MVA: Reinforcement Learning (2020/2021)	**Homework 3**

Exploration in Reinforcement Learning (theory)

Lecturers: *A. Lazaric, M. Pirotta* *(December 10, 2020)*

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 $S_{j,t} = \sum_{k=1}^{t} X_{i_k,k} \cdot \mathbb{1}(i_k = a)$ 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 $\widehat{\mu}_{j,t} = \frac{S_{j,t}}{N_{j,t}}$ the estimated mean. Recall that, at each timestep t, UCB plays the arm i_t such that

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

Is $\widehat{\mu}_{j,t}$ an unbiased estimator (i.e., $\mathbb{E}_{UCB}[\widehat{\mu}_{j,t}] = \mu_j$)? 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 $i^\star$ 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.

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

```
Input: k arms, confidence δ
S = {1, ..., k}
for t = 1, ... do
    Pull all arms in S
    S = S \ { i ∈ S : ∃j ∈ S, μ̂_{j,t} − U(t,δ) ≥ μ̂_{i,t} + U(t,δ) }
    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 $\widehat{\mu}_{i,t} = \frac{1}{t}\sum_{j=1}^{t} X_{i,j}$.

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

$$\mathbb{P}\left(\bigcup_{t=1}^{\infty} \{|\widehat{\mu}_{i,t} - \mu_i| > U(t,\delta)\}\right) \leq \delta$$

  Use Hoeffding's inequality.

- Let $\mathcal{E} = \bigcup_{i=1}^{k} \bigcup_{t=1}^{\infty} \{|\widehat{\mu}_{i,t} - \mu_i| > U(t,\delta')\}$. 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 $i^\star = \arg\max_i\{\mu_i\}$ 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 $\Delta_i \geq C_1 U(t,\delta')$ 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 $i^\star$.

- 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 $X_t \sim Bern(\mu_{I_t})$.

- Implement KL-UCB and UCB

  KL-UCB:

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

  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:

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

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 $\mu_1 = 9/10$.
- Discuss your results.

4 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

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

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

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

- 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 $V_{H+1,k}(s) = V^\star_{H+1}(s) = 0$. Prove that under event $\mathcal{E}$, Q_k is optimistic, i.e.,

$$Q_{h,k}(s,a) \geq Q^\star_h(s,a), \forall s, a$$

  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 $Q_{H,k}(s,a) \geq Q^\star_H(s,a)$ (for a properly defined bonus). Then use induction to prove that this holds for all the stages h.

- In class we have seen that

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

  where $\delta_{hk}(s) = V_{hk}(s) - V^{\pi_k}_h(s)$ 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 $V^{\pi_k}_h(s_{hk}) = r(s_{hk}, a_{hk}) + \mathbb{E}_p[V_{h+1,k}(s')] - \delta_{h+1,k}(s_{h+1,k}) - m_{h,k}$

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 π_{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

Algorithm 1: UCBVI

2. Show that $V_{h,k}(s_{hk}) \le Q_{h,k}(s_{hk}, a_{hk})$.
3. Putting everything together prove Eq. 1.

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

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

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

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

- Finally, we have that

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

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

$$\mathbb{P}(\|\widehat{p}_h(\cdot|s,a) - p_h(\cdot|s,a)\|_1 \ge \epsilon) \le (2^S - 2) \exp\Big(-\frac{n\epsilon^2}{2}\Big)$$

References