

Exploration in Reinforcement Learning (theory)

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Solution by **FILL** fullname command at the beginning of latex document

Instructions

- The deadline is **January 10, 2021. 23h00**
- 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 UCB

Denote by $S_{j,t} = \sum_{k=1}^t X_{i_k,k} \cdot \mathbb{1}(i_k = j)$ and by $N_{j,t} = \sum_{k=1}^t \mathbb{1}(i_k = j)$ the cumulative reward and number of pulls of arm j at time t . Denote by $\hat{\mu}_{j,t} = \frac{S_{j,t}}{N_{j,t}}$ the estimated mean. Recall that, at each timestep t , UCB plays the arm i_t such that

$$i_t \in \arg \max_j \hat{\mu}_{j,t} + U(N_{j,t}, \delta)$$

Is $\hat{\mu}_{j,t}$ an unbiased estimator (i.e., $\mathbb{E}_{UCB}[\hat{\mu}_{j,t}] = \mu_j$)? Justify your answer.

2 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^* the best arm and by \hat{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 $\mathbb{P}_{\mu_1, \dots, \mu_k}(\hat{i} \neq i^*) \leq \delta$ and $\tau_\delta < \infty$ almost surely for any μ_1, \dots, μ_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.

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

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

Consider the following algorithm

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

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

- Compute the function $U(t, \delta)$ that satisfy the any-time confidence bound. For any arm $i \in [k]$

$$\mathbb{P}(\{|\hat{\mu}_{i,t} - \mu_i| > U(t, \delta)\}) \leq \delta$$

Use Hoeffding's inequality.

- Let $\mathcal{E} = \bigcup_{i=1}^k \bigcup_{t=1}^{\infty} \{|\hat{\mu}_{i,t} - \mu_i| > U(t, \delta')\}$. Using previous result 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 $i^* = \arg \max_i \{\mu_i\}$ 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 $i \neq i^*$ will be removed from the active set when $\Delta_i \geq C_1 U(t, \delta')$ where $C_1 > 1$ is a constant. Compute the time required to have such condition for each non-optimal arm. Use the condition of arm elimination applied to arm i^* .
- Compute a bound on the sample complexity (after how many rounds the algorithm stops) for identifying the optimal arm w.p. $1 - \delta$.

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

3 Bernoulli Bandits

In this exercise, you compare KL-UCB and UCB empirically with Bernoulli rewards $X_t \sim \text{Bern}(\mu_{I_t})$.

- Implement KL-UCB and UCB

KL-UCB:

$$I_t = \arg \max_i \max \left\{ \mu \in [0, 1] : d(\hat{\mu}_{i,t}, \mu) \leq \frac{\log(1 + t \log^2(t))}{N_{i,t}} \right\}$$

where d is the Kullback–Leibler divergence (see closed form for Bernoulli). A way of computing the inner max is through bisection (finding the zero of a function).

UCB:

$$I_t = \arg \max_i \hat{\mu}_{i,t} + \sqrt{\frac{\log(1 + t \log^2(t))}{2N_{i,t}}}$$

that has been tuned for 1/2-subgaussian problems.

- Let $n = 10000$ and $k = 2$. Plot the expected regret of each algorithm as a function of Δ when $\mu_1 = 1/2$ and $\mu_2 = 1/2 + \Delta$.
- Repeat the above experiment with $\mu_1 = 1/10$ and $\mu_2 = 9/10$.
- Discuss your results.

4 Regret Minimization in RL

Consider a finite-horizon MDP $M^* = (S, A, p_h, r_h)$ 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 ($T = KH$)

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

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 $\mathcal{E} = \{\forall k, M^* \in \mathcal{M}_k\}$. 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

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

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

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

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

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

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

- In class we have seen that

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

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.

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

for  $k = 1, \dots, K$  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  $\pi_{hk}$  using  $\widehat{M}_k$ 
  for  $h = H, \dots, 1$  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  $h = 1, \dots, H$  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

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Algorithm 1: UCBVI

- 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

$$\sum_{h,k} \frac{1}{\sqrt{N_{hk}(s_{hk}, a_{hk})}} = \sum_{h=1}^H \sum_{s,a} \sum_{i=1}^{N_{h,K}(s,a)} \frac{1}{\sqrt{i}} \leq 2 \sum_{h=1}^H \sum_{s,a} \sqrt{N_{hk}(s, a)}$$

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