Exploration in Tabular MDPs

Sham Kakade and Wen Sun

CS 6789: Foundations of Reinforcement Learning

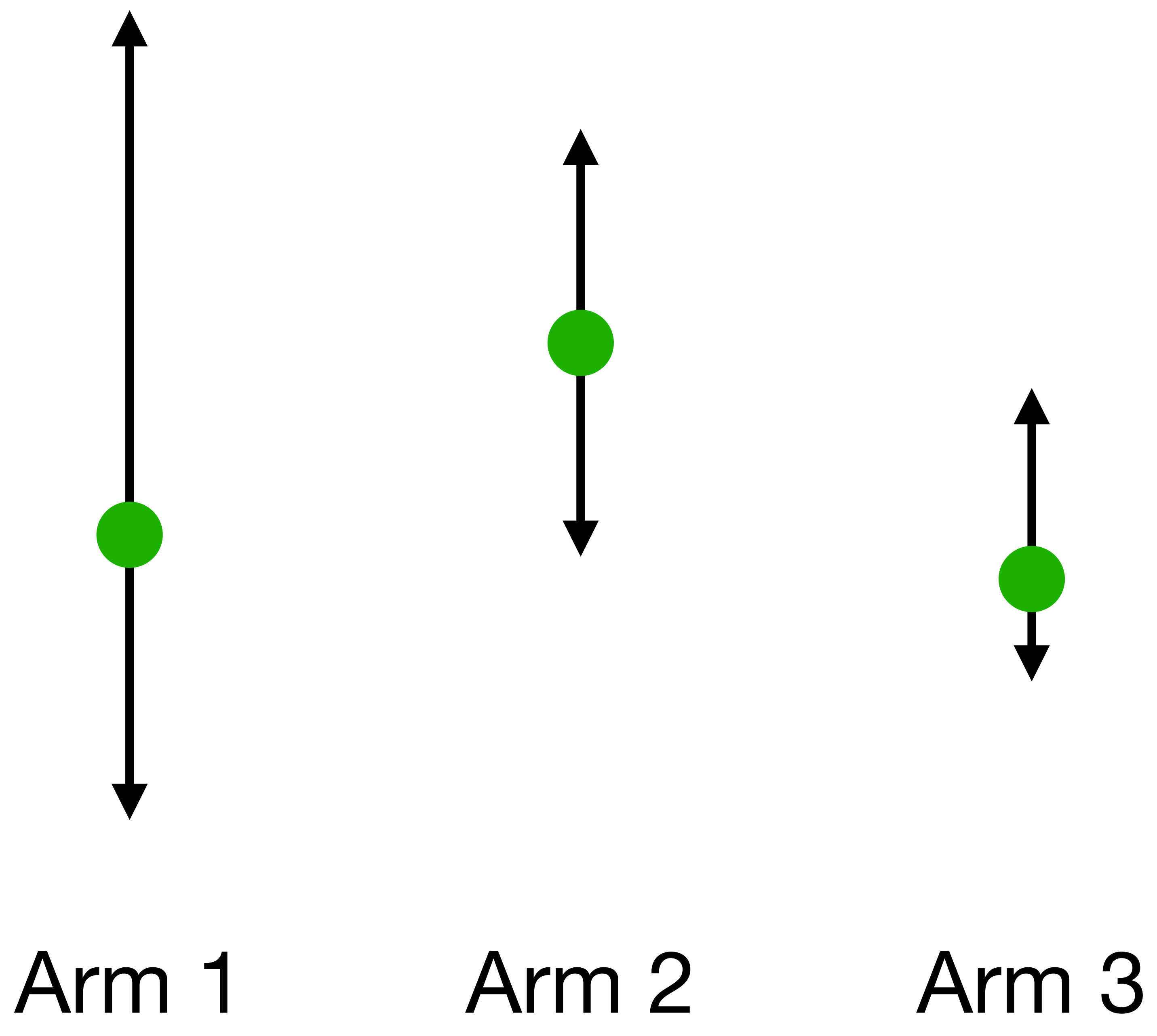
Announcements

Course Project Website
https://wensun.github.io/CS6789projects.html

(Please start thinking about potential projects and feel free to discuss w/ me and TA during office hours)

Recap:

Multi-armed Bandits and UCB Algorithm



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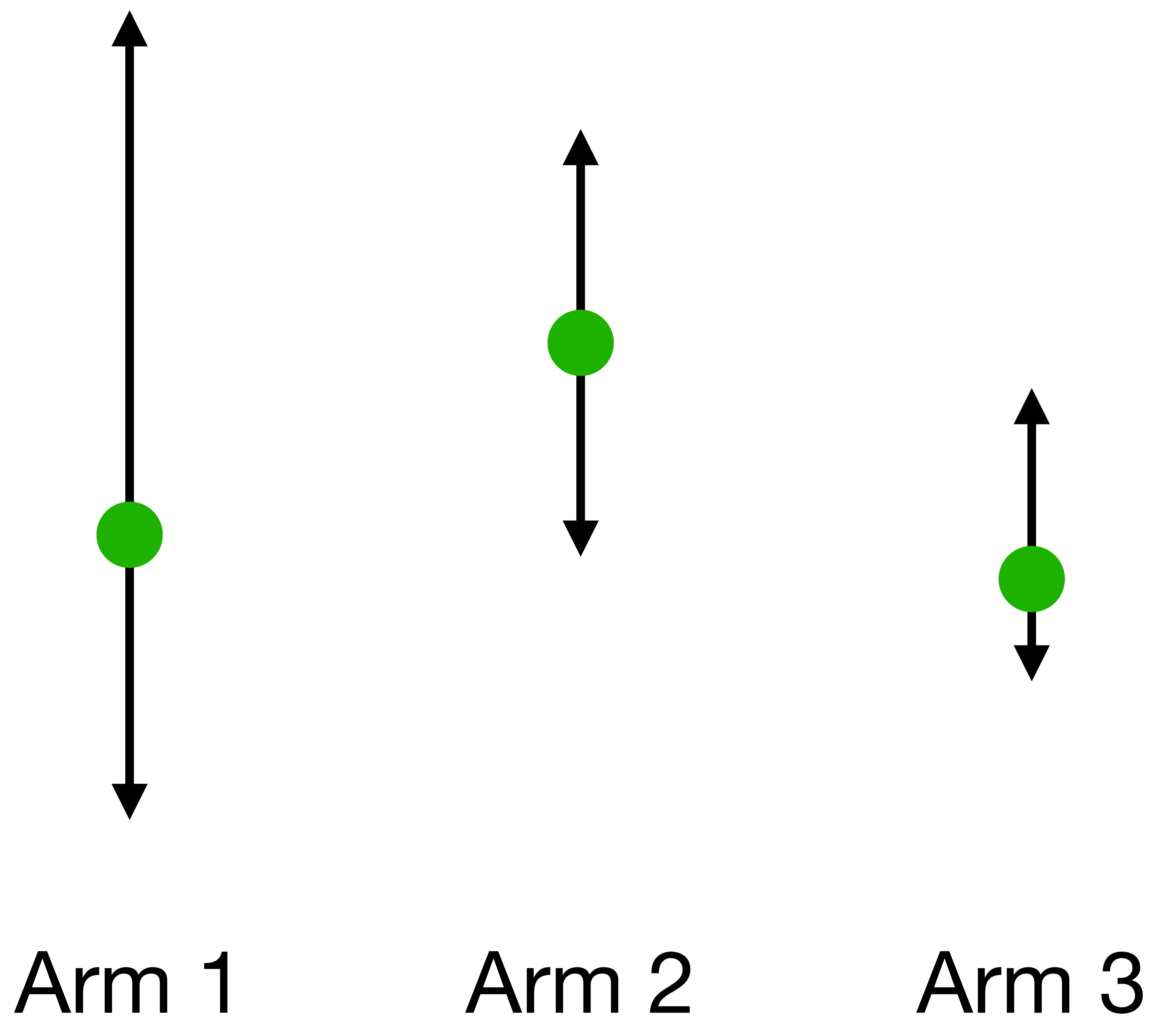

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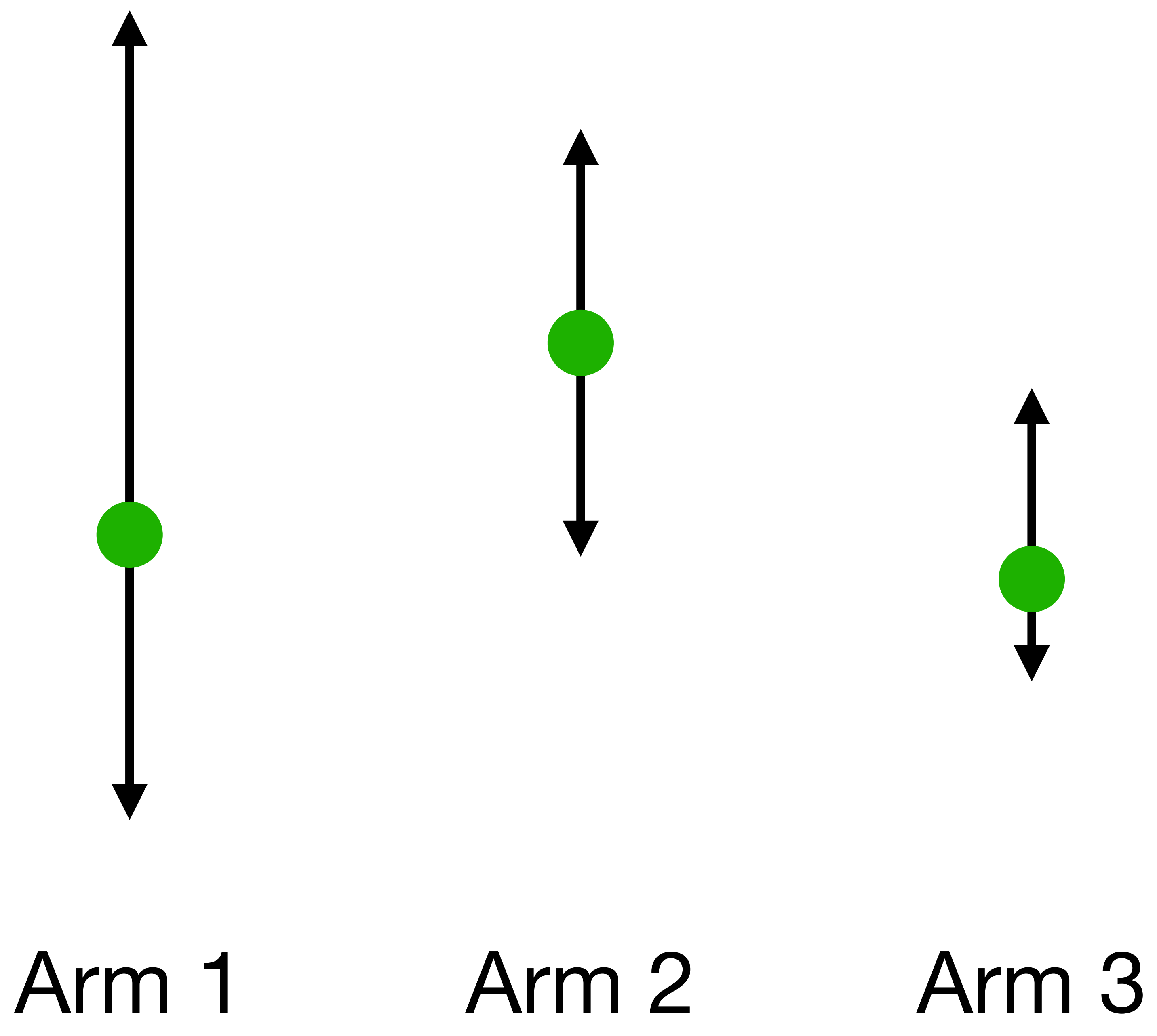

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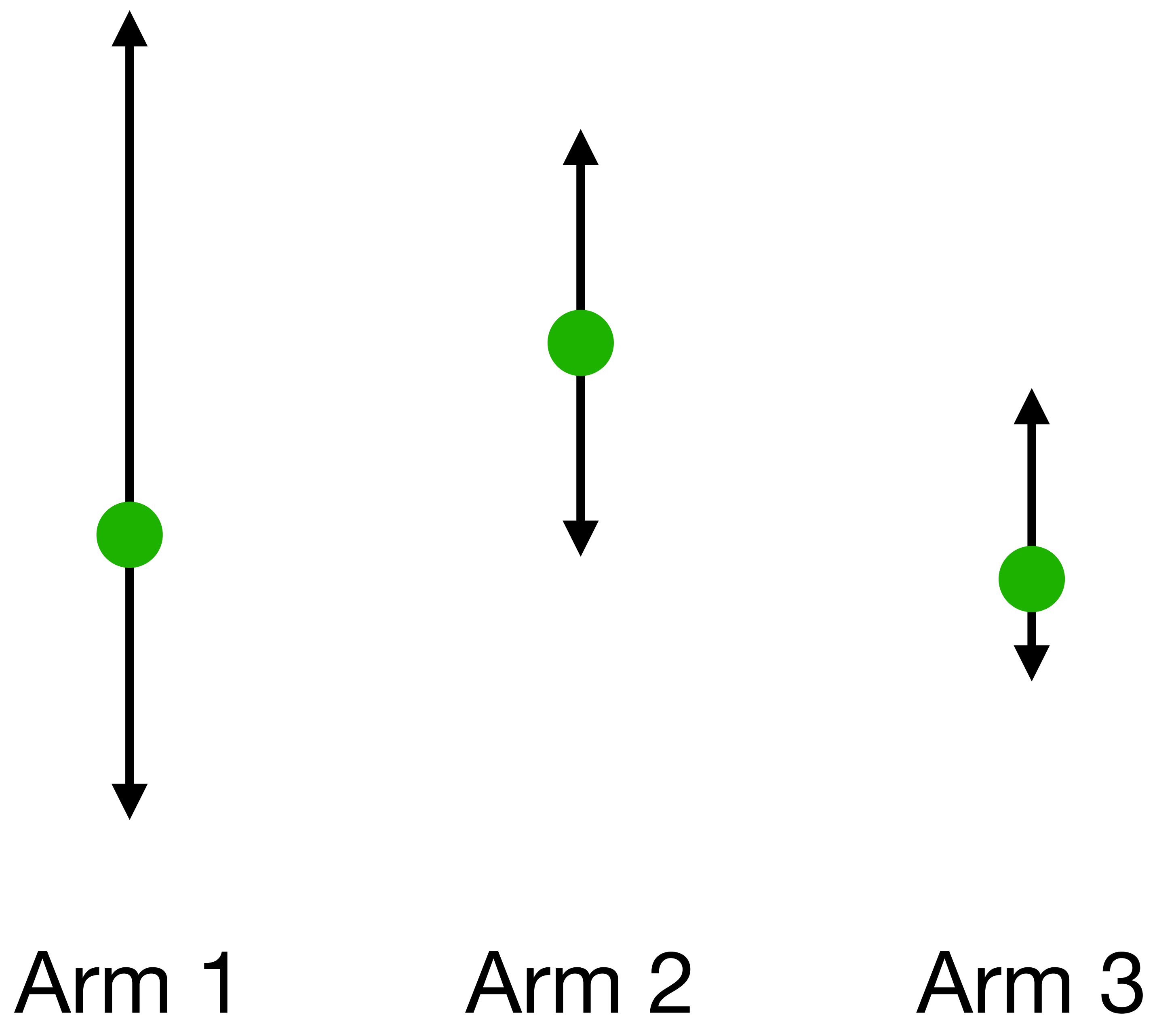

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Key step in the proof:

$$\mu(a^\star) - \mu(a^n) \leq \widehat{\mu}(a^n) + \sqrt{\frac{\ln(KN/\delta)}{N^n(a_n)}} - \mu(a^n)$$

Today: Efficient Learning in Finite Horizon tabular MDPs

Finite horizon episode (time-dependent) discrete MDP $\mathscr{M} = \left\{ \{r_h\}_{h=0}^{H-1}, \{P_h\}_{h=0}^{H}, H, \mu, S, A \right\}$

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EXPLORATION!

Why we need strategic exploration?

Initialization: s_0

Length of chain is H

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Probability of random walk hitting reward 1 is $(1/3)^{-H}$

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2. At episode n, learner executes π^n:
$\{s_h^n, a_h^n, r_h^n\}_{h=0}^{H-1}$, with $a_h^n = \pi^n(s_h^n), r_h^n = r(s_h^n, a_h^n),\ s_{h+1}^n \sim P(\cdot \mid s_h^n, a_h^n)$

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Performance measure: REGRET

$$\mathbb{E}\left[\sum_{n=1}^{N}\left(V^\star - V^{\pi^n}\right)\right] = \text{poly}(S, A, H)\sqrt{N}$$

Notations for Today

$$\mathbb{E}_{s' \sim P(\cdot|s,a)}\left[f(s')\right] := P(\cdot \mid s, a) \cdot f$$

$d_h^\pi(s, a)$: state-action distribution induced by π at time step h
(i.e., probability of π visiting (s, a) at time step h starting from s_0)

$$\pi = \{\pi_0, \ldots, \pi_{H-1}\}$$

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1. Attempt 2: The Upper Confidence Bound Value Iteration Algorithm (UCB-VI)

2. UCB-VI’s regret bound and the analysis

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Key lesson: shouldn't treat policies as independent arms — they do share information

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Collect a new trajectory by executing π^n in the real world $\{P_h\}_{h=0}^{H-1}$ starting from s_0

UCBVI—Part 1: Model Estimation

Let us consider the **very beginning** of episode n:

$$\mathcal{D}_h^n = \{s_h^i, a_h^i, s_{h+1}^i\}_{i=1}^{n-1}, \forall h$$

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Estimate model $\widehat{P}_h^n(s' \mid s, a), \forall s, a, s', h$:

$$\widehat{P}_h^n(s' \mid s, a) = \frac{N_h^n(s,a,s')}{N_h^n(s,a)}$$

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$$\left\| \widehat{V}_h^n \right\|_\infty \leq H, \forall h, n$$

UCBVI: Put All Together

For $n = 1 \to N$:

1. Set $N_h^n(s,a) = \sum_{i=1}^{n-1} \mathbf{1}\{(s_h^i, a_h^i) = (s,a)\}, \forall s, a, h$

2. Set $N_h^n(s,a,s') = \sum_{i=1}^{n-1} \mathbf{1}\{(s_h^i, a_h^i, s_{h+1}^i) = (s,a,s')\}, \forall s, a, a', h$

3. Estimate $\widehat{P}^n$: $\widehat{P}_h^n(s' | s,a) = \dfrac{N_h^n(s,a,s')}{N_h^n(s,a)}, \forall s, a, s', h$

4. Plan: $\pi^n = VI\left(\{\widehat{P}_h^n, r_h + b_h^n\}_h\right)$, with $b_h^n(s,a) = cH\sqrt{\dfrac{\ln(SAHN/\delta)}{N_h^n(s,a)}}$

5. Execute π^n : $\{s_0^n, a_0^n, r_0^n, \ldots, s_{H-1}^n, a_{H-1}^n, r_{H-1}^n, s_H^n\}$

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Theorem: UCBVI Regret Bound

$$\mathbb{E}\left[\text{Regret}_N\right] := \mathbb{E}\left[\sum_{n=1}^{N}\left(V^\star - V^{\pi^n}\right)\right] \leq \widetilde{O}\left(H^2\sqrt{S^2AN}\right)$$

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Remarks:

Note that we consider expected regret here (policy π^n is a random quantity).
High probability version is not hard to get (need to do a martingale argument)

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Dependency on H and S are suboptimal; but the **same** algorithm can achieve $H^2\sqrt{SAN}$ in the leading term [Azar et.al 17 ICML, and the book Chapter 7]

Outline of Proof

Bonus $b_h^n(s,a)$ is related to $\left(\left(\widehat{P}_h^n(\cdot \mid s,a) - P_h(\cdot \mid s,a)\right) \cdot V_{h+1}^{\star}\right)$

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VI with bonus inside the learned model gives optimism, i.e., $\widehat{V}_h^n(s) \geq V_h^\star(s), \forall h, n, s, a$

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Upper bound per-episode regret: $V_0^\star(s_0) - V_0^{\pi^n}(s_0) \leq \widehat{V}_0^n(s_0) - V_0^{\pi^n}(s_0)$

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Apply simulation lemma: $\widehat{V}_0^n(s_0) - V^{\pi^n}(s_0)$

1. Model Error using Hoeffing's inequality & Union Bound

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Given a fixed function $f : S \mapsto [0,H]$, w/ prob $1-\delta$:

$$\left| \left(\widehat{P}_h^n(\cdot|s,a) - P_h(\cdot|s,a) \right)^\top f \right| \leq O(H\sqrt{\ln(SAHN/\delta)/N_h^n(s,a)}), \forall s, a, h, N$$

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Intuition:

1. Assume for some i, $s_h^i = s, a_h^i = a$, then $f(s_{h+1}^i)$ is an unbiased estimate of $\mathbb{E}_{s' \sim P_h(\cdot|s,a)} f(s')$

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From now on, assume this event being true

Intuition:

1. Assume for some i, $s_h^i = s, a_h^i = a$, then $f(s_{h+1}^i)$ is an unbiased estimate of $\mathbb{E}_{s'\sim P_h(\cdot|s,a)} f(s')$

2. Note $\widehat{P}_h^n(\cdot|s,a)\cdot f = \dfrac{1}{N_h^n(s,a)} \displaystyle\sum_{i=1}^{n-1} \mathbf{1}[(s_h^i, a_h^i) = (s,a)] f(s_{h+1}^i)$

2. Proving Optimism via Induction

Lemma [Optimism]: $\widehat{V}_h^n(s) \geq V_h^\star(s), \forall n, h, s$

Recall Bonus-enhanced Value Iteration at episode n:

$$\widehat{V}_H^n(s) = 0, \quad \widehat{Q}_h^n(s,a) = \min\left\{ r_h(s,a) + b_h^n(s,a) + \widehat{P}_h^n(\cdot \mid s,a) \cdot \widehat{V}_{h+1}^n, H \right\}$$

$$\widehat{V}_h^n(s) = \max_a \widehat{Q}_h^n(s,a), \quad \pi_h^n(s) = \arg\max_a \widehat{Q}_h^n(s,a), \forall s$$

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$$\widehat{Q}_h^n(s,a) - Q_h^\star(s,a) = r_h(s,a) + b_h^n(s,a) + \widehat{P}_h^n(\cdot \mid s,a) \cdot \widehat{V}_{h+1}^n - r_h(s,a) - P_h(\cdot \mid s,a) \cdot V_{h+1}^\star$$

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Inductive hypothesis: $\widehat{V}^n_{h+1}(s) \geq V^\star_{h+1}(s), \quad \forall s$

$$\widehat{Q}^n_h(s,a) - Q^\star_h(s,a) = r_h(s,a) + b^n_h(s,a) + \widehat{P}^n_h(\cdot \mid s,a) \cdot \widehat{V}^n_{h+1} - r_h(s,a) - P_h(\cdot \mid s,a) \cdot V^\star_{h+1}$$

$$\geq b^n_h(s,a) + \widehat{P}^n_h(\cdot \mid s,a) \cdot V^\star_{h+1} - P_h(\cdot \mid s,a) \cdot V^\star_{h+1}$$

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$$\geq b_h^n(s,a) + \widehat{P}_h^n(\cdot \mid s,a) \cdot V_{h+1}^\star - P_h(\cdot \mid s,a) \cdot V_{h+1}^\star$$

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$$= b_h^n(s,a) + \left(\widehat{P}_h^n(\cdot \mid s,a) - P_h(\cdot \mid s,a) \right) \cdot V_{h+1}^\star$$

$$\geq b_h^n(s,a) - b_h^n(s,a) = 0, \quad \forall s, a$$

3. Upper Bounding Regret using Optimism

per-episode regret $:= V_0^\star(s_0) - V_0^{\pi_n}(s_0) \leq \widehat{V}_0^n(s_0) - V_0^{\pi_n}(s_0)$

This is something
we can control!
And this is related
to our policy π^n

4. Upper bounding Regret via Simulation Lemma

$$\widehat{V}^n_H(s) = 0, \quad \widehat{Q}^n_h(s,a) = \min\left\{ r_h(s,a) + b^n_h(s,a) + \widehat{P}^n_h(\cdot \mid s,a) \cdot \widehat{V}^n_{h+1}, H \right\}$$

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Lemma [Simulation lemma]:

$$\widehat{V}^n_0(s_0) - V^{\pi^n}_0(s_0) \leq \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d^{\pi^n}_h}\left[b^n_h(s,a) + \left(\widehat{P}^n_h(\cdot \mid s,a) - P_h(\cdot \mid s,a)\right) \cdot \widehat{V}^n_{h+1} \right]$$

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$$\le r_0(s_0, \pi^n(s_0)) + b^n_h(s_0, \pi^n(s_0)) + \widehat{P}^n_0(\cdot \mid s_0, \pi^n(s_0)) \cdot \widehat{V}^n_1 - r_0(s_0, \pi^n(s_0)) - P_0(\cdot \mid s_0, \pi^n(s_0)) \cdot V^{\pi^n}_1$$

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$$= b^n_h(s_0, \pi^n(s_0)) + \widehat{P}^n_0(\cdot \mid s_0, \pi^n(s_0)) \cdot \widehat{V}^n_1 - P_0(\cdot \mid s_0, \pi^n(s_0)) \cdot V^{\pi^n}_1$$

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$$\widehat{V}^n_0(s_0) - V_0^{\pi^n}(s_0) \le \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}} \left[b_h^n(s,a) + (\widehat{P}^n_h(\cdot \mid s,a) - P_h(\cdot \mid s,a)) \cdot \widehat{V}^n_{h+1} \right]$$

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$$\le r_0(s_0, \pi^n(s_0)) + b_h^n(s_0, \pi^n(s_0)) + \widehat{P}^n_0(\cdot \mid s_0, \pi^n(s_0)) \cdot \widehat{V}^n_1 - r_0(s_0, \pi^n(s_0)) - P_0(\cdot \mid s_0, \pi^n(s_0)) \cdot V_1^{\pi^n}$$

$$= b_h^n(s_0, \pi^n(s_0)) + \widehat{P}^n_0(\cdot \mid s_0, \pi^n(s_0)) \cdot \widehat{V}^n_1 - P_0(\cdot \mid s_0, \pi^n(s_0)) \cdot V_1^{\pi^n}$$

$$= b_h^n(s_0, \pi^n(s_0)) + \left(\widehat{P}^n_0(\cdot \mid s_0, \pi^n(s_0)) - P_0(\cdot \mid s_0, \pi^n(s_0)) \right) \cdot \widehat{V}^n_1 + P_0(\cdot \mid s_0, \pi^n(s_0)) \cdot \left(\widehat{V}^n_1 - V_1^{\pi^n} \right)$$

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$$\widehat{V}^n_H(s) = 0, \quad \widehat{Q}^n_h(s,a) = \min\left\{ r_h(s,a) + b^n_h(s,a) + \widehat{P}^n_h(\cdot \mid s,a) \cdot \widehat{V}^n_{h+1}, H \right\}$$

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$$\leq r_0(s_0, \pi^n(s_0)) + b^n_h(s_0, \pi^n(s_0)) + \widehat{P}^n_0(\cdot \mid s_0, \pi^n(s_0)) \cdot \widehat{V}^n_1 - r_0(s_0, \pi^n(s_0)) - P_0(\cdot \mid s_0, \pi^n(s_0)) \cdot V^{\pi^n}_1$$

$$= b^n_h(s_0, \pi^n(s_0)) + \widehat{P}^n_0(\cdot \mid s_0, \pi^n(s_0)) \cdot \widehat{V}^n_1 - P_0(\cdot \mid s_0, \pi^n(s_0)) \cdot V^{\pi^n}_1$$

$$= b^n_h(s_0, \pi^n(s_0)) + \left(\widehat{P}^n_0(\cdot \mid s_0, \pi^n(s_0)) - P_0(\cdot \mid s_0, \pi^n(s_0)) \right) \cdot \widehat{V}^n_1 + P_0(\cdot \mid s_0, \pi^n(s_0)) \cdot \left(\widehat{V}^n_1 - V^{\pi^n}_1 \right)$$

$$= \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d^{\pi^n}_h}\left[b^n_h(s,a) + (\widehat{P}^n_h(\cdot \mid s,a) - P_h(\cdot \mid s,a)) \cdot \widehat{V}^n_{h+1} \right]$$

4. Upper bounding Regret via Simulation Lemma

per-episode regret $:= V_0^\star(s_0) - V_0^{\pi_n}(s_0) \leq \widehat{V}_0^n(s_0) - V_0^{\pi_n}(s_0)$

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But $\widehat{V}_h^n$ is data-dependent

(this is different from $V_h^\star$) !!!

$$\leq \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}}\left[b_h^n(s,a) + (\widehat{P}_h^n(\cdot \mid s,a) - P_h(\cdot \mid s,a)) \cdot \widehat{V}_{h+1}^n\right]$$

Let's do Holder's inequality

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$$\left(\widehat{P}_h^n(\cdot|s,a) - P_h(\cdot|s,a)\right) \cdot \widehat{V}_{h+1}^n \leq \|P_h(\cdot|s,a) - \widehat{P}_h^n(\cdot|s,a)\|_1 \|\widehat{V}_{h+1}^n\|_\infty$$

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$$\left(\widehat{P}_h^n(\cdot|s,a) - P_h(\cdot|s,a) \right) \cdot \widehat{V}_{h+1}^n \le \| P_h(\cdot|s,a) - \widehat{P}_h^n(\cdot|s,a) \|_1 \| \widehat{V}_{h+1}^n \|_\infty$$

$$\le H \| P_h(\cdot|s,a) - \widehat{P}_h^n(\cdot|s,a) \|_1 \le H \sqrt{\frac{S \ln(SAHN/\delta)}{N_h^n(s,a)}}, \forall s, a, h, n, \text{with prob} 1 - \delta$$

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$$\leq \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}}\left[b_h^n(s,a) + (\widehat{P}_h^n(\cdot\,|\,s,a) - P_h(\cdot\,|\,s,a))\cdot \widehat{V}_{h+1}^n\right]$$

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$$\leq \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}}\left[b_h^n(s,a) + H\sqrt{\frac{S\ln(SAHN/\delta)}{N_h^n(s,a)}}\right]$$

$$\left(\widehat{P}_h^n(\cdot\,|\,s,a) - P_h(\cdot\,|\,s,a)\right)\cdot \widehat{V}_{h+1}^n \leq \|P_h(\cdot\,|\,s,a) - \widehat{P}_h^n(\cdot\,|\,s,a)\|_1 \|\widehat{V}_{h+1}^n\|_\infty$$

$$\leq H\|P_h(\cdot\,|\,s,a) - \widehat{P}_h^n(\cdot\,|\,s,a)\|_1 \leq H\sqrt{\frac{S\ln(SAHN/\delta)}{N_h^n(s,a)}}, \forall s,a,h,n, \text{with prob} 1-\delta$$

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Let's do Holder's inequality

$$\leq \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}} \left[b_h^n(s,a) + H\sqrt{\frac{S\ln(SAHN/\delta)}{N_h^n(s,a)}} \right]$$

$$\leq 2\sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}} \left[H\sqrt{\frac{S\ln(SAHN/\delta)}{N_h^n(s,a)}} \right]$$

$$\left(\widehat{P}_h^n(\cdot|s,a) - P_h(\cdot|s,a)\right) \cdot \widehat{V}_{h+1}^n \leq \|P_h(\cdot|s,a) - \widehat{P}_h^n(\cdot|s,a)\|_1 \|\widehat{V}_{h+1}^n\|_\infty$$

$$\leq H\|P_h(\cdot|s,a) - \widehat{P}_h^n(\cdot|s,a)\|_1 \leq H\sqrt{\frac{S\ln(SAHN/\delta)}{N_h^n(s,a)}}, \forall s,a,h,n, \text{with prob} 1-\delta$$

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$$\leq \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}} \left[b_h^n(s,a) + H\sqrt{\frac{S\ln(SAHN/\delta)}{N_h^n(s,a)}} \right]$$

$$\leq 2\sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}} \left[H\sqrt{\frac{S\ln(SAHN/\delta)}{N_h^n(s,a)}} \right] = 2H\sqrt{S\ln(SAHN/\delta)} \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}} \left[\sqrt{\frac{1}{N_h^n(s,a)}} \right]$$

$$\left(\widehat{P}_h^n(\cdot|s,a) - P_h(\cdot|s,a) \right) \cdot \widehat{V}_{h+1}^n \leq \|P_h(\cdot|s,a) - \widehat{P}_h^n(\cdot|s,a)\|_1 \|\widehat{V}_{h+1}^n\|_\infty$$

$$\leq H\|P_h(\cdot|s,a) - \widehat{P}_h^n(\cdot|s,a)\|_1 \leq H\sqrt{\frac{S\ln(SAHN/\delta)}{N_h^n(s,a)}}, \forall s,a,h,n, \text{ with prob} 1-\delta$$

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$$\mathbb{E}\left[\text{Regret}_N\right] = \mathbb{E}\left[\mathbf{1}\{\text{events hold}\}\sum_{n=1}^{N}\left(V_0^{\star}(s_0) - V_0^{\pi^n}(s_0)\right)\right] + \mathbb{E}\left[\mathbf{1}\{\text{events don't hold}\}\sum_{n=1}^{N}\left(V_0^{\star}(s_0) - V_0^{\pi^n}(s_0)\right)\right]$$

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$$\leq H\sqrt{S\ln(SANH/\delta)}\,\mathbb{E}\left[\sum_{n=1}^{N}\sum_{h=0}^{H-1}\frac{1}{\sqrt{N_h^n(s_h^n, a_h^h)}}\right] + 2\delta NH$$

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$$\sum_{n=1}^{N} \sum_{h=0}^{H-1} \frac{1}{\sqrt{N_h^n(s_h^n, a_h^n)}}$$

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$$\mathbb{E}\left[\mathrm{Regret}_N\right] \le 2H^2S\sqrt{AN\ln(SAHN/\delta)} + 2\delta NH$$

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$$\sum_{n=1}^{N}\sum_{h=0}^{H-1}\frac{1}{\sqrt{N_h^n(s_h^n,a_h^n)}} = \sum_{h=0}^{H-1}\sum_{s,a}\sum_{i=1}^{N_h^N(s,a)}\frac{1}{\sqrt{i}} \leq \sum_{h=0}^{H-1}\sum_{s,a}\sqrt{N_h^N(s,a)} \leq \sum_{h=0}^{H-1}\sqrt{SA\sum_{s,a}N_h^N(s,a)}$$

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Set $\delta = 1/(HN)$

$$\leq 2H^2S\sqrt{AN\cdot\ln(SAH^2N^2)} = \widetilde{O}\left(H^2S\sqrt{AN}\right)$$

High-level Idea: Exploration or Exploitation Tradeoff

Upper bound per-episode regret: $V_0^\star(s_0) - V_0^{\pi^n}(s_0) \leq \widehat{V}_0^n(s_0) - V_0^{\pi^n}(s_0)$

1. What if $\widehat{V}_0^n(s_0) - V_0^{\pi^n}(s_0) \leq \epsilon$?

Then π^n is close to $\pi^\star$, i.e., we are doing exploitation

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We collect data at steps where bonus is large or model is wrong, i.e., exploration