathbb{P}\left(\|p - \widehat{p}_n\|_1 \ge \sqrt{\frac{2}{n}\log\left(\frac{2^{|\mathcal{X}|} - 2}{\delta}\right)}\right) \le \delta$$



# Recap: Confidence Sets

Consider a distribution p over a set  $\mathcal{X}$ .

- p is unknown.
- Consider n i.i.d. samples from p:  $X_1, \ldots, X_n \sim_{\text{i.i.d.}} p$ .
- Empirical estimate of p:

$$\widehat{p}_n(x) := \frac{1}{n} \sum_{i=1}^n \mathbb{I}\{X_i = x\} \quad \forall x \in \mathcal{X}.$$

What if n is not deterministic?

Weissman's inequality (for random stopping time n) For  $\delta \in (0,1)$ .

$$\mathbb{P}\left(\exists n: \left\|p-\widehat{p}_n\right\|_1 \geq \sqrt{\frac{2}{n}\left(1+\frac{1}{n}\right)\log\left(\frac{(2^{|\mathcal{X}|}-2)\sqrt{n+1}}{\delta}\right)}\right) \leq \delta$$



# Step 1: Confidence Sets

 $\delta \in (0,1)$  is given.

#### Confidence Set for P:

ullet Define a confidence set for  $P(\cdot|s,a)$  as

$$C'_{s,a} = \left\{ q \in \Delta(\mathcal{S}) : \left\| \widehat{P}_t(\cdot|s,a) - q \right\|_1 \le \beta'_{N_t(s,a)} \right\}$$

for some suitable function  $\beta'_{N_t(s,a)}$ .

• For example, using Weissman's inequality (combined with Laplace's methods):

$$\beta'_n = \sqrt{\frac{2}{n}(1 + \frac{1}{n})\log\frac{SA(2^S - 2)\sqrt{n+1}}{\delta}}$$

$$\mathbb{P}\Big(\forall t \ge 1, \, \forall (s, a) : \, P(\cdot | s, a) \in C'_{s, a}\Big) \ge 1 - \delta$$



# Step 1: Set of Models

Confidence sets  $\{C_{s,a},C'_{s,a}\}_{s\in\mathcal{S},a\in\mathcal{A}}$  yield a set of models (i.e., MDPs) consistent with the history  $h_t=(s_1,a_1,r_1,\ldots,s_{t-1},a_{t-1},r_{t-1},s_t)$ :

$$\mathcal{M}_t = \left\{ M' = (\mathcal{S}, \mathcal{A}, P', R', \gamma) : 
ight.$$
  $P'(\cdot|s,a) \in C'_{s,a} ext{ and } R'(s,a) \in C_{s,a}, \; orall s, a 
ight\}$ 

- $\mathcal{M}_t$  collects all MDPs that could be a candidate for the true Model M (in view of  $h_t$ ).
- Moreover, M is trapped in  $\mathcal{M}_t$  with high probability, simultaneously for all t:

$$\mathbb{P}(\forall t > 1 : M \in \mathcal{M}_t) > 1 - 2\delta$$



## Step 2: Planning

### Step 2: Planning. To implement OFU, we wish to find

$$\pi_t \in \arg\max_{\mathbf{M'} \in \mathcal{M}_t} \max_{\pi \in \Pi^{\mathsf{SD}}} V_{\mathbf{M'}}^{\pi}$$

and then we choose  $a_t = \pi_t(s_t)$ .

Alternatively, by Bellman's optimality equation, we wish to find  $\widetilde{Q}(s,a)$  satisfying: For all (s,a),

$$\widetilde{Q}(s,a) = \max_{R'(s,a) \in C_{s,a}} R'(s,a) + \gamma \max_{P'(\cdot|s,a) \in C'_{s,a}} \sum_{x} P'(x|s,a) \max_{a'} \widetilde{Q}(x,a')$$

where  $\widetilde{Q}(s,a)$  is indeed the optimal Q-function of  $\mathcal{M}_t$ .



## Step 2: Planning

$$\widetilde{Q}(s,a) = \max_{R'(s,a) \in C_{s,a}} R'(s,a) + \gamma \max_{P'(\cdot|s,a) \in C'_{s,a}} \sum_{\boldsymbol{x}} P'(\boldsymbol{x}|s,a) \max_{a'} \widetilde{Q}(\boldsymbol{x},a')$$

Compared to optimality equations for MDPs, we have two extra maximizations.

• The one in blue admits a closed-form solution:

$$\max_{R'(s,a) \in C_{s,a}} R'(s,a) = \widehat{R}_t(s,a) + \beta_{N_t(s,a)}$$

 $\bullet$  No closed-form solution to the second. However, for a fixed  $u \in \mathbb{R}^{S \times A}$  , the problem

$$\max_{p \in C'(s,a)} \sum_{x} p(x) \max_{a'} u(x,a')$$

can be solve using a simple procedure thanks to the shape of  $C'_{s,a}$ .

The second optimization problem can be efficiently solved using Extended Value Iteration (EVI).

### **MBIE**

- input:  $\varepsilon, \delta$
- initialization: For all (s, a),
  - -N(s,a) = 0
  - $-\widetilde{Q}(s,a) = \frac{R_{\max}}{1-\gamma}$
- for t = 1, 2, ...
  - Compute estimates  $\widehat{P}_t$  and  $\widehat{R}_t$
  - Find  $\widetilde{Q}$  by solving Bellman's equation for  $\mathcal{M}_t$  using EVI
  - Choose  $a_t \in \operatorname{argmax}_a \widetilde{Q}(s_t, a)$
  - Receive reward  $r_t \sim R(s_t, a_t)$  and next-state  $s_{t+1} \sim P(\cdot|s_t, a_t)$
  - Update  $N(s_t, a_t) \leftarrow N(s_t, a_t) + 1$ .



### MBIE: EVI

- ullet input: arepsilon
- initialization: Select  $\widetilde{Q}_0 \in \mathbb{R}^{S \times A}$  arbitrarily. Set n = -1.
- repeat:
  - Increment n
  - Compute, for each (s, a),

$$\begin{aligned} & \pmb{R'(s,a)} = \widehat{R}_t(s,a) + \beta_{N(s,a)} \\ & \pmb{P'(\cdot|s,a)} \in \operatorname{argmax} \Big\{ \sum_{x \in \mathcal{S}} q(x) \max_{a'} \widetilde{Q}_n(x,a') : q \in C'_{s,a} \Big\} \end{aligned}$$
e, for each  $(s,a)$ .

– Update, for each (s,a),

$$\begin{split} \widetilde{Q}_{n+1}(s,a) &= \underline{R'(s,a)} + \gamma \sum_{x \in \mathcal{S}} \underline{P'(x|s,a)} \max_{a'} \widetilde{Q}_n(x,a') \\ \text{until } \|\widetilde{Q}_{n+1} - \widetilde{Q}_n\|_{\infty} &< \frac{\varepsilon(1-\gamma)}{2\alpha} \end{split}$$

ullet output:  $\widetilde{Q}_n$ 



### MBIE: EVI

Algorithm for solving

$$\max_{q \in C_{s,a}'} \sum_{x \in \mathcal{S}} q(x) u(x)$$

Index  $S = \{s_1, s_2, \dots, s_S\}$ , and assume w.l.o.g. that

$$u(s_1) \ge u(s_2) \ge \ldots \ge u(s_S)$$

- initialization:  $q = \widehat{P}_t(\cdot|s,a)$
- Set  $q(s_1) = \widehat{P}_t(s_1|s,a) + \frac{1}{2}\beta'_{N_t(s,a)}$
- $\bullet \ \ell = S$
- while:  $\sum_{x \in \mathcal{S}} q(x) > 1$ 
  - Set  $q(s_{\ell}) = \max \left\{ 0, 1 \sum_{x \neq s_{\ell}} q(x) \right\}$
  - Decrement  $\ell$
- output: q



## MBIE: Sample Complexity

Sample complexity of MBIE in any discounted MDP with S states and A actions:

## Theorem (Sample Complexity of MBIE)

For any  $\varepsilon > 0$ ,  $\delta \in (0,1)$ , the sample complexity of MBIE is bounded by

$$\widetilde{\mathcal{O}}\left(\frac{S^2A}{\varepsilon^3(1-\gamma)^6}\log\left(\frac{1}{\delta}\right)\right), \quad \textit{w.p.} \geq 1-\delta,$$

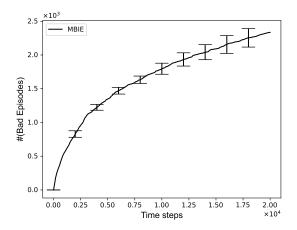
where  $\widetilde{\mathcal{O}}(\cdot)$  hides poly-logarithmic terms in  $SA, \varepsilon^{-1}$  , and  $\frac{1}{1-\gamma}.$ 

⇒ MBIE is PAC-MDP. More precisely:

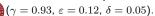
$$\mathbb{P}\bigg\{\sum_{t=1}^{\infty} \underbrace{\mathbb{I}\big\{V^{\star}(s_t) - V^{\pi_t}(s_t) > \varepsilon\big\}}_{t \text{ is } \varepsilon \text{-bad}} > \widetilde{O}\left(\frac{S^2 A}{\varepsilon^3 (1-\gamma)^6} \log \frac{1}{\delta}\right)\bigg\} < \delta,$$



## Numerical Experiments



The number of  $\varepsilon\text{-steps}$  under MBIE in RiverSwim



# Worst-Case Lower Bound on Sample Complexity



### Worst-Case Lower Bound

How good is the sample complexity bound of UCB-QL? Could it be improved?

To answer these, we need to derive lower bounds on sample complexity.

- Problem-dependent lower bound
- Worst-case lower bound



### Worst-Case Lower Bound

The following lower bound on sample complexity is due to (Lattimore & Hutter, 2014).

### Theorem (Worst-Case Lower Bound)

Let  $S \geq 4$ , A,  $\gamma$ ,  $\delta$ , and  $\varepsilon$ , with  $\varepsilon(1-\gamma)$  being sufficiently small. For any learning algorithm  $\mathbb A$ , there exists a discounted MDP M with S states, A actions, and discount factor  $\gamma$  such that with probability at least  $\delta$ , the number of  $\varepsilon$ -bad steps of  $\mathbb A$  is larger than

$$c_1 \cdot \frac{SA}{\varepsilon^2 (1 - \gamma)^3} \log \left( \frac{c_2 S}{\delta} \right)$$

for some universal constants  $c_1, c_2 > 0$ . Namely, w.p. higher than  $\delta$ ,

$$\sum_{t=1}^{\infty} \mathbb{I}\{V^{\mathbb{A}_t}(s_t) < V^{\star}(s_t) - \varepsilon\} \ge c_1 \cdot \frac{SA}{\varepsilon^2 (1-\gamma)^3} \log\left(\frac{c_2 S}{\delta}\right)$$

• The theorem asserts a fundamental performance limit on sample complexity which no algorithm can beat.



### Worst-Case Lower Bound

$$\underbrace{\Omega\!\left(\frac{SA}{\varepsilon^2(1-\gamma)^3}\log\left(\frac{S}{\delta}\right)\right)}_{\text{worst-case LB}} \quad \text{vs.} \quad \underbrace{\widetilde{\mathcal{O}}\!\left(\frac{SA}{\varepsilon^2(1-\gamma)^7}\log\left(\frac{SA}{\delta}\right)\right)}_{\text{UCB-QL UB}}$$

The sample complexity of UCB-QL

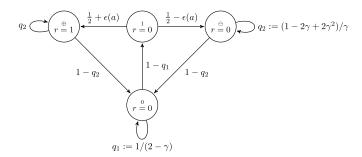
- ullet Has optimal dependence on S, A, and arepsilon,  $\delta$  (ignoring poly-log factors).
- Could be improved by a factor of  $1/(1-\gamma)^4$ .
- $\bullet$  UCRL $\gamma$  (Lattimore & Hutter, 2014), a variant of UCRL2 for discounted MDPs, achieves:

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

• This gap was closed in 2021.



### Worst-Case MDP: S=4



A family of worst-case 4-state MDPs (Lattimore & Hutter, 2014):

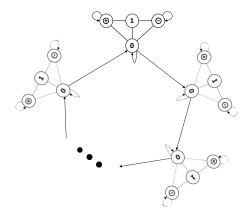
- $S = \{ \oplus, \ominus, 1, 0 \}$  and A actions per each state.
- All actions have identical rewards, and the rewarding state is +.
- $\bullet \ \varepsilon(a^\star) = 16\varepsilon(1-\gamma) \text{ for some } a = a^\star \text{, and } \varepsilon(a) = 0 \text{ for } a \neq a^\star.$
- $s=\oplus,\ominus$  are highly abosorbing. s=0 traps the agent for around  $\frac{1}{1-\gamma}$  steps (in expectation).



### Worst-Case MDP: S > 4

A worst-case instance for S>4 can be constructed by chaining S/4 of the previous 4-state MDPs together

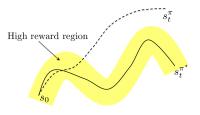
- ullet State 0 of k-th one transits with a very small probability to state 0 of the (k+1)-th.
- $q_1$  must be slightly modified too; see (Lattimore & Hutter, 2014).





## An Important Remark

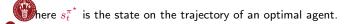
Defining Sample Complexity w.r.t. the trajectory of the algorithm is not always meaningful:



$$\mathbb{P}\left(V^{\pi_t}(\boldsymbol{s_t}) \ge V^{\star}(\boldsymbol{s_t}) - \varepsilon\right) \ge 1 - \delta$$

Due to exploration, we can end up in states with very low rewards, and being optimal from there may not mean much. A more meaningful criterion would be

$$\mathbb{P}\left(V^{\pi_t}(\boldsymbol{s_t}) \geq V^{\star}(\boldsymbol{s_t^{\pi^{\star}}}) - \varepsilon\right) \geq 1 - \delta$$



### References

- Sham Kakade, "On the sample complexity of reinforcement learning," PhD Thesis, University of London, University College London, 2003.
- Ronen Brafman and Moshe Tennenholtz, "R-max -A general polynomial time algorithm for near-optimal reinforcement learning," Journal of Machine Learning Research, 2002.
- Alexander Strehl et al., "PAC model-free reinforcement learning" International Conference on Machine Learning, 2006.
- Chi Jin, Zeyuan Allen-Zhu, Sebastien Bubeck, and Michael Jordan, "Is Q-learning provably efficient?" Advances in Neural Information Processing Systems 31, 2018.
- Kefan Dong, Yuanhao Wang, Xiaoyu Chen, and Liwei Wang, "Q-learning with UCB exploration is sample efficient for infinite-horizon MDP" International Conference on Learning Representations, 2020.
- Tor Lattimore and Marcus Hutter, "Near-optimal PAC bounds for discounted MDPs" Theoretical Computer Science, 2014.
- Eyal Even-Dar and Yishay Mansour, "Convergence of optimistic and incremental Q-learning," Advances in Neural Information Processing Systems 14, 2001.

