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Artificial Intelligence Research

Exploration-Exploitation in Reinforcement Learning

Finite-Horizon MDPs

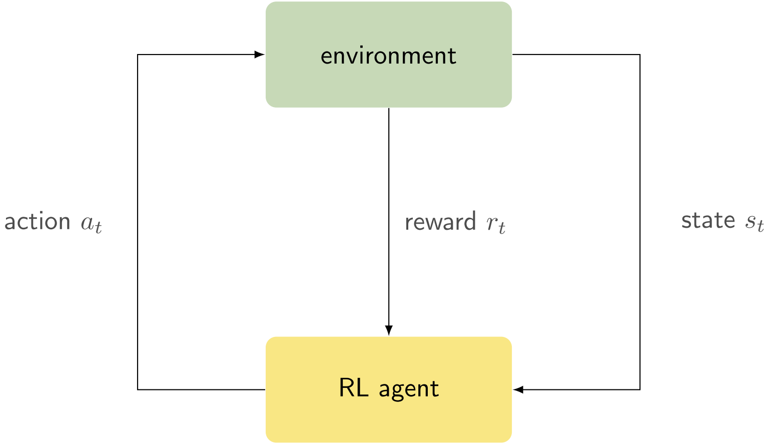
Matteo Pirotta
Facebook AI Research

Acknowledgements

These slides are part of a longer tutorial on exploration-exploitation in RL.

`https://rlgammazero.github.io/`

RL Agent-Environment Interaction



Website

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Markov Decision Process

[Puterman, 1994]

A **finite-horizon** Markov decision process (MDP) is a tuple $M = \langle \mathcal{S}, \mathcal{A}, r_h, p_h, H \rangle$

- State space $\mathcal{S}$
- Action space $\mathcal{A}$
- Horizon H
- Transition distribution $p_h(\cdot|s,a) \in \Delta(\mathcal{S})$, $h = 1, \dots, H$
- Reward distribution with expectation $r_h(s,a) \in [0,1]$, $h = 1, \dots, H$

An agent acts according to a *time-variant policy*

$$\pi_h : \mathcal{S} \to \mathcal{A} \qquad h = 1, \dots, H$$

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An agent acts according to a *time-variant policy*

$$\pi_h : \mathcal{S} \to \mathcal{A} \qquad h = 1, \ldots, H$$

In (contextual) bandit, actions do not influence the evolution of states

Value Functions and Optimality

Value functions

$$Q_h^{\pi}(s,a) = r_h(s,a) + \mathbb{E}\left[\sum_{l=h+1}^{H} r_l(s_l, \pi_l(s_l))\right]$$

$$V_h^{\pi}(s) = Q_h^{\pi}(s, \pi_h(s))$$

Optimality

$$Q_h^{\star}(s,a) = \sup_{\pi} Q_h^{\pi}(s,a)$$

$$\pi_h^{\star}(s) = \arg\max_{a \in \mathcal{A}} Q_h^{\star}(s,a)$$

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Remark: given $r_h(s,a) \in [0,1]$, then $Q_h(s,a), V_h(s) \in [0, H-(h-1)]$

Bellman Equations

Policy Bellman equation

$$\begin{aligned} Q_h^\pi(s,a) &= r_h(s,a) + \mathbb{E}_{s' \sim p_h(\cdot|s,a)}\left[Q_{h+1}^\pi(s', \pi_{h+1}(s'))\right] \\ &= r_h(s,a) + \mathbb{E}_{s' \sim p_h(\cdot|s,a)}\left[V_{h+1}^\pi(s')\right] \end{aligned}$$

Optimal Bellman equation

$$\begin{aligned} Q_h^\star(s,a) &= r_h(s,a) + \mathbb{E}_{s' \sim p_h(\cdot|s,a)}\left[\max_{a' \in \mathcal{A}} Q_{h+1}^\star(s', a')\right] \\ &= r_h(s,a) + \mathbb{E}_{s' \sim p_h(\cdot|s,a)}\left[V_{h+1}^\star(s')\right] \end{aligned}$$

Value Iteration (aka Backward Induction)

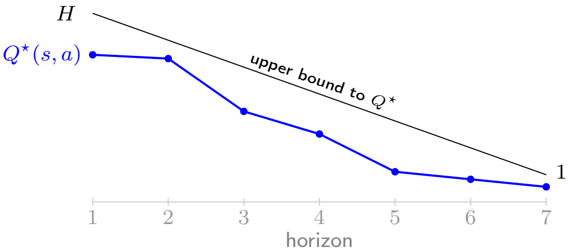
Input: $\mathcal{S}$, $\mathcal{A}$, r_h, p_h
Set $Q^\star_{H+1}(s,a) = 0$ for all $(s,a) \in \mathcal{S} \times \mathcal{A}$

for $h = H, \dots, 1$ **do**
  for $(s,a) \in \mathcal{S} \times \mathcal{A}$ **do**
    Compute

$$
\begin{aligned}
Q^\star_h(s,a) &= r_h(s,a) + \mathbb{E}_{s' \sim p_h(\cdot|s,a)}\left[\max_{a' \in \mathcal{A}} Q^\star_{h+1}(s',a')\right] \\
&= r_h(s,a) + \mathbb{E}_{s' \sim p_h(\cdot|s,a)}\left[V^\star_{h+1}(s')\right]
\end{aligned}
$$

  end
end
return $\pi^\star_h(s) = \arg\max_{a \in \mathcal{A}} Q^\star_h(s,a)$

Value Iteration (aka Backward Induction)



$$Q^\star_h(s,a) = \max_a \left\{ r_h(s,a) + \mathbb{E}_{s'|s,a}[V^\star_{h+1}(s')] \right\}$$

Online Learning Problem

Input: $\mathcal{S}, \mathcal{A}$ $\cancel{r_h, p_h}$

Initialize $Q_{h1}(s,a) = 0$ for all $(s,a) \in \mathcal{S} \times \mathcal{A}$ and $h = 1, \dots, H$, $\mathcal{D}_1 = \emptyset$

for $k = 1, \dots, K$ **do** `// episodes`

  Define π_k based on $(Q_{hk})_{h=1}^H$

  Observe initial state s_{1k} *(arbitrary)*

  for $h = 1, \dots, H$ **do**

    Execute $a_{hk} = \pi_{hk}(s_{hk})$

    Observe r_{hk} and $s_{h+1,k}$

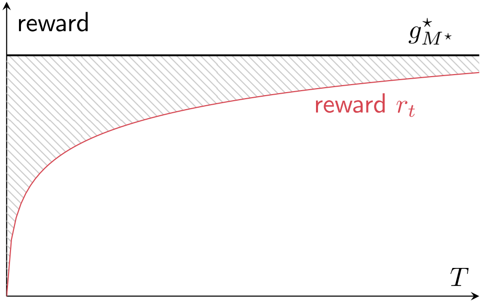
  end

  Add trajectory $(s_{hk}, a_{hk}, r_{hk})_{h=1}^H$ to $\mathcal{D}_{k+1}$

  Compute $(Q_{h,k+1})_{h=1}^H$ from $\mathcal{D}_{k+1}$

end

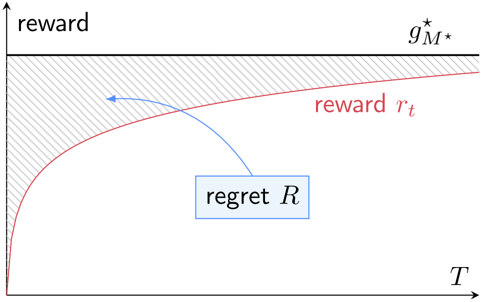
Frequentist Regret



$$R(K,\ M^\star,\ \mathfrak{A}) = \sum_{k=1}^{K} \Big(V^\star(s_{1k}) - V^{\pi_k}(s_{1k}) \Big)$$

Let $T = HK$ total number of steps executed in the environment

Frequentist Regret



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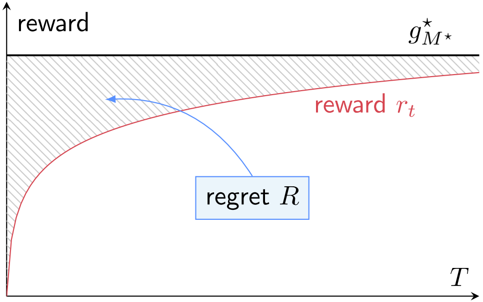

unknown true MDP
$M^\star = \langle \mathcal{S}, \mathcal{A}, r, p, H \rangle$

algorithm $\mathfrak{A} = \{\pi_k\}_{k=1}^K$

$$R(K, M^\star, \mathfrak{A}) = \sum_{k=1}^{K} \left(V^\star(s_{1k}) - V^{\pi_k}(s_{1k}) \right)$$

policy selected by $\mathfrak{A}$

Let $T = HK$ total number of steps executed in the environment

Alternative Models

- Infinite-horizon undiscounted MDPs (average reward)
  $\Rightarrow$ regret minimization

- Infinite-horizon discounted MDPs
  $\Rightarrow$ PAC-MDPs

$$N(M^\star, \mathfrak{A}) = \sum_{t=0}^{\infty} \mathbb{I}\left\{ V^{\pi_t}(s_t) \leq V^\star(s_t) - \epsilon \right\}$$

What is Wrong with Q-learning with ϵ-greedy?

- ϵ-greedy strategy

$$a_{hk} = \begin{cases} \arg\max_{a \in \mathcal{A}} Q_{hk}(s_{hk}, a) & \text{w.p. } 1 - \epsilon_{hk}, \\ \mathcal{U}(\mathcal{A}) & \text{otherwise.} \end{cases}$$

- Q-learning update

$$Q_{h,k+1}(s_{hk}, a_{hk}) = (1 - \alpha_t) Q_{hk}(s_{hk}, a_{hk}) + \alpha_t \Big(r_{hk} + \max_{a' \in \mathcal{A}} Q_{h+1,k}(s_{h+1,k}, a') \Big)$$

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- **Dithering effect:** exploration is not effective in covering the state space
- **Policy shift:** the policy changes at each step

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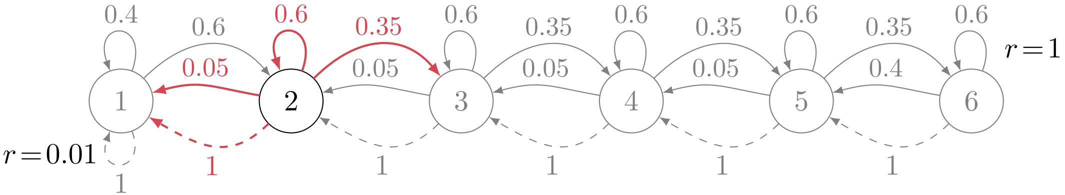
- The exploration strategy relies on **biased** estimates Q_{hk}
- Samples are used **once**
- **Dithering effect:** exploration is not effective in covering the state space
- **Policy shift:** the policy changes at each step
- **Regret:** $\Omega\Big(\min\{T, A^{H/2}\}\Big)$ [Jin et al., 2018]

River Swim: Markov Decision Processes

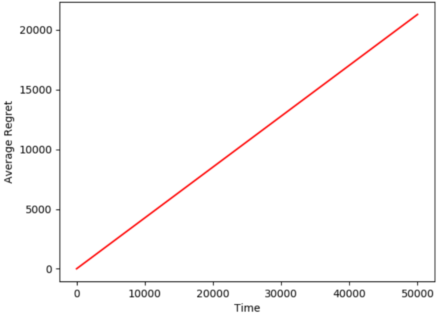
Strehl and Littman [2008]

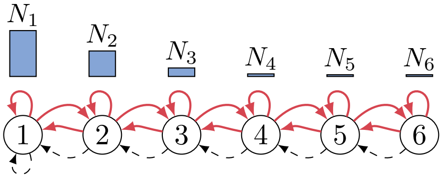


- $\mathcal{S} = \{1, 2, 3, 4, 5, 6\}$, $\mathcal{A} = \{L, R\}$
- $\pi_L(s) = L$, $\pi_R(s) = R$

River Swim: Q-learning w\ ϵ-greedy Exploration

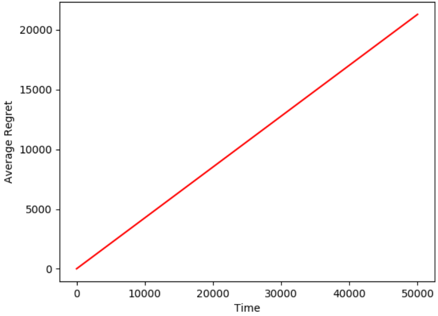
- $\epsilon_t = 1.0$

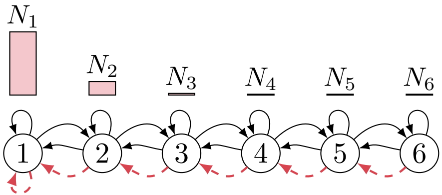




River Swim: Q-learning w\ ϵ-greedy Exploration

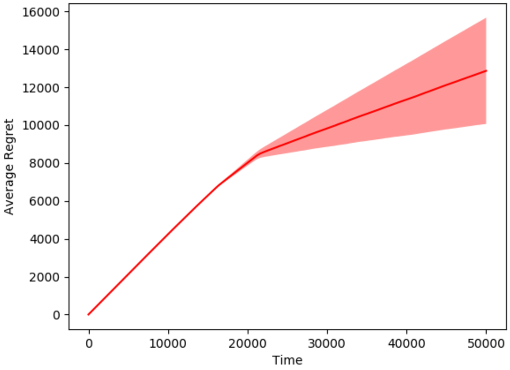
- $\epsilon_t = 1.0$
- $\epsilon_t = 0.5$





River Swim: Q-learning w\ ϵ-greedy Exploration

- $\epsilon_t = 1.0$
- $\epsilon_t = 0.5$
- $\epsilon_t = \dfrac{\epsilon_0}{(N(s_t) - 1000)^{2/3}}$



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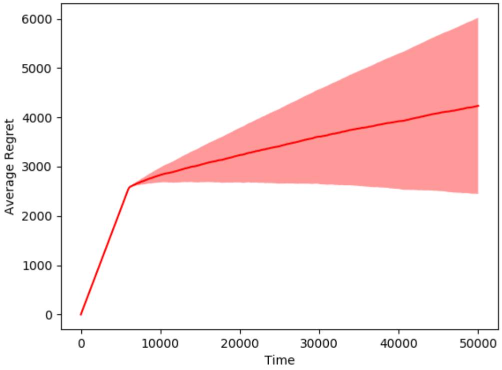

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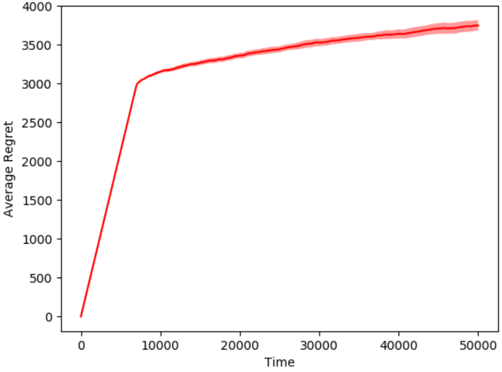

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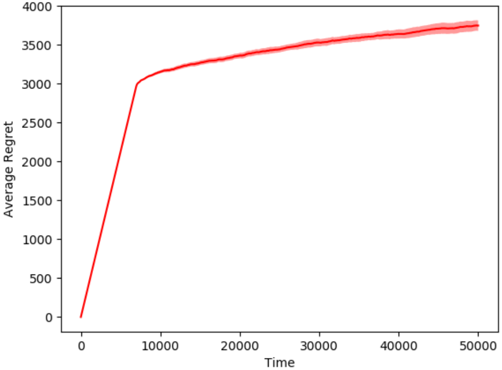


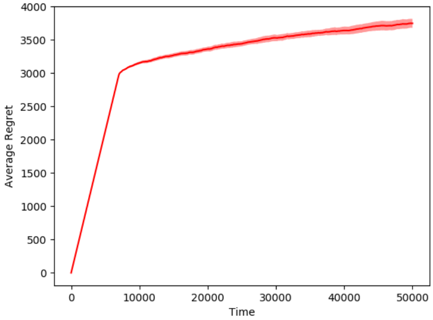
Tuning the ϵ schedule is difficult and problem dependent

River Swim: Q-learning w\ ϵ-greedy Exploration

Main drawbacks of Q-learning with ϵ-greedy

- ϵ-greedy performs *undirected* exploration
- *Inefficient use* of samples

Regret: $\Omega\Big(\min\{T, A^{H/2}\}\Big)$



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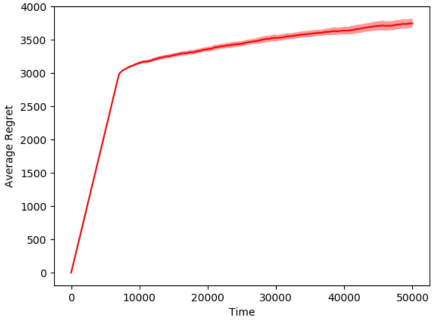


Uncertainty-driven exploration-exploitation

Minimax Lower Bound

Theorem (adapted from Jaksch et al. [2010])

For any MDP $M^\star = \langle \mathcal{S}, \mathcal{A}, p_h, r_h, H \rangle$ with stationary $(p_1 = p_2 = \ldots = p_H)$ transitions, any algorithm $\mathfrak{A}$ at any episode K suffers a regret of at least

$$\Omega\left(\sqrt{HSAT}\right)$$

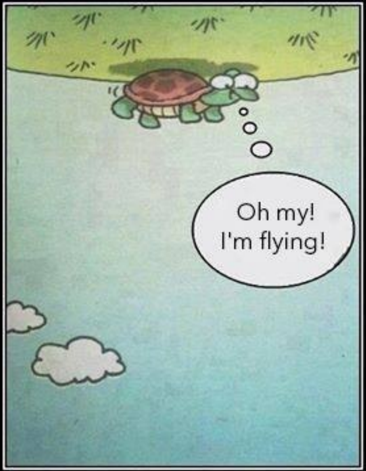
with $T = HK$.

- If *non-stationary* transitions
  - $p_1, \ldots, p_H$ can be arbitrary different
  - Effective number of states is $S' = HS$
  - Lower bound

$$\Omega\left(H\sqrt{SAT}\right)$$

Tabular MDPs: Outline

The Optimism Principle: Intuition



OPTIMISM
It's the best way to see life.

The Optimism Principle: Intuition

Exploration vs. Exploitation

The Optimism Principle: Intuition

Exploration vs. Exploitation

Optimism in Face of Uncertainty

When you are uncertain, consider the **best possible world (reward-wise)**

The Optimism Principle: Intuition

Exploration vs. Exploitation

Optimism in Face of Uncertainty

When you are uncertain, consider the **best possible world (reward-wise)**

If the best possible world is **correct**

$\Longrightarrow$ **no regret**

Exploitation

If the best possible world is **wrong**

$\Longrightarrow$ **learn useful information**

Exploration

The Optimism Principle: Intuition

Exploration vs. Exploitation

Optimism in **value function**

Optimism in Face of Uncertainty

When you are uncertain, consider the **best possible world (reward-wise)**

If the best possible world is **correct**

$\Longrightarrow$ **no regret**

Exploitation

If the best possible world is **wrong**

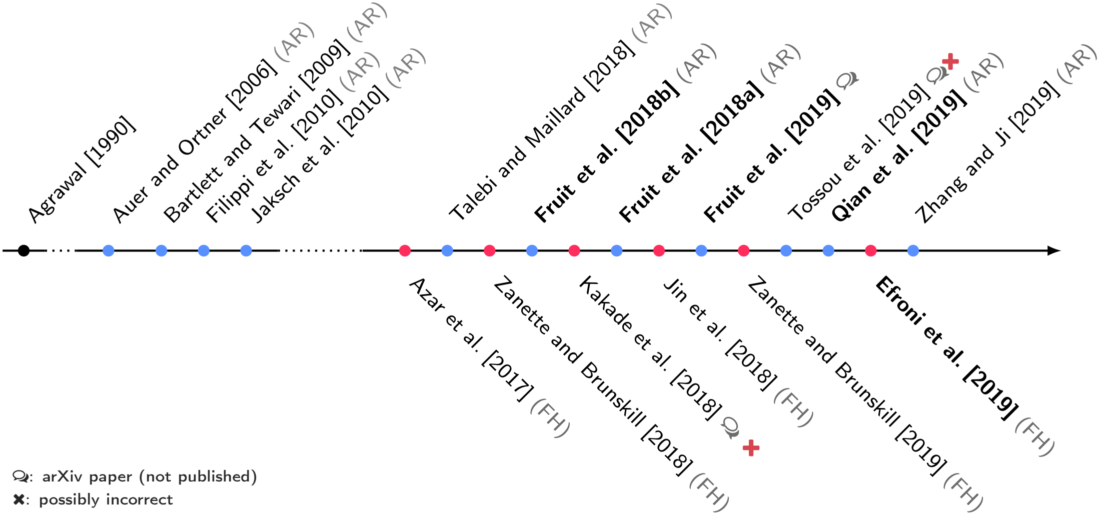
$\Longrightarrow$ **learn useful information**

Exploration

History: *OFU* for Regret Minimization

Tabular MDPs

FH: finite-horizon
AR: average reward



: arXiv paper (not published)
✖: possibly incorrect

Learning Problem

Input: $\mathcal{S}$, $\mathcal{A}$ $\cancel{r_h, p_h}$

Initialize $Q_{h1}(s,a) = 0$ for all $(s,a) \in \mathcal{S} \times \mathcal{A}$ and $h = 1, \dots, H$, $\mathcal{D}_1 = \emptyset$

for $k = 1, \dots, K$ **do** // `episodes`

Observe initial state s_{1k} *(arbitrary)*

Compute $(Q_{h,k})_{h=1}^{H}$ from $\mathcal{D}_k$

Define π_k based on $(Q_{hk})_{h=1}^{H}$

for $h = 1, \dots, H$ **do**

Execute $a_{hk} = \pi_{hk}(s_{hk})$

Observe r_{hk} and $s_{h+1,k}$

end

Add trajectory $(s_{hk}, a_{hk}, r_{hk})_{h=1}^{H}$ to $\mathcal{D}_{k+1}$

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Learning Problem

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for $k = 1, \dots, K$ **do** `// episodes`
    Observe initial state s_{1k} *(arbitrary)*
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    Define π_k based on $(Q_{hk})_{h=1}^{H}$
    for $h = 1, \dots, H$ **do**
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        Observe r_{hk} and $s_{h+1,k}$
    end
    Add trajectory $(s_{hk}, a_{hk}, r_{hk})_{h=1}^{H}$ to $\mathcal{D}_{k+1}$
end

Defines the type of algorithm

Model-based Learning

Input: $\mathcal{S}$, $\mathcal{A}$ $\cancel{r_h, p_h}$

Initialize $Q_{h1}(s,a) = 0$ for all $(s,a) \in \mathcal{S} \times \mathcal{A}$ and $h = 1, \dots, H$, $\mathcal{D}_1 = \emptyset$

for $k = 1, \dots, K$ **do** `// episodes`

Observe initial state s_{1k} *(arbitrary)*

Estimate empirical MDP $\widehat{M}_k = (\mathcal{S}, \mathcal{A}, \widehat{p}_{hk}, \widehat{r}_{hk}, H)$ from $\mathcal{D}_k$

$$\widehat{p}_{hk}(s'|s,a) = \frac{\sum_{i=1}^{k-1} \mathbb{1}\left((s_{hi}, a_{hi}, s_{h+1,i}) = (s,a,s')\right)}{N_{hk}(s,a)}, \quad \widehat{r}_{hk}(s,a) = \frac{\sum_{i=1}^{k-1} r_{hi} \cdot \mathbb{1}\left((s_{hi}, a_{hi}) = (s,a)\right)}{N_{hk}(s,a)}$$

Planning (by backward induction) for π_{hk}

for $h = 1, \dots, H$ **do**

Execute $a_{hk} = \pi_{hk}(s_{hk})$

Observe r_{hk} and $s_{h+1,k}$

end

Add trajectory $(s_{hk}, a_{hk}, r_{hk})_{h=1}^{H}$ to $\mathcal{D}_{k+1}$

end

Measuring Uncertainty

Bounded parameter MDP [Strehl and Littman, 2008]

$$\mathcal{M}_k = \Big\{ \langle \mathcal{S}, \mathcal{A}, r_h, p_h, H \rangle : \forall h \in [H]$$

$$r_h(s,a) \in B^r_{hk}(s,a),\; p_h(\cdot|s,a) \in B^p_{hk}(s,a), \forall (s,a) \in \mathcal{S} \times \mathcal{A} \Big\}$$

Compact *confidence sets*

$$B^r_{hk}(s,a) := \left[\widehat{r}_{hk}(s,a) - \beta^r_{hk}(s,a),\; \widehat{r}_{hk}(s,a) + \beta^r_{hk}(s,a) \right]$$

$$B^p_{hk}(s,a) := \left\{ p(\cdot|s,a) \in \Delta(\mathcal{S}) :\; \|p(\cdot|s,a) - \widehat{p}_{hk}(\cdot|s,a)\|_1 \leq \; \beta^p_{hk}(s,a) \right\}$$

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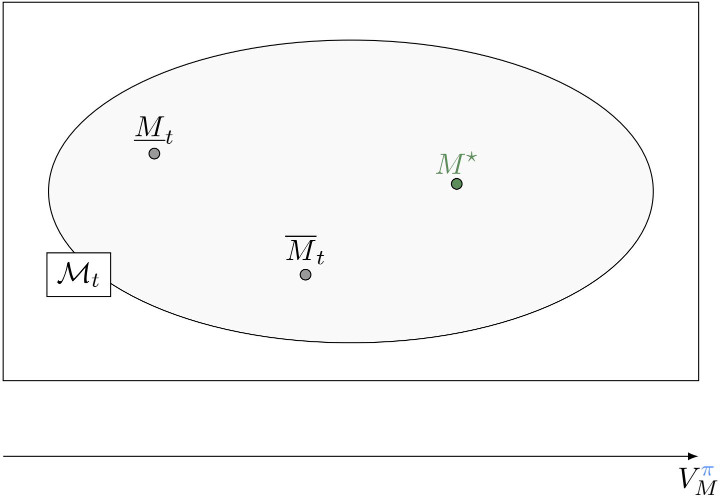
Compact *confidence sets*

$$B^r_{hk}(s,a) := \Big[\widehat{r}_{hk}(s,a) - \beta^r_{hk}(s,a),\ \widehat{r}_{hk}(s,a) + \beta^r_{hk}(s,a) \Big]$$
$$B^p_{hk}(s,a) := \Big\{ p(\cdot|s,a) \in \Delta(\mathcal{S}) :\ \|p(\cdot|s,a) - \widehat{p}_{hk}(\cdot|s,a)\|_1 \leq\ \beta^p_{hk}(s,a) \Big\}$$

Confidence bounds based on [Hoeffding, 1963] and [Weissman et al., 2003]

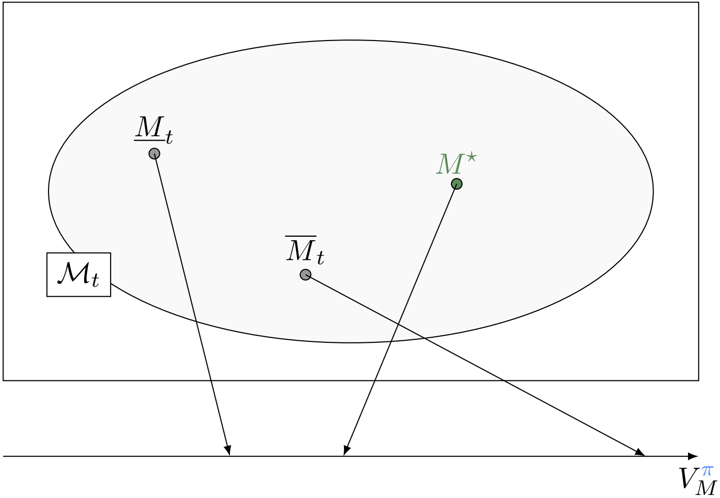
$$\beta^r_{hk}(s,a) \propto \sqrt{\frac{\log(N_{hk}(s,a)/\delta)}{N_{hk}(s,a)}}, \qquad \beta^p_{hk}(s,a) \propto \sqrt{\frac{S \log(N_{hk}(s,a)/\delta)}{N_{hk}(s,a)}}$$

Bounded Parameter MDP: Optimism



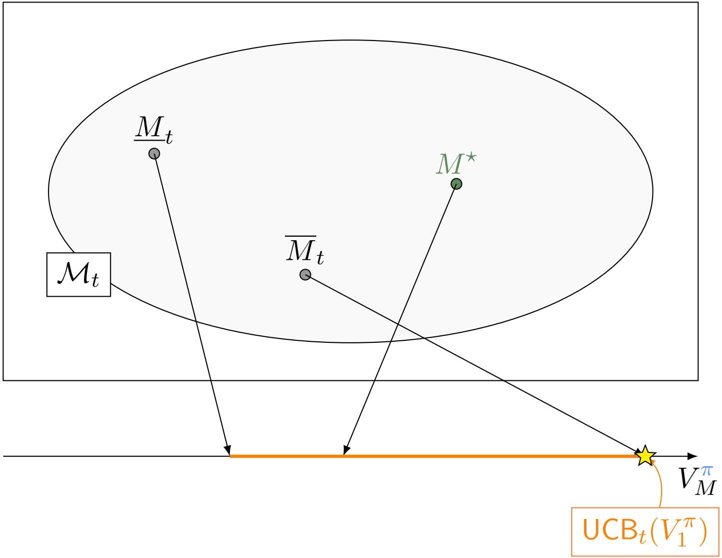
Fix a *policy* π

Bounded Parameter MDP: Optimism



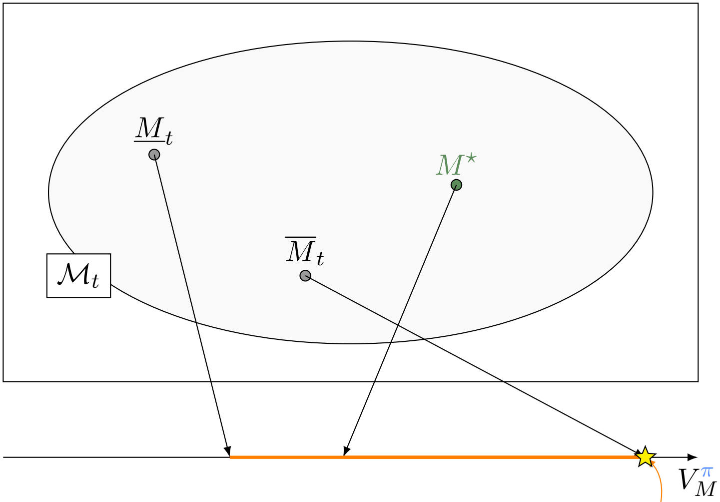
Fix a *policy* π

Bounded Parameter MDP: Optimism



Fix a *policy* π

Bounded Parameter MDP: Optimism



Fix a *policy* π

Optimism: $\mathsf{UCB}_t(V_1^\pi) = \max_{M \in \mathcal{M}_t} V_{1,M}^\pi \geq V_{1,M^\star}^\pi$ $\boxed{\mathsf{UCB}_t(V_1^\pi)}$

Extended Value Iteration

[Jaksch et al., 2010]

Input: $\mathcal{S}$, $\mathcal{A}$, B^r_{hk}, B^p_{hk}

Set $Q_{H+1}(s,a) = 0$ for all $(s,a) \in \mathcal{S} \times \mathcal{A}$

for $h = H, \dots, 1$ **do**

  for $(s,a) \in \mathcal{S} \times \mathcal{A}$ **do**

    Compute

$$Q_{hk}(s,a) = \max_{r_h \in B^r_{hk}(s,a)} r_h(s,a) + \max_{p_h \in B^p_{hk}(s,a)} \mathbb{E}_{s' \sim p_h(\cdot|s,a)} \Big[V_{h+1,k}(s') \Big]$$

$$= \widehat{r}_{hk}(s,a) + \beta^r_{hk}(s,a) + \max_{p_h \in B^p_{hk}(s,a)} \mathbb{E}_{s' \sim p_h(\cdot|s,a)} \Big[V_{h+1,k}(s') \Big]$$

$$V_{hk}(s) = \min\Big\{ H - (h-1), \max_{a \in \mathcal{A}} Q_{hk}(s,a) \Big\}$$

  end

end

return $\pi_{hk}(s) = \arg\max_{a \in \mathcal{A}} Q_{hk}(s,a)$

Extended Value Iteration

[Jaksch et al., 2010]

Input: $\mathcal{S}$, $\mathcal{A}$, B^r_{hk}, B^p_{hk}

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$$V_{hk}(s) = \min \Big\{ H - (h-1),\ \max_{a \in \mathcal{A}} Q_{hk}(s,a) \Big\}$$

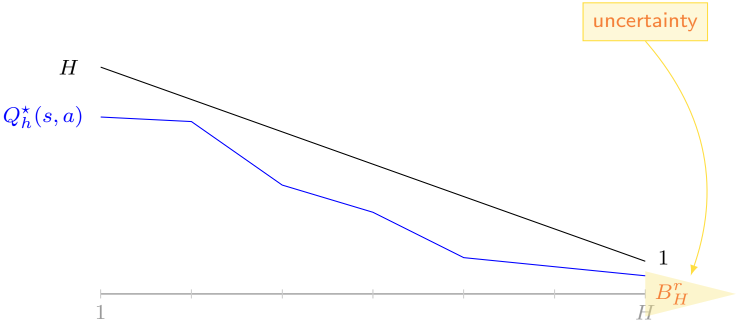
  end

end

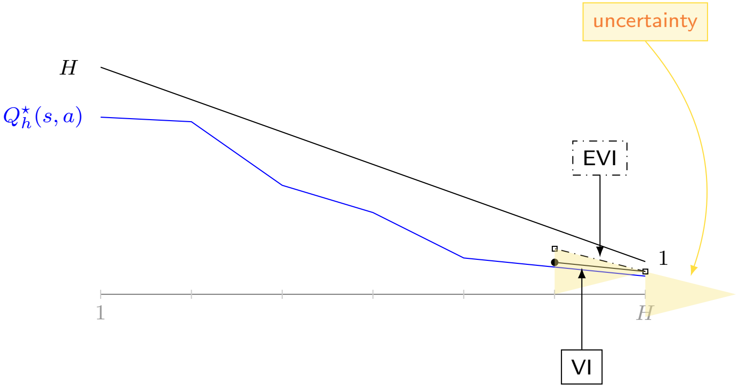
return $\pi_{hk}(s) = \arg\max_{a \in \mathcal{A}} Q_{hk}(s,a)$

Policy **executed** at episode k

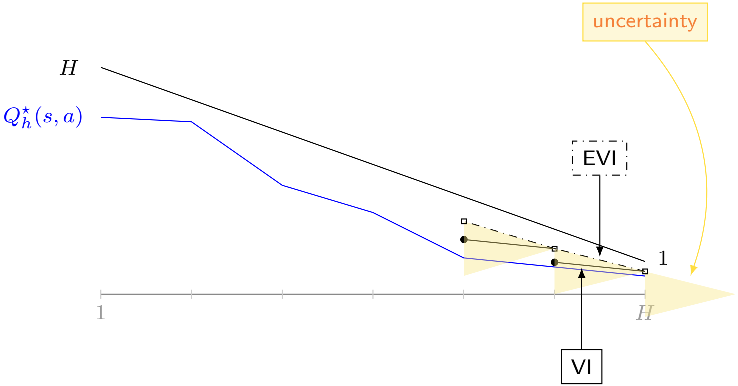
Optimism



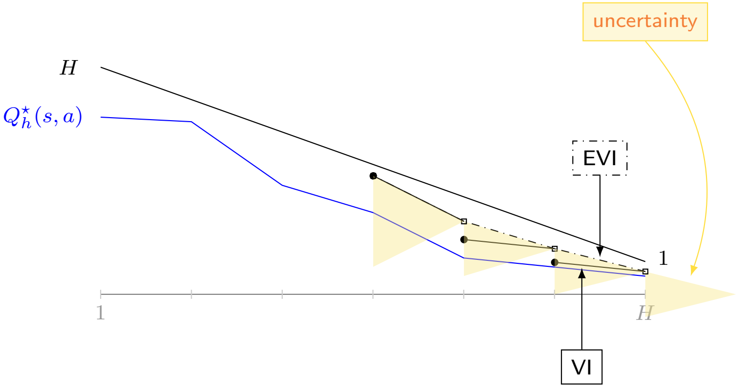
Optimism



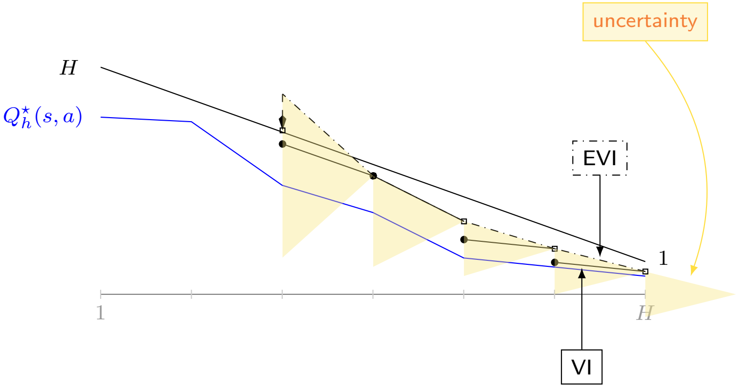
Optimism



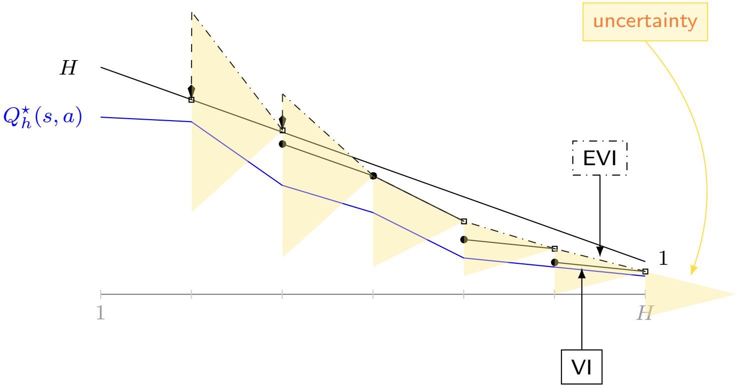
Optimism



Optimism



Optimism



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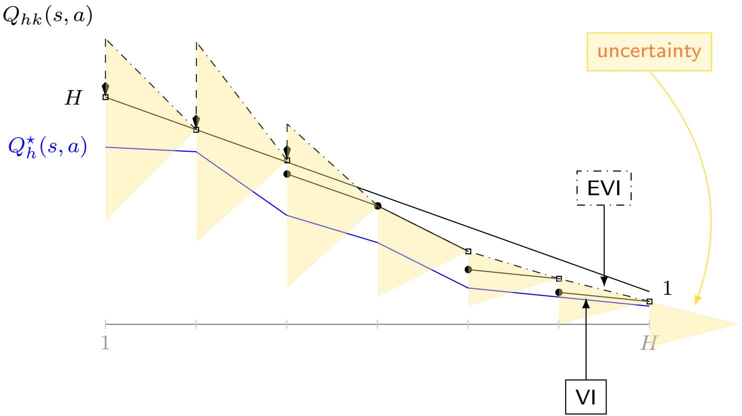
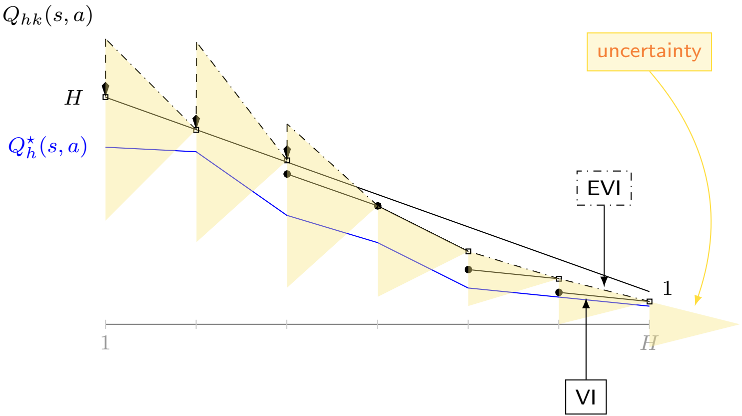


Optimism



$$\forall h \in [H], \forall (s,a), \qquad Q_{hk}(s,a) \geq Q^\star_h(s,a)$$

UCRL2-CH for Finite Horizon

Theorem (adapted from [Jaksch et al., 2010])

For any tabular MDP with stationary transitions, UCRL2 *with Chernoff-Hoeffding confidence intervals (UCRL2-CH), with high-probability, suffers a regret*

$$R(K, M^\star, \text{UCRL2-CH}) = \widetilde{\mathcal{O}}\left(HS\sqrt{AT} + H^2SA\right)$$

- Order optimal $\sqrt{AT}$
- $\sqrt{HS}$ factor worse than the lower-bound

Lower-bound: $\Omega(\sqrt{HSAT})$ ***(stationary transitions)***

Extended Value Iteration

$$Q_{hk}(s,a) = \max_{(r,p)\in B^r_{hk}(s,a)\times B^p_{hk}(s,a)} \left\{ r + p^\mathsf{T} V_{h+1,k} \right\}$$

$$= \max_{r\in B^r_{hk}(s,a)} r + \max_{p\in B^p_{hk}(s,a)} p^\mathsf{T} V_{h+1,k}$$

$$= \widehat{r}_{hk}(s,a) + \beta^r_{hk}(s,a) + \max_{p\in B^p_{hk}(s,a)} p^\mathsf{T} V_{h+1,k}$$

$$\leq \widehat{r}_{hk}(s,a) + \beta^r_{hk}(s,a) + \|p - \widehat{p}_{hk}(\cdot|s,a)\|_1 \|V_{h+1,k}\|_\infty + \widehat{p}_{hk}(\cdot|s,a)^\mathsf{T} V_{h+1,k}$$

$$\leq \widehat{r}_{hk}(s,a) + \beta^r_{hk}(s,a) + H\beta^p_{hk}(s,a) + \widehat{p}_{hk}(\cdot|s,a)^\mathsf{T} V_{h+1,k}$$

Extended Value Iteration

$$Q_{hk}(s,a) = \max_{(r,p)\in B^r_{hk}(s,a)\times B^p_{hk}(s,a)} \left\{ r + p^\mathsf{T} V_{h+1,k} \right\}$$

$$= \max_{r\in B^r_{hk}(s,a)} r + \max_{p\in B^p_{hk}(s,a)} p^\mathsf{T} V_{h+1,k}$$

$$= \widehat{r}_{hk}(s,a) + \beta^r_{hk}(s,a) + \max_{p\in B^p_{hk}(s,a)} p^\mathsf{T} V_{h+1,k}$$

$$\leq \widehat{r}_{hk}(s,a) + \beta^r_{hk}(s,a) + \|p - \widehat{p}_{hk}(\cdot|s,a)\|_1 \|V_{h+1,k}\|_\infty + \widehat{p}_{hk}(\cdot|s,a)^\mathsf{T} V_{h+1,k}$$

$$\leq \widehat{r}_{hk}(s,a) + \beta^r_{hk}(s,a) + H\beta^p_{hk}(s,a) + \widehat{p}_{hk}(\cdot|s,a)^\mathsf{T} V_{h+1,k}$$

Exploration bonus $(1 + H\sqrt{S})\beta^r_{hk}(s,a)$ for the reward

UCBVI

[Azar et al., 2017]

Replace EVI with *Exploration Bonus*

Input: $\mathcal{S}$, $\mathcal{A}$, $\cancel{B^r_{hk}, B^p_{hk}}$, $\widehat{r}_{hk}, \widehat{p}_{hk}, b_{hk}$

Set $Q_{H+1,k}(s,a) = 0$ for all $(s,a) \in \mathcal{S} \times \mathcal{A}$

for $h = H, \dots, 1$ **do**

  for $(s,a) \in \mathcal{S} \times \mathcal{A}$ **do**

    Compute

$$Q_{hk}(s,a) = \widehat{r}_{hk}(s,a) + b_{hk}(s,a) + \mathbb{E}_{s' \sim \widehat{p}_{hk}(\cdot|s,a)}\Big[V_{h+1,k}(s')\Big]$$

$$V_{hk}(s) = \min\Big\{H - (h-1), \max_{a' \in \mathcal{A}} Q_{hk}(s',a')\Big\}$$

  end

end

return $\pi_{hk}(s) = \arg\max_{a \in \mathcal{A}} Q_{hk}(s,a)$

Equivalent to value iteration on $\overline{M}_k = (\mathcal{S}, \mathcal{A}, \widehat{r}_{hk} + b_{hk}, \widehat{p}_{hk}, H)$

UCBVI: Measuring Uncertainty

- *Combine uncertainties* in rewards and transitions
- In a smart way

$$b_{hk}(s,a) = (H+1)\sqrt{\frac{\log(N_{hk}(s,a)/\delta)}{N_{hk}(s,a)}} < \beta^r_{hk} + H\beta^p_{hk}$$

UCBVI: Measuring Uncertainty

- *Combine uncertainties* in rewards and transitions
- In a smart way

$$b_{hk}(s,a) = (H+1)\sqrt{\frac{\log(N_{hk}(s,a)/\delta)}{N_{hk}(s,a)}} < \beta^r_{hk} + H\beta^p_{hk}$$

Save a $\sqrt{S}$ factor

$$\left| (p_h(\cdot|s,a) - \widehat{p}_{hk}(\cdot|s,a))^\mathsf{T} \underbrace{V^\star_h}_{\leq H} \right| \leq H \underbrace{\sqrt{\frac{\log(N_{hk}(s,a)/\delta)}{N_{hk}(s,a)}}}_{=\beta^p_{hk}/\sqrt{S}}$$

UCBVI-CH: Regret

Theorem (Thm. 1 of Azar et al. [2017])

For any tabular MDP with stationary transitions, UCBVI *with Chernoff-Hoeffding confidence intervals (UCBVI-CH), with high-probability, suffers a regret*

$$R(K, M^\star, \text{UCBVI-CH}) = \widetilde{\mathcal{O}}\left(H\sqrt{SAT} + H^2 S^2 A\right)$$

- Order optimal $\sqrt{SAT}$
- $\sqrt{H}$ factor worse than the lower-bound
- Long "warm up" phase
- If *non-stationary*, then $\widetilde{\mathcal{O}}\left(H^{3/2}\sqrt{SAT}\right)$

Lower-bound: $\Omega(\sqrt{HSAT})$ ***(stationary transitions)***

Refined Confidence Bounds

- UCRL2 with *Bernstein-Freedman bounds* (instead of Hoeffding/Weissman): *
  - see tutorial website

$$R(K, M^\star, \mathsf{UCRL2B}) = \widetilde{\mathcal{O}}\left(\sqrt{H\ \Gamma\ SAT} + H^2 S^2 A\right)$$

$$\Gamma = \max_{h,s,a} \|p_h(\cdot|s,a)\|_0 \leq S$$

Still not matching the lower-bound!

* **stationary model** $(p_1 = \ldots = p_H)$

Refined Confidence Bounds

- UCRL2 with *Bernstein-Freedman bounds* (instead of Hoeffding/Weissman): *
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$$R(K, M^\star, \text{UCRL2B}) = \widetilde{\mathcal{O}}\left(\sqrt{H\,\Gamma\,SAT} + H^2S^2A\right)$$

$$\Gamma = \max_{h,s,a} \|p_h(\cdot|s,a)\|_0 \leq S$$

  - Still not matching the lower-bound!

- UCBVI with *Bernstein-Freedman bounds*: *

$$R(K, M^\star, \text{UCBVI-BF}) = \widetilde{\mathcal{O}}\left(\sqrt{HSAT} + H^2S^2A + H\sqrt{T}\right)$$

  - Matching the Lower-Bound!
  - Long "warm up" phase

* **stationary model** $(p_1 = \ldots = p_H)$

Refined Confidence Bounds

- EULER [Zanette and Brunskill, 2019]
  keeps upper and lower bounds on $V_h^\star$

$$R(K, M^\star, \text{EULER}) = \mathcal{O}\left(\sqrt{\mathbb{Q}^\star SAT} + \sqrt{S}SAH^2(\sqrt{S} + \sqrt{H})\right)$$

Problem-dependent bound based on *environmental norm* [Maillard et al., 2014]

$$\mathbb{Q}^\star = \max_{s,a,h}\left(\mathbb{V}(r_h(s,a)) + \mathbb{V}_{x\sim p_h(\cdot|s,a)}(V_{h+1}^\star(x))\right)$$

$$\mathbb{V}_{x\sim p}(f(x)) = \mathbb{E}_{x\sim p}\left[\left(f(x) - \mathbb{E}_{y\sim p}[f(y)]\right)^2\right]$$

Can remove the dependence on H

Matching lower-bound in the worst case

UCRL2: RiverSwim

Hoeffding

$$b^r_{hk}(s,a) = r_{\max}\sqrt{\frac{L}{N}}$$

$$b^p_{hk}(s,a) = \sqrt{\frac{SL}{N}}$$

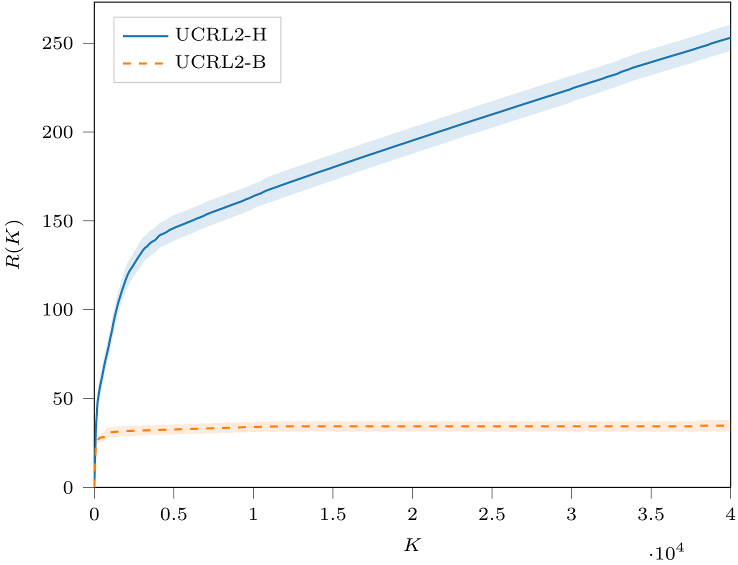
Bernstein

$$b^r_{hk}(s,a) = \sqrt{\frac{L\widehat{\mathbb{V}}(\widehat{r}_{hk})}{N}} + r_{\max}\frac{L}{N}$$

$$b^p_{hk}(s,a) = \sqrt{\frac{L\widehat{\mathbb{V}}(\widehat{p}_{hk})}{N}} + \frac{L}{N}$$

$$\widehat{\mathbb{V}}(\widehat{r}_{hk}) = \frac{1}{N}\sum_i (r_{h,i} - \widehat{r}_{hk})^2$$

is the population variance



$N = N_{hk}(s,a) \vee 1$
$L = \log(SAN/\delta)$

UCBVI: RiverSwim

Hoeffding

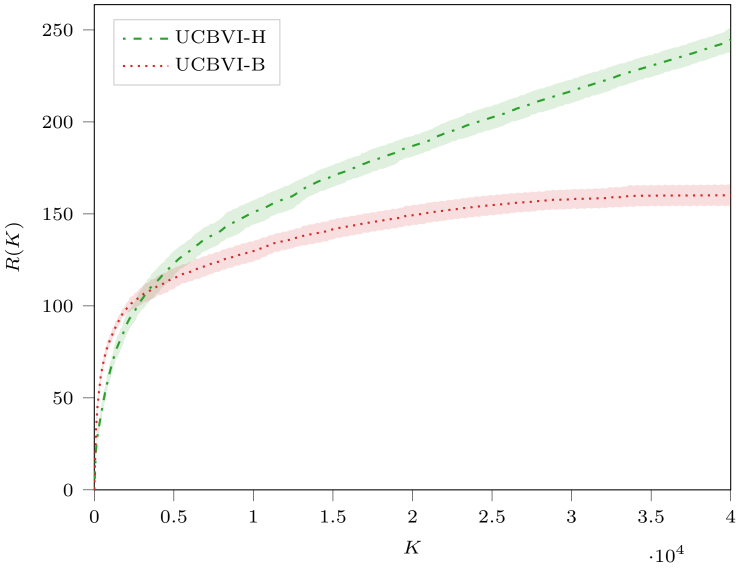
$$b_{hk}(s,a) = \frac{(H-h)L}{\sqrt{N}}$$

Bernstein

$$b_{hk}(s,a) = \sqrt{\frac{L\mathbb{V}_{\widehat{p}_{hk}}(V_{h+1,k})}{N}} + \frac{(H-h)L}{N} + \frac{(H-h)}{\sqrt{N}}$$

$\mathbb{V}_p(V) = \mathbb{E}_{x\sim p}[(V(x)-\mu)^2]$
with $\mu = \mathbb{E}_{x\sim p}[V(x)]$

$N = N_{hk}(s,a) \vee 1$
$L = \log(SAN/\delta)$



UCBVI: RiverSwim

Hoeffding

$$b_{hk}(s,a) = \frac{(H-h)L}{\sqrt{N}}$$

Bernstein

$$b_{hk}(s,a) = \sqrt{\frac{L\mathbb{V}_{\widehat{p}_{hk}}(V_{h+1,k})}{N}} + \frac{(H-h)L}{N} + \frac{(H-h)}{\sqrt{N}}$$

$\mathbb{V}_p(V) = \mathbb{E}_{x\sim p}[(V(x)-\mu)^2]$
with $\mu = \mathbb{E}_{x\sim p}[V(x)]$

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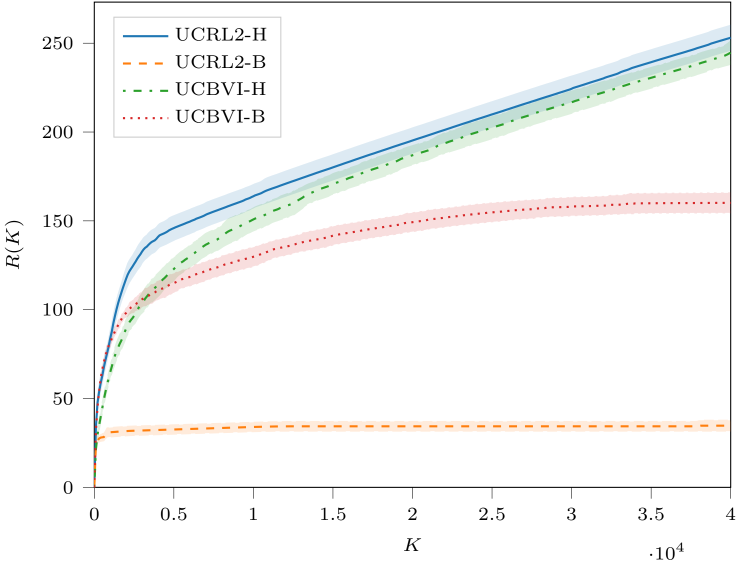
$L = \log(SAN/\delta)$



Model-Based *Advantages*

Learning efficiency

- First order optimal
- Matching lower-bound

Counterfactual reasoning

- Optimistic/Pessimistic value estimate for any π
- Usefull for inference (e.g., safety)

Model-Based *Issues*

Complexity

- Space $O(HS^2A)$

$$\textit{non-stationary model} \implies H(\underbrace{S^2A}_{\textit{transitions}} + \underbrace{SA}_{\textit{rewards}})$$

- Time $O(K \underbrace{HS^2A}_{\textit{planning by VI}})$

Model-Based *Issues*

Complexity

- Space $O(HS^2A)$

$$\text{non-stationary model} \implies H(\underbrace{S^2A}_{\text{transitions}} + \underbrace{SA}_{\text{rewards}})$$

- Time $O(K \underbrace{HS^2A}_{\text{planning by VI}})$

incremental updates

Tabular MDPs: Outline

Posterior Sampling (PS)

a.k.a. Thompson Sampling [Thompson, 1933]

Keep Bayesian posterior for the *unknown* MDP

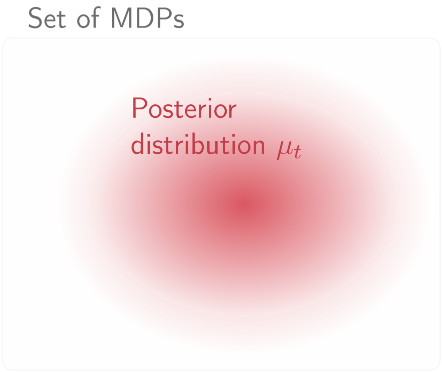
👉 A sample from the posterior is used as an estimate of the unknown MDP

Exploration

Few samples $\Longrightarrow$ uncertainty in the estimate

More samples $\Longrightarrow$ posterior concentrates on the true MDP

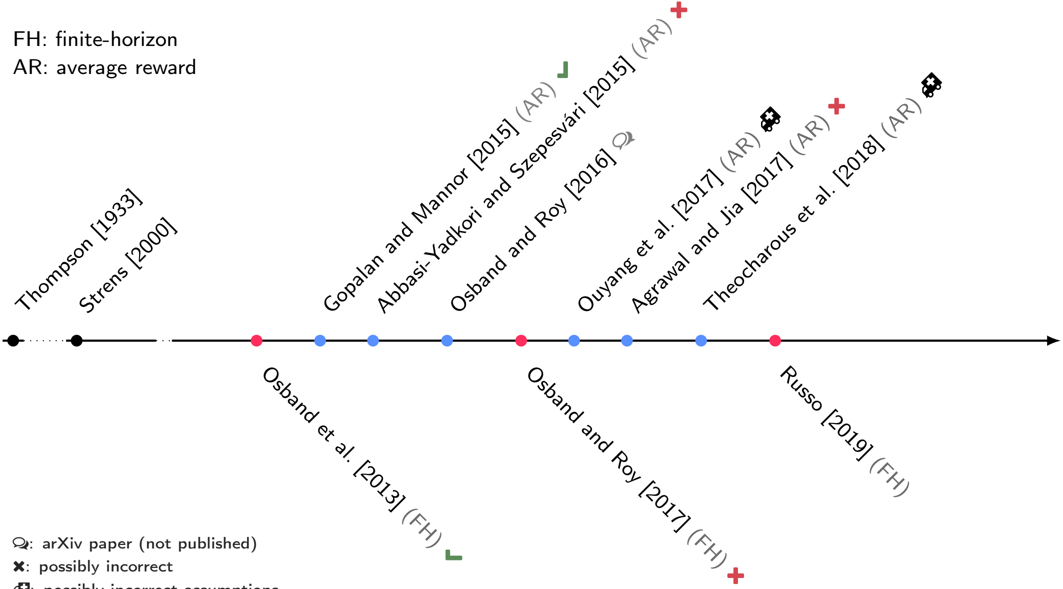
Exploitation



History: PS for Regret Minimization

Tabular MDPs

FH: finite-horizon
AR: average reward



: arXiv paper (not published)
✖: possibly incorrect
: possibly incorrect assumptions

Bayesian Regret

$$R^B(K, \mu_1, \mathfrak{A}) = \mathbb{E}_{M^\star \sim \mu_1}\left[\underbrace{\overline{R}(K, M^\star, \mathfrak{A})}_{:=\mathbb{E}\left[R(K, M^\star, \mathfrak{A})\right]} \right] = \mathbb{E}_{M^\star}\left[\sum_{k=1}^{K} V^\star_{1,M^\star}(s_{1k}) - V^{\pi_k}_{1,M^\star}(s_{1k})\right]$$

Posterior Sampling

[Osband and Roy, 2017]

Input: $\mathcal{S}$, $\mathcal{A}$, $\cancel{r_h, p_h}$, *prior* μ_1
Initialize $\mathcal{D}_1 = \emptyset$

for $k = 1, \ldots, K$ **do** `// episodes`

Observe initial state s_{1k} *(arbitrary)*

Sample $M_k \sim \mu_k(\cdot|\mathcal{D}_k)$
Compute

$$\pi_k \in \arg\max_{\pi}\{V^{\pi}_{1,M_k}\}$$

for $h = 1, \ldots, H$ **do**

Execute $a_{hk} = \pi_{hk}(s_{hk})$
Observe r_{hk} and $s_{h+1,k}$

end

Add trajectory $(s_{hk}, a_{hk}, r_{hk})_{h=1}^{H}$ to $\mathcal{D}_{k+1}$

end

Posterior Sampling

[Osband and Roy, 2017]

Input: $\mathcal{S}$, $\mathcal{A}$, $\cancel{r_h, p_h}$, *prior* μ_1
Initialize $\mathcal{D}_1 = \emptyset$

for $k = 1, \dots, K$ **do** `// episodes`
  Observe initial state s_{1k} *(arbitrary)*

  Sample $M_k \sim \mu_k(\cdot|\mathcal{D}_k)$
  Compute

$$\pi_k \in \arg\max_{\pi}\{V^{\pi}_{1,M_k}\}$$

  for $h = 1, \dots, H$ **do**
    Execute $a_{hk} = \pi_{hk}(s_{hk})$
    Observe r_{hk} and $s_{h+1,k}$
  end
  Add trajectory $(s_{hk}, a_{hk}, r_{hk})_{h=1}^{H}$ to $\mathcal{D}_{k+1}$
end

Prior distribution:

$$\forall \Theta, \quad \mathbb{P}(M^* \in \Theta) = \mu_1(\Theta)$$

Posterior distribution:

$$\forall \Theta, \quad \mathbb{P}(M^* \in \Theta | \mathcal{D}_k, \mu_1) = \mu_k(\Theta)$$

Priors

- Dirichlet (transitions)
- Beta, Normal-Gamma, etc. (rewards)

Model Update with Dirichlet Priors

⚠ *assume r is known*

$$\underbrace{\left\{\mu_t,\ (s_t, a_t, s_{t+1})\right\}}_{\sim H_t} \mapsto \mu_{t+1}$$

Model Update with Dirichlet Priors

⚠ *assume r is known*

$$\underbrace{\{\mu_t,\ (s_t, a_t, s_{t+1})\}}_{\sim H_t} \mapsto \mu_{t+1}$$

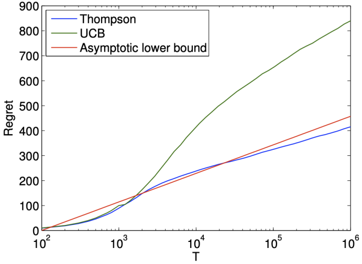
- $\mu_t(s,a) = \text{Dirichlet}(\alpha_1, \dots, \alpha_S)$ on $p(\cdot|s,a)$
- Observe $s_{t+1} \sim p(\cdot|s_t, a_t)$ (outcome of a multivariate Bernoulli) such that $s_{t+1} = i$. The Bayesian posterior is

$$\mu_{t+1}(s,a) = \text{Dirichlet}(\ \alpha_1, \dots, \alpha_i + 1, \dots, \alpha_S\ )$$

- Posterior mean vector $\widehat{p}_{t+1}(s_i|s,a) = \frac{\alpha_i}{n}$
- Variance bounded by $\frac{1}{n}$

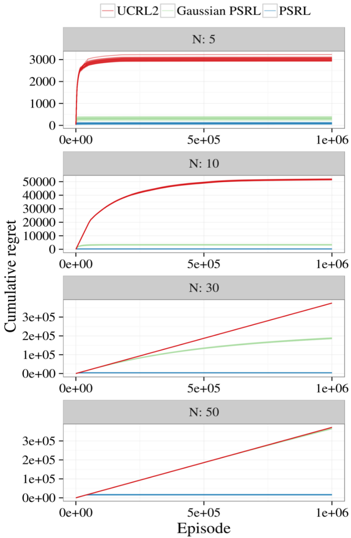
$$n = \sum_{i=1}^{S} \alpha_i$$

Posterior Sampling is Usually Better



Bandit

[Chapelle and Li, 2011]



Finite horizon RL

[Osband and Roy, 2017]

PSRL: Regret

Theorem (Osband and Roy [2017] revisited)

For any prior μ_1 with any independent Dirichlet prior over stationary transitions, the Bayesian regret of PSRL is bounded as

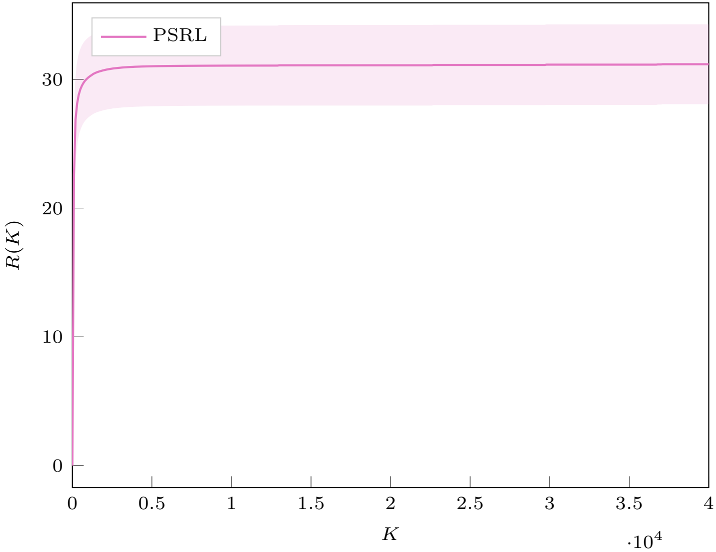
$$R^B(K, \mu_1, PSRL) = \widetilde{O}(HS\sqrt{AT})$$

- Order optimal $\sqrt{AT}$
- $\sqrt{HS}$ factor suboptimal

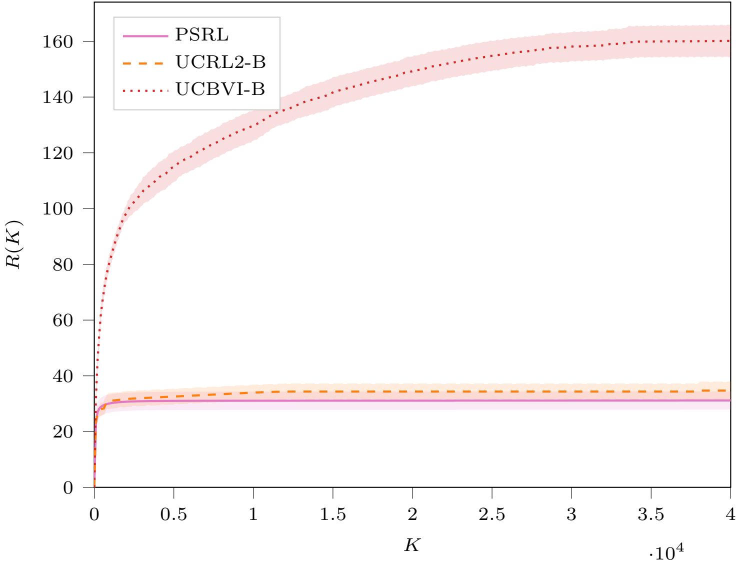
Lower-bound: $\Omega(\sqrt{HSAT})$ ***(stationary transitions)***

* in [Osband and Roy, 2017] is $\widetilde{O}(H\sqrt{SAT})$ for stationary MDPs
but there is a mistake in Lem. 3 (see [Qian et al., 2020])

PSRL: RiverSwim



PSRL: RiverSwim



Tabular MDPs: Outline

Model-Based *Issues*

Complexity

- Space $O(HS^2A)$

nonstationary model $\Longrightarrow H(\underbrace{S^2A}_{\textit{transitions}} + \underbrace{SA}_{\textit{rewards}})$

- Time $O(K \underbrace{HS^2A}_{\textit{planning by VI}})$

Solutions

1. Time complexity: incremental planning (e.g.,Opt-RTDP)

Model-Based *Issues*

Complexity

- Space $O(HS^2A)$

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1. Time complexity: incremental planning (e.g.,Opt-RTDP)
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Model-Based *Issues*

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Solutions

1. Time complexity: incremental planning (e.g.,Opt-RTDP)
2. Space complexity: avoid to estimate rewards and transitions

Optimistic Q-learning (Opt-QL)

Space: $\mathcal{O}(HSA)$ Time: $\mathcal{O}(HAK)$

Optimistic Q-learning

Input: $\mathcal{S}$, $\mathcal{A}$, $\cancel{r_h, p_h}$

Initialize $Q_h(s,a) = H - (h-1)$ and $N_h(s,a) = 0$ for all $(s,a) \in \mathcal{S} \times \mathcal{A}$ and $h = [H]$

for $k = 1, \dots, K$ **do** `// episodes`

  Observe initial state s_{1k} *(arbitrary)*

  for $h = 1, \dots, H$ **do**

    Execute $a_{hk} = \pi_{hk}(s_{hk}) = \arg\max_a \widehat{Q}_h(s_{hk}, a)$

    Observe r_{hk} and $s_{h+1,k}$

    Set $N_h(s_{hk}, a_{hk}) = N_h(s_{hk}, a_{hk}) + 1$

    Update

$$Q_h(s_{hk}, a_{hk}) = (1-\alpha_t) Q_h(s_{hk}, a_{hk}) + \alpha_t \left(r_{hk} + \widehat{V}_{h+1}(s_{h+1,k}) + b_t \right)$$

Upper-Confidence Bound

    Set $\widehat{V}_h(s_{hk}) = \min \left\{ H - (h-1), \max_{a \in \mathcal{A}} Q_h(s_{hk}, a) \right\}$

  end

end

Step size and bonus for Opt-Qlearning

Let $t = N_{hk}(s,a)$

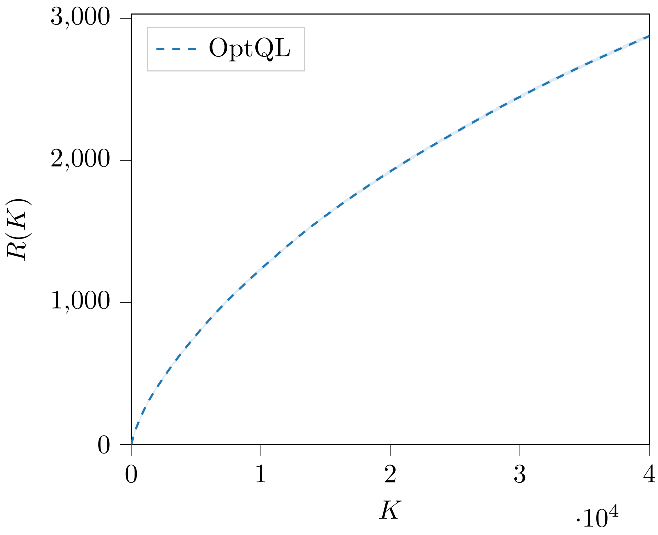
$$\alpha_t = \frac{H+1}{H+t}$$

Bonus

$$\left| \sum_{i=1}^{t} \alpha_t^i \Big(V_{h+1}^{\star}(s_{h+1,k_i}) - \mathbb{E}_{s'|s,a}[V_{h+1}^{\star}(s')] \Big) \right| \le \underbrace{c\sqrt{\frac{H^3 \log(SAT/\delta)}{t}}}_{:= b_t}$$

Opt-Qlearning: Example

Not so good!



Thank you!

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