Exploration in Reinforcement Learning (theory)

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Instructions

- The deadline is **January 20, 2023. 23h59**

- By doing this homework you agree to the *late day policy, collaboration and misconduct rules* reported on Piazza.

- **Mysterious or unsupported answers will not receive full credit**. A correct answer, unsupported by calculations, explanation, or algebraic work will receive no credit; an incorrect answer supported by substantially correct calculations and explanations might still receive partial credit.

- Answers should be provided in **English**.

1   Best Arm Identification

In best arm identification (BAI), the goal is to identify the best arm in as few samples as possible. We will focus on the fixed-confidence setting where the goal is to identify the best arm with high probability $1 - \delta$ in as few samples as possible. A player is given k arms with expected reward μ_i. At each timestep t, the player selects an arm to pull (I_t), and they observe some reward ($X_{I_t,t}$) for that sample. At any timestep, once the player is confident that they have identified the best arm, they may decide to stop.

δ-correctness and fixed-confidence objective.   Denote by τ_δ the stopping time associated to the stopping rule, by $i^\star$ the best arm and by $\widehat{i}$ an estimate of the best arm. An algorithm is δ-correct if it predicts the correct answer with probability at least $1 - \delta$. Formally, if $\mathbb{P}_{\mu_1,\ldots,\mu_k}(\widehat{i} \neq i^\star) \leq \delta$ and $\tau_\delta < \infty$ almost surely for any $\mu_1,\ldots,\mu_k$. Our goal is to find a δ-correct algorithm that minimizes the sample complexity, that is, $\mathbb{E}[\tau_\delta]$ the expected number of sample needed to predict an answer. Assume that the best arm $i^\star$ is *unique* (i.e., there exists only one arm with maximum mean reward).

Notation

- I_t: the arm chosen at round t.

- $X_{i,t} \in [0,1]$: reward observed for arm i at round t.

- μ_i: the expected reward of arm i.

- $\mu^\star = \max_i \mu_i$.

- $\Delta_i = \mu^\star - \mu_i$: suboptimality gap.

Consider the following algorithm
The algorithm maintains an active set S and an estimate of the empirical reward of each arm $\widehat{\mu}_{i,t} = \frac{1}{t}\sum_{j=1}^{t} X_{i,j}$.

- Compute the function $U(t,\delta)$ that satisfy the any-time confidence bound. Let

$$\mathcal{E} = \bigcup_{i=1}^{k} \bigcup_{t=1}^{\infty} \{|\widehat{\mu}_{i,t} - \mu_i| > U(t,\delta')\}.$$

Input: k arms, confidence δ
$S = \{1, \ldots, k\}$
for $t = 1, \ldots$ **do**
 Pull **all** arms in S
 $S = S \setminus \left\{ i \in S \ : \ \exists j \in S, \ \widehat{\mu}_{j,t} - U(t, \delta') \geq \widehat{\mu}_{i,t} + U(t, \delta') \right\}$
 if $|S| = 1$ **then**
  STOP
  return S
 end
end

Using Hoeffding's inequality and union bounds, shows that $\mathbb{P}(\mathcal{E}) \leq \delta$ for a particular choice of δ'. This is called "bad event" since it means that the confidence intervals do not hold.

- Show that with probability at least $1 - \delta$, the optimal arm $i^\star = \arg\max_i\{\mu_i\}$ remains in the active set S. Use your definition of δ' and start from the condition for arm elimination. From this, use the definition of $\neg\mathcal{E}$.

- Under event $\neg\mathcal{E}$, show that an arm $i \neq i^\star$ will be removed from the active set when $\Delta_i \geq C_1 U(t, \delta')$ for some constant $C_1 \in \mathbb{N}$. Compute the time required to have such condition for each non-optimal arm. Use the condition of arm elimination applied to arm $i^\star$.[1]

- Compute a bound on the sample complexity (after how many *pulls* the algorithm stops) for identifying the optimal arm w.p. $1 - \delta$.

- We assumed that the optimal arm $i^\star$ is unique. Would the algorithm still work if there exist multiple best arms? Why?

Note that also a variations of UCB are effective in pure exploration.

2 Regret Minimization in RL

Consider a finite-horizon MDP $M^\star = (S, A, p_h, r_h)$ with stage-dependent transitions and rewards. Assume rewards are bounded in $[0, 1]$. We want to prove a regret upper-bound for UCBVI. We will aim for the suboptimal regret bound ($T = KH$)

$$R(T) = \sum_{k=1}^{K} V_1^\star(s_{1,k}) - V_1^{\pi_k}(s_{1,k}) = \widetilde{O}(H^2 S \sqrt{AK})$$

Define the set of plausible MDPs as

$$\mathcal{M}_k = \{M = (S, A, p_{h,k}, r_{h,k}) \ : \ r_{h,k}(s,a) \in \beta_{h,k}^r(s,a), p_{h,k}(\cdot|s,a) \in \beta_{h,k}^p(s,a)\}$$

Confidence intervals can be anytime or not.

- Define the event $\mathcal{E} = \{\forall k, M^\star \in \mathcal{M}_k\}$. Prove that $\mathbb{P}(\neg\mathcal{E}) \leq \delta/2$. First step, construct a confidence interval for rewards and transitions for each (s, a) using Hoeffding and Weissmain inequality (see appendix), respectively. So, we want that

$$\mathbb{P}\left(\forall k, h, s, a : \widehat{r}_{hk}(s,a) - r_h(s,a)| \leq \beta_{hk}^r(s,a) \wedge \|\widehat{p}_{hk}(\cdot|s,a) - p_h(\cdot|s,a)\|_1 \leq \beta_{hk}^p(s,a)\right) \geq 1 - \delta/2$$

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[1] Note that $at \geq \log(bt)$ can be solved using Lambert W function. We thus have $t \geq \frac{-W_{-1}(-a/b)}{a}$ since, given $a = \Delta_i^2$ and $b = 2k/\delta$, $-a/b \in (-1/e, 0)$. We can make the bound more explicit by noticing that $-1 - \sqrt{2u} - u \leq W_{-1}(-e^{-u-1}) \leq -1 - \sqrt{2u} - 2u/3$ for $u > 0$ [Chatzigeorgiou, 2016]. Then $t \geq \frac{1 + \sqrt{2u} + u}{a}$ with $u = \log(b/a) - 1$.

- Define the bonus function and consider the Q-function computed at episode k

$$Q_{h,k}(s,a) = \widehat{r}_{h,k}(s,a) + b_{h,k}(s,a) + \sum_{s'} \widehat{p}_{h,k}(s'|s,a)V_{h+1,k}(s')$$

with $V_{h,k}(s) = \min\{H, \max_a Q_{h,k}(s,a)\}$. Recall that $V_{H+1,k}(s) = V_{H+1}^{\star}(s) = 0$. Prove that under event $\mathcal{E}$, Q_k is optimistic, i.e.,

$$Q_{h,k}(s,a) \geq Q_h^{\star}(s,a), \forall s,a$$

where $Q^{\star}$ is the optimal Q-function of the unknown MDP $M^{\star}$. Note that $\widehat{r}_{H,k}(s,a) + b_{H,k}(s,a) \geq r_{H,k}(s,a)$ and thus $Q_{H,k}(s,a) \geq Q_H^{\star}(s,a)$ (for a properly defined bonus). Then use induction to prove that this holds for all the stages h.

- In class we have seen that

$$\delta_{1k}(s_{1,k}) \leq \sum_{h=1}^{H} Q_{hk}(s_{hk}, a_{hk}) - r(s_{hk}, a_{hk}) - \mathbb{E}_{Y \sim p(\cdot|s_{hk}, a_{hk})}[V_{h+1,k}(Y)]) + m_{hk} \tag{1}$$

where $\delta_{hk}(s) = V_{hk}(s) - V_h^{\pi_k}(s)$ and $m_{hk} = \mathbb{E}_{Y \sim p(\cdot|s_{hk}, a_{hk})}[\delta_{h+1,k}(Y)] - \delta_{h+1,k}(s_{h+1,k})$. We now want to prove this result. Denote by a_{hk} the action played by the algorithm (you will have to use the greedy property).

  1. Show that $V_h^{\pi_k}(s_{hk}) = r(s_{hk}, a_{hk}) + \mathbb{E}_p[V_{h+1,k}(s')] - \delta_{h+1,k}(s_{h+1,k}) - m_{h,k}$
  2. Show that $V_{h,k}(s_{hk}) \leq Q_{h,k}(s_{hk}, a_{hk})$.
  3. Putting everything together prove Eq. 1.

- Since $(m_{hk})_{hk}$ is an MDS, using Azuma-Hoeffding we show that with probability at least $1 - \delta/2$

$$\sum_{k,h} m_{hk} \leq 2H\sqrt{KH \log(2/\delta)}$$

Show that the regret is upper bounded with probability $1 - \delta$ by

$$R(T) \leq 2\sum_{kh} b_{hk}(s_{hk}, a_{hk}) + 2H\sqrt{KH \log(2/\delta)}$$

- Finally, we have that [Domingues et al., 2021]

$$\sum_{h,k} \frac{1}{\sqrt{N_{hk}(s_{hk}, a_{hk})}} \lesssim H^2 S^2 A + 2\sum_{h=1}^{H} \sum_{s,a} \sqrt{N_{hK}(s,a)}$$

Complete this by showing an upper-bound of $H\sqrt{SAK}$, which leads to $R(T) \lesssim H^2 S\sqrt{AK}$

A   Weissmain inequality

Denote by $\widehat{p}(\cdot|s,a)$ the estimated transition probability build using n samples drawn from $p(\cdot|s,a)$. Then we have that

$$\mathbb{P}(\|\widehat{p}_h(\cdot|s,a) - p_h(\cdot|s,a)\|_1 \geq \epsilon) \leq (2^S - 2)\exp\left(-\frac{n\epsilon^2}{2}\right)$$

References

Ioannis Chatzigeorgiou. Bounds on the lambert function and their application to the outage analysis of user cooperation. *CoRR*, abs/1601.04895, 2016.

Omar Darwiche Domingues, Pierre Ménard, Matteo Pirotta, Emilie Kaufmann, and Michal Valko. Kernel-based reinforcement learning: A finite-time analysis. In *ICML*, volume 139 of *Proceedings of Machine Learning Research*, pages 2783–2792. PMLR, 2021.

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

for $k = 1, \ldots, K$ **do**
    Observe initial state s_{1k} *(arbitrary)*
    Estimate empirical MDP $\widehat{M}_k = (S, A, \widehat{p}_{hk}, \widehat{r}_{hk}, H)$ from $\mathcal{D}_k$

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

    Planning (by backward induction) for π_{hk} using $\widehat{M}_k$
    for $h = H, \ldots, 1$ **do**
        $Q_{h,k}(s,a) = \widehat{r}_{h,k}(s,a) + b_{h,k}(s,a) + \sum_{s'} \widehat{p}_{h,k}(s'|s,a) V_{h+1,k}(s')$
        $V_{h,k}(s) = \min\{H, \max_a Q_{h,k}(s,a)\}$
    end
    Define $\pi_{h,k}(s) = \arg\max_a Q_{h,k}(s,a)$, $\forall s, h$
    for $h = 1, \ldots, H$ **do**
        Execute $a_{hk} = \pi_{hk}(s_{hk})$
        Observe r_{hk} and $s_{h+1,k}$
        $N_{h,k+1}(s_{hk}, a_{hk}) = N_{h,k}(s_{hk}, a_{hk}) + 1$
    end
end

Algorithm 1: UCBVI