

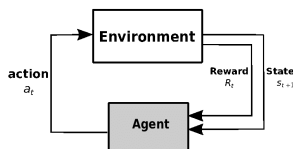
# On the complexity of learning good policies with and without rewards

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Mathematics of Online Decision Making, Simons Institute  
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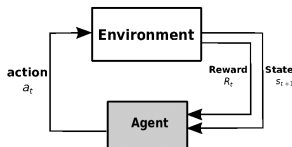
**RL setup:** an agent interacts with an environment (MDP)



**Several Performance measures:**

- 1 the agent should *adopt* a good behavior
  - maximize the total rewards (*regret minimization*)
  - use as much as possible an  $\epsilon$ -optimal policy (*PAC-MDP*)
- 2 the agent should *learn* a good behavior
  - learn an optimal policy for a **given reward function**
  - learn the dynamics so that to be robust to find the optimal policy for **any reward function**

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two Pure Exploration problems

**Episodic MDP:** horizon  $H$  and MDP  $(\mathcal{S}, \mathcal{A}, P, r)$  for

- a state space  $\mathcal{S}$  of size  $S < \infty$
- an action space  $\mathcal{A}$  of size  $A < \infty$
- a transition kernel  $P = (p_h(s'|s, a))_{\substack{(s,a,s') \in \mathcal{S} \times \mathcal{A} \times \mathcal{S} \\ h \in [H]}}$
- a reward function  $r = (r_h(s, a))_{\substack{(s,a) \in \mathcal{S} \times \mathcal{A} \\ h \in [H]}}$

Value of a policy  $\pi = (\pi_h)_{h=1}^H$ ,  $\pi_h : \mathcal{S} \rightarrow \mathcal{A}$ :

$$V_h^\pi(s; r) \triangleq \mathbb{E}^\pi \left[ \sum_{\ell=h}^H r_\ell(s_\ell, \pi_\ell(s_\ell)) \middle| s_{\ell+1} \sim p_\ell(\cdot | s_\ell, \pi_\ell(s_\ell)), s_h = s \right]$$

**Optimal policy:**  $\pi_r^*$  such that  $V_h^{\pi_r^*}(s; r) \geq V_h^\pi(s; r)$  for all  $\pi, s, h$ .

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# Setting: Episodic Markov Decision Process

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Q-value of a **policy**  $\pi = (\pi_h)_{h=1}^H$ ,  $\pi_h : \mathcal{S} \rightarrow \mathcal{A}$ :

$$Q_h^\pi(s, a; r) \triangleq \mathbb{E}^\pi \left[ r_h(s, a) + \sum_{\ell=h+1}^H r_\ell(s_\ell, \pi_\ell(s_\ell)) \mid \substack{s_h=s, a_h=a \\ s_{\ell+1} \sim p_\ell(\cdot | s_\ell, \pi_\ell(s_\ell))} \right]$$

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- a reward function  $r = (r_h(s, a))_{\substack{(s,a) \in \mathcal{S} \times \mathcal{A} \\ h \in [H]}}$  (**step-dependent**)

Q-value of a **policy**  $\pi = (\pi_h)_{h=1}^H$ ,  $\pi_h : \mathcal{S} \rightarrow \mathcal{A}$ :

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- 1 The BPI and RFE objectives
- 2 Reward-Free UCRL
- 3 BPI Algorithms



# Online episodic algorithm

Collect data from the MDP by generating **trajectories** (episodes)  
 $\neq$  generative model

In each episode  $t = 1, 2, \dots$ , the agent

- selects an **exploration policy**  $\pi^t$
- generates an episode under this policy

$$(s_1^t, a_1^t, s_2^t, a_2^t, \dots, s_H^t, a_H^t)$$

where  $s_1^t \sim \rho$ ,  $a_h^t = \pi_h^t(s_h^t)$  and  $s_{h+1}^t \sim p_h(\cdot | s_h^t, a_h^t)$

- can decide to **stop exploration**
- if decides to stop, **outputs a prediction**

→ three **data-dependent** components

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where  $\mathbf{s}_1^t = \mathbf{s}_1$ ,  $a_h^t = \pi_h^t(s_h^t)$  and  $s_{h+1}^t \sim p_h(\cdot | s_h^t, a_h^t)$

- can decide to **stop exploration**
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→ three **data-dependent** components

# Best Policy Identification (BPI)

→ Learn the optimal policy for a **known reward function**  $r$

[Fiechter, 1994]

## BPI algorithm

- **exploration policy**  $\pi^t$ : may depend on past data  $\mathcal{D}_{t-1}$  and  $r$

$$\mathcal{D}_t = \mathcal{D}_{t-1} \cup \{(s_1^t, a_1^t, s_2^t, a_2^t, \dots, s_H^t, a_H^t)\}$$

- **stopping rule**  $\tau$ : stopping time w.r.t.  $(\mathcal{D}_t)_{t \in \mathbb{N}}$   
(can depend on  $r$ )
- **prediction**  $\hat{\pi}$ : a **policy** that may depend on  $\mathcal{D}_\tau$  and  $r$

## $(\varepsilon, \delta)$ -PAC algorithm for Best Policy Identification

$$\mathbb{P} \left( V_1^*(\mathbf{s}_1; r) - V_1^{\hat{\pi}}(\mathbf{s}_1; r) \leq \varepsilon \right) \geq 1 - \delta$$

**Wanted:**  $(\varepsilon, \delta)$ -PAC algorithm with a small sample complexity  $\tau$

# Reward-Free Exploration (RFE)

→ Learn the optimal policy for **any** reward function  $r$

[Jin et al., 2020]

## RFE algorithm

- exploration policy  $\pi^t$ : may depend on past data  $\mathcal{D}_{t-1}$

$$\mathcal{D}_t = \mathcal{D}_{t-1} \cup \{(s_1^t, a_1^t, s_2^t, a_2^t, \dots, s_H^t, a_H^t)\}$$

- stopping rule  $\tau$ : stopping time w.r.t.  $(\mathcal{D}_t)_{t \in \mathbb{N}}$
- prediction  $\hat{P} = (\hat{p}_h(\cdot | s, a))_{h,s,a}$ : a **transition kernel** that may depend on  $\mathcal{D}_\tau$

$\hat{\pi}_r^*$ : optimal policy in the MDP  $(\hat{P}, r)$

## $(\varepsilon, \delta)$ -PAC algorithm for Reward-Free Exploration

$$\mathbb{P} \left( \text{for all reward function } r, V_1^*(\mathbf{s}_1; r) - V_1^{\hat{\pi}_r^*}(\mathbf{s}_1; r) \leq \varepsilon \right) \geq 1 - \delta$$

**Wanted:**  $(\varepsilon, \delta)$ -PAC algorithm with a small sample complexity  $\tau$

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# A model-based algorithm

Based on the available data  $\mathcal{D}_t$ , builds estimates of the transition probabilities  $p_h(s, a)$

→ estimates of the Q-values  $Q_h^\pi(s, a; r)$

**Number of visits:**

$$n_h^t(s, a) = \sum_{k=1}^t \mathbb{1}_{\{(s_h^k, a_h^k) = (s, a)\}} \quad n_h^t(s, a, s') = \sum_{k=1}^t \mathbb{1}_{\{(s_h^k, a_h^k, s_{h+1}^k) = (s, a, s')\}}$$

**Empirical transitions:**  $\hat{P}^t = (\hat{p}_h^t(s'|s, a))_{h,s,a,s'}$

$$\hat{p}_h^t(s'|s, a) = \begin{cases} \frac{n_h^t(s, a, s')}{n_h^t(s, a)} & \text{if } n_h^t(s, a) > 0 \\ \frac{1}{S} & \text{else} \end{cases}$$

**Empirical values:**

- $\hat{V}_h^{t,\pi}(s; r)$  values in the empirical MDP  $(\mathcal{S}, \mathcal{A}, \hat{P}^t, r)$
- $\hat{Q}_h^{t,\pi}(s; r)$  Q-values in the empirical MDP  $(\mathcal{S}, \mathcal{A}, \hat{P}^t, r)$

## Central observation

A sufficient condition to be  $(\varepsilon, \delta)$ -PAC is to have **accurate estimates of the value function for all  $\pi$  and  $r$** :

$$\mathbb{P} \left( \forall \pi, \forall r, |\hat{V}_1^{\tau, \pi}(s_1; r) - V_1^{\pi}(s_1; r)| \leq \varepsilon/2 \right) \geq 1 - \delta.$$

## RF-UCRL:

- builds upper bounds on the errors

$$\hat{e}_h^{t, \pi}(s, a; r) := |\hat{Q}_h^{t, \pi}(s, a; r) - Q_h^{\pi}(s, a; r)|$$

... that are **independent of  $\pi$  and  $r$** !

- greedily reduces the upper bounds

$$\hat{e}_h^{t,\pi}(s, a; r) := |\hat{Q}_h^{t,\pi}(s, a; r) - Q_h^\pi(s, a; r)|$$

We define inductively  $\bar{E}_{H+1}^t(s, a) = 0$  and

$$\bar{E}_h^t(s, a) = \min \left[ (H-h); (H-h) \sqrt{\frac{2\beta(n_h^t(s, a), \delta)}{n_h^t(s, a)}} + \sum_{s'} \hat{p}_h^t(s'|s, a) \max_b \bar{E}_{h+1}^t(s', b) \right]$$

for some **threshold function**  $\beta(n, \delta)$ .

→ like in UCRL [Jaksch et al. 10], this construction relies on **confidence regions on the transitions probabilities**

## Upper Bound Property

On the event

$$\mathcal{E} = \left\{ \forall t \in \mathbb{N}, \forall h \in [H], \forall (s, a), \text{KL}(\hat{p}_h^t(\cdot|s, a), p_h(\cdot|s, a)) \leq \frac{\beta(n_h^t(s, a), \delta)}{n_h^t(s, a)} \right\},$$

for all  $\pi$  and  $r$ , for all  $h, s, a$ ,  $\hat{e}_h^{t,\pi}(s, a; r) \leq \bar{E}_h^t(s, a)$ .



$$\hat{e}_h^{t,\pi}(s, a; r) := |\hat{Q}_h^{t,\pi}(s, a; r) - Q_h^\pi(s, a; r)|$$

A simple consequence of **Bellman equations**:

$$\hat{Q}_h^{t,\pi}(s, a; r) = r_h(s, a) + \sum_{s'} \hat{p}_h^t(s'|s, a) \hat{Q}_{h+1}^{t,\pi}(s', \pi(s'); r)$$

$$\text{and } Q_h^\pi(s, a; r) = r_h(s, a) + \sum_{s'} p_h(s'|s, a) Q_{h+1}^\pi(s', \pi(s'); r).$$

**Error decomposition:**

$$\begin{aligned} \hat{e}_h^{t,\pi}(s, a; r) &\leq \sum_{s'} |\hat{p}_h^t(s'|s, a) - p_h(s'|s, a)| Q_{h+1}^\pi(s', \pi(s'); r) \\ &\quad + \sum_{s'} \hat{p}_h^t(s'|s, a) \left| \hat{Q}_{h+1}^{t,\pi}(s', \pi(s'); r) - Q_{h+1}^\pi(s', \pi(s'); r) \right| \\ &\leq (H-h) \underbrace{\|\hat{p}_h^t(\cdot|s, a) - p_h(\cdot|s, a)\|_1}_{\leq \sqrt{\frac{2\beta(n_h^t(s,a), \delta)}{n_h^t(s,a)}} \text{ (Pinsker} + \mathcal{E})} + \sum_{s'} \hat{p}_h^t(s'|s, a) \underbrace{\hat{e}_{h+1}^{t,\pi}(s', \pi(s'); r)}_{\leq \max_b \bar{E}_{h+1}^t(s', b) \text{ (induction)}}. \end{aligned}$$

$$\bar{E}_h^t(s, a) = \min \left[ (H-h); (H-h) \sqrt{\frac{2\beta(n_h^t(s, a), \delta)}{n_h^t(s, a)}} + \sum_{s'} \hat{p}_h^t(s'|s, a) \max_b \bar{E}_{h+1}^t(s', b) \right]$$

## Reward-Free UCRL

- **exploration policy:**  $\pi^{t+1}$  is the greedy policy wrt  $\bar{E}^t(s, a)$ :

$$\forall s \in \mathcal{S}, \forall h \in [H], \quad \pi_h^{t+1}(s) = \arg \max_{a \in \mathcal{A}} \bar{E}_h^t(s, a).$$

- **stopping rule:**  $\tau = \inf \{ t \in \mathbb{N} : \bar{E}_1^t(s_1, \pi_1^{t+1}(s_1)) \leq \varepsilon/2 \}$
- **prediction:** transition kernel  $\hat{P}^\tau$

→ very close to an old algorithm by [Fiechter, 1994]  
... originally proposed for Best Policy Identification!

## Theorem [Kaufmann et al. 2020]

With  $\beta(n, \delta) \simeq \log\left(\frac{1}{\delta}\right) + S \log(n)$ , RF-UCRL is  $(\varepsilon, \delta)$ -PAC for Reward-Free Exploration and satisfies, w.p.  $1 - \delta$ ,

$$\tau^{\text{RF-UCRL}} = \tilde{O}\left(\frac{H^4 SA}{\varepsilon^2} \left[\log\left(\frac{1}{\delta}\right) + S\right]\right)$$

→ improves over the state-of-the art bound of [Jin et al. 20]

$$\tau^{\text{RF-RL-Explore}} = \tilde{O}\left(\frac{S^2 AH^5}{\varepsilon^2} \log\left(\frac{1}{\delta}\right) + \frac{S^4 AH^7}{\varepsilon^2} \log^3\left(\frac{1}{\delta}\right)\right)$$

→ RF-UCRL is a natural *adaptive* approach to RFE  
... with a simple sample complexity analysis

- 1 The BPI and RFE objectives
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**First observation:** RF-UCRL is also  $(\varepsilon, \delta)$ -PAC for Best Policy Identification with the updated

- **prediction rule:**  $\hat{\pi}$ , the optimal policy if the MDP  $(\mathcal{S}, \mathcal{A}, \hat{P}^\tau, r)$

$$\tau^{\text{RF-UCRL}} = \tilde{O} \left( \frac{H^4 SA}{\varepsilon^2} \left[ \log \left( \frac{1}{\delta} \right) + S \right] \right) \text{ w.h.p.}$$

## Lower bound for BPI [Domingues et al. 2020]

For every  $(\varepsilon, \delta)$ -PAC BPI algorithm, there exists an MDP (with stage-dependent transitions) such that

$$\mathbb{E}[\tau] \geq c_1 \frac{H^3 SA}{\varepsilon^2} \log \left( \frac{1}{\delta} \right),$$

where  $c_1$  is an absolute constant.

→ some room for improvement...

# Building on Regret Minimizing algorithm

The UCB-VI algorithm of [Azar et al. 17] satisfies

$$\mathbb{E} \left[ \sum_{t=1}^T \left( V_1^*(s_1; r) - V_1^{\pi^t}(s_1; r) \right) \right] \leq C \left( \sqrt{H^3 SAT} \right)$$

(minimax optimal **cumulative regret**)

From UCB-VI to a BPI algorithm [Jin et al. 18]

- **exploration policy:** that of the UCB-VI algorithm
- **stopping rule:**  $T = \frac{C^2 SAH^3}{\epsilon^2 \delta^2}$   
( $\tau = T$  is fixed in advance)
- **prediction rule:**  $\hat{\pi}$  is **one of the policies used by UCB-VI**, chosen uniformly at random:  $\hat{\pi} = \hat{\pi}^n \quad n \sim \mathcal{U}(\{1, \dots, T\})$

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→ optimal dependency in  $\varepsilon$ , **sub-optimal dependency in  $\delta$**

A more *adaptive* conversion from a regret minimizer:

→ associate a **data-dependent stopping rule** to a UCRL algorithm

## BPI-UCRL

- **exploration policy:**  $\pi^{t+1}(s) = \arg \max_{a \in \mathcal{A}} \bar{Q}_h^t(s, a; r)$
- **stopping rule:**  $\tau = \inf \{ t \in \mathbb{N} : \bar{V}_1^t(s_1; r) - \underline{V}_1^t(s_1; r) \leq \epsilon \}$
- **prediction rule:**  $\hat{\pi}_h(s) = \arg \max_{a \in \mathcal{A}} \underline{Q}_h^r(s, a; r)$

where we have built upper and lower confidence bounds

$$\begin{aligned} \underline{Q}_h^t(s, a; r) &\leq Q_h^*(s, a; r) \leq \bar{Q}_h^t(s, a; r) \\ \underline{V}_h^t(s; r) &\leq V_h^*(s; r) \leq \bar{V}_h^t(s; r). \end{aligned}$$



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## Theorem [Kaufmann et al. 2020]

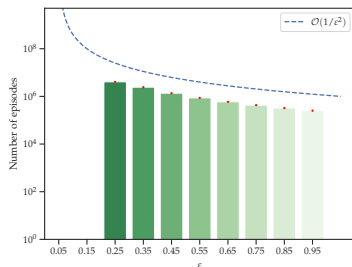
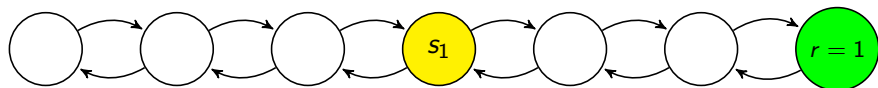
With  $\beta(n, \delta) \simeq \log\left(\frac{1}{\delta}\right) + S \log(n)$ , BPI-UCRL is  $(\varepsilon, \delta)$ -PAC for Best Policy Identification and satisfies, w.p.  $\geq 1 - \delta$ ,

$$\tau^{\text{BPI-UCRL}} = \tilde{O}\left(\frac{H^4 SA}{\varepsilon^2} \left[\log\left(\frac{1}{\delta}\right) + S\right]\right)$$

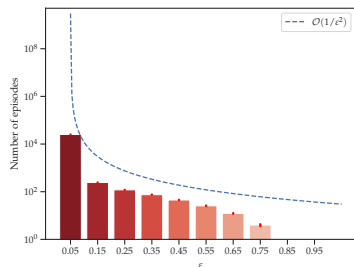
- similar sample complexity bound as RF-UCRL (obtained with a similar proof)
- yet the practical story is different...

# RF-UCRL versus BPI-UCRL

Double Chain MDP with  $L = 31, H = 20$ :



$\mathbb{E}[\tau | \tau < 10^8]$  for RF-UCRL



$\mathbb{E}[\tau | \tau < 10^6]$  for BPI-UCRL

→ BPI-UCRL has a much smaller sample complexity!

- The sample complexity of...

	Upper Bound	Lower Bound
<b>BPI</b>	$\frac{H^4 SA}{\epsilon^2} \left[ \log \left( \frac{1}{\delta} \right) + S \right]$ BPI-UCRL / RF-UCRL	$\frac{H^3 SA}{\epsilon^2} \log \left( \frac{1}{\delta} \right)$ [Darwiche Domingues et al. 2020]
<b>RFE</b>	$\frac{H^4 SA}{\epsilon^2} \left[ \log \left( \frac{1}{\delta} \right) + S \right]$ RF-UCRL	$\frac{H^3 SA}{\epsilon^2} \left[ \log \left( \frac{1}{\delta} \right) + S \right]$ + [Jin et al. 2020]

**Follow-up work:** shaving the remaining  $H$  factor for BPI and RFE for more sophisticated algorithms using Bernstein bonuses

- BPI-UCBVI for Best Policy Identification
- RF-Express for Reward Free Exploration

Ménard et al. 2020, *Fast active learning for pure exploration in reinforcement learning*, arXiv:2007.13442

- The sample complexity of...

	Upper Bound	Lower Bound
<b>BPI</b>	$\frac{H^4 SA}{\epsilon^2} \left[ \log \left( \frac{1}{\delta} \right) + S \right]$ BPI-UCRL / RF-UCRL	$\frac{H^3 SA}{\epsilon^2} \log \left( \frac{1}{\delta} \right)$ [Darwiche Domingues et al. 2020]
<b>RFE</b>	$\frac{H^4 SA}{\epsilon^2} \left[ \log \left( \frac{1}{\delta} \right) + S \right]$ RF-UCRL	$\frac{H^3 SA}{\epsilon^2} \left[ \log \left( \frac{1}{\delta} \right) + S \right]$ + [Jin et al. 2020]

**Future work:** beyond worst-case guarantees

- problem-dependent sample complexity for the simpler *planning* problem (= find the best first action)  
[Jonsson et al., 2020]
- problem-dependent regret guarantees  
[Simchowitz and Jamieson, 2019]

... how about BPI?

- Azar et al., *Minimax Regret Bounds for Reinforcement Learning*, ICML 2017
- Darwiche Domingues et al., *Episodic Reinforcement Learning in Finite MDPs: Minimax Lower Bounds Revisited*, arXiv:2010.03531, 2020
- Jaksch et al., *Near-optimal Regret Bounds for Reinforcement Learning*, JMLR 2010
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- Jin et al., *Is Q-Learning Provably Efficient?*, NeurIPS 2018
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- Fiechter, *Efficient Reinforcement Learning*, COLT 1994
- Kaufmann et al., *Adaptive Reward-Free Exploration*, arXiv:2006.06294, 2020
- Ménard et al., *Fast active learning for pure exploration in reinforcement learning*, arXiv:2007.13442, 2020
- Simchowitz and Jamieson, *Non-Asymptotic Gap-Dependent Regret Bounds for Tabular MDPs*, NeurIPS 2019