Exploration in Tabular MDPs:

Upper Confidence Bound Value Iteration (UCBVI)

Announcements

1. Scribing Lecture Notes (see Piazza for details)

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

Recap:

Generative Model and Statistical Limits

Theorem: (Azar et al. '13) With probability greater than $1-\delta$,

$$\|Q^\star - \widehat{Q}^\star\|_\infty \le \gamma\sqrt{\frac{c}{(1-\gamma)^3}\frac{\log(cSA/\delta)}{N}} + \frac{c\gamma}{(1-\gamma)^3}\frac{\log(cSA/\delta)}{N},$$

where c is an absolute constant.

Corollary: for $\epsilon < 1$, provided $N \ge \frac{c}{(1-\gamma)^3}\frac{\log(cSA/\delta)}{\epsilon^2}$ then

$\|Q^\star - \widehat{Q}^\star\|_\infty \le \epsilon$ (with prob. greater than $1-\delta$)

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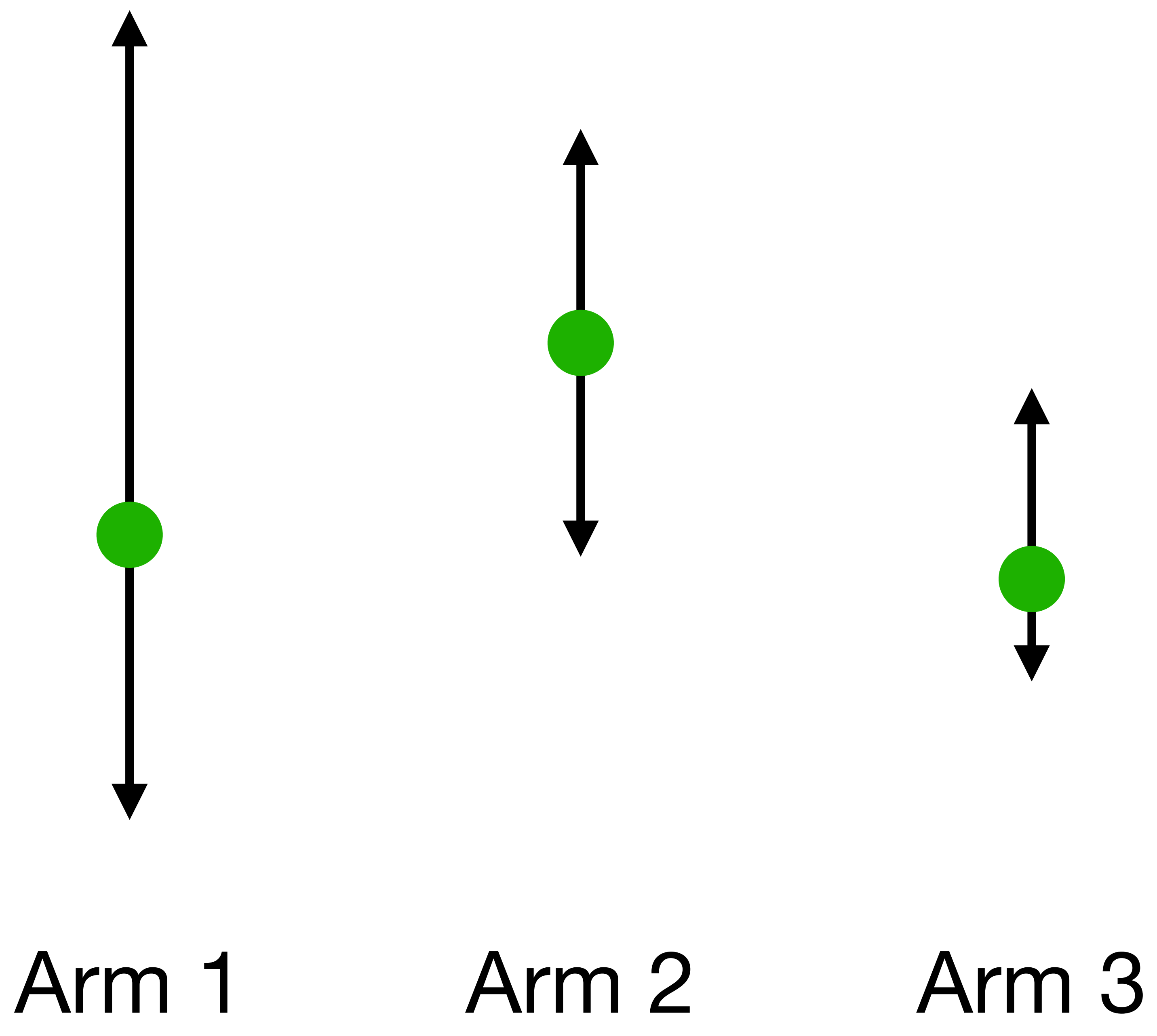
Generative Model: we can reset to anywhere we want (may not be realistic)

Recap:

Multi-armed Bandits and UCB Algorithm



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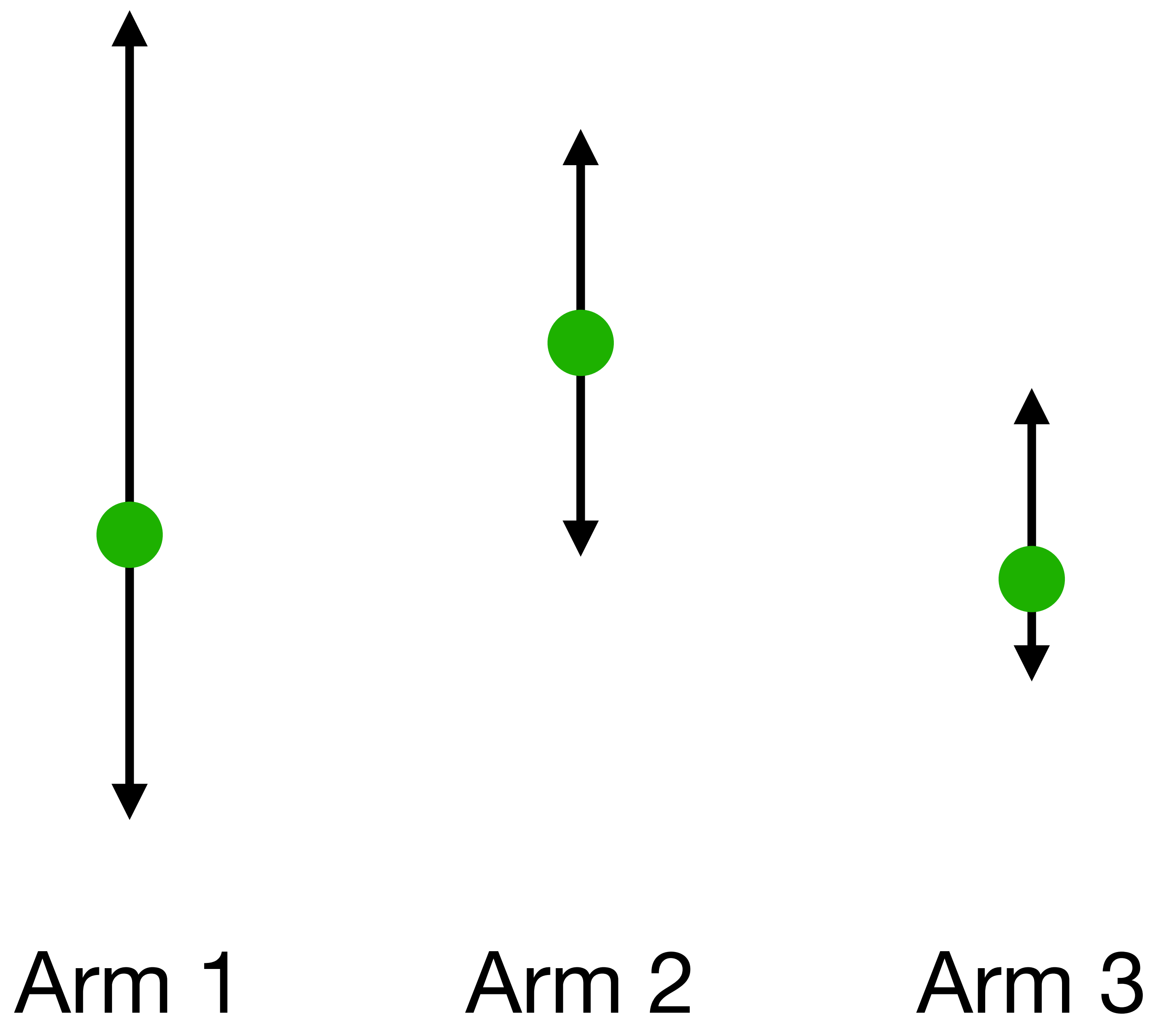

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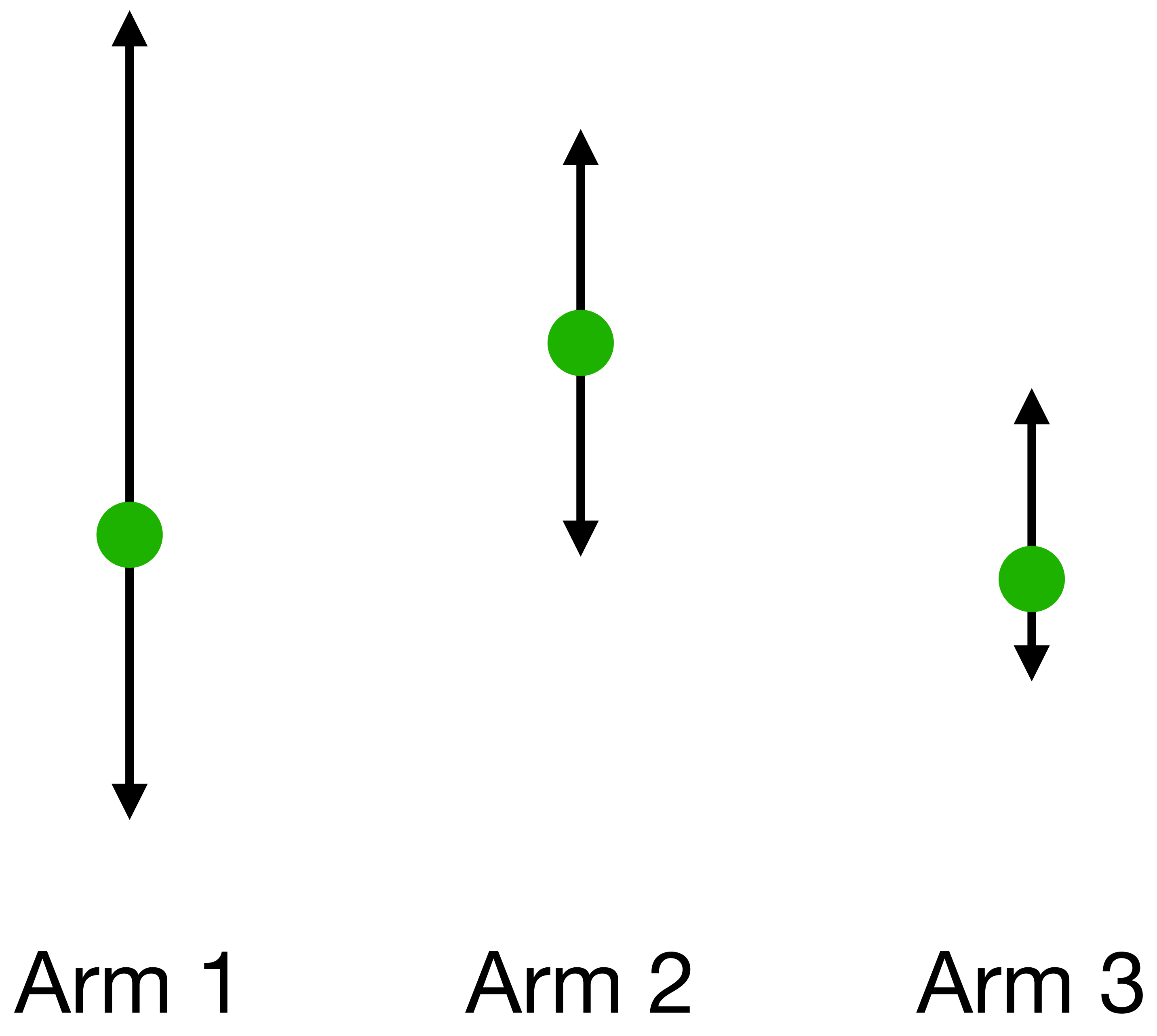

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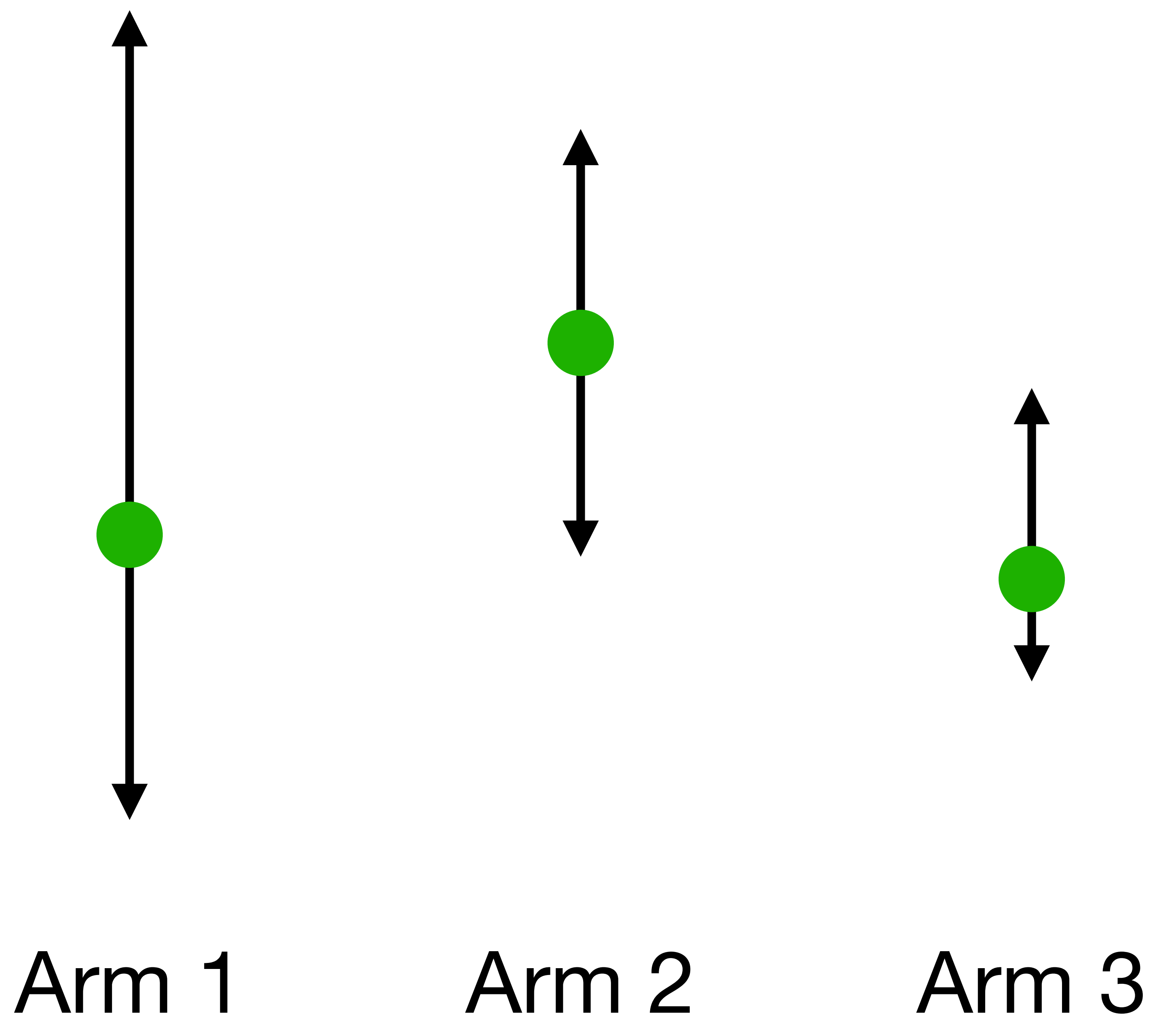

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Key step in the proof:

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

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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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Unknown Transition P (for simplicity assume reward is known)

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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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Optimistic planning with learned model: $\pi^n = \text{Value-Iter}\left(\{ \widehat{P}_h^n, r_h + b_h^n \}_{h=1}^{H-1} \right)$

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

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

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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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]

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

High-level Idea: Exploration or Exploitation Tradeoff

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

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

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:

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

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

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

Recall simulation lemma — the lemma measures the difference of a policy under two MDPs

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

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

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

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

4. Upper bounding Regret via Simulation Lemma

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

But $\widehat{V}_h^n$ is data-dependent
(this is different from $V_h^\star$) !!!

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

Let's do Holder's inequality

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

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

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

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

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

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

5. Final Step

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

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

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

$$\leq \sum_{h=0}^{H-1}\sqrt{SAN} = H\sqrt{SAN}$$

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

$$\le \sum_{h=0}^{H-1}\sqrt{SAN} = H\sqrt{SAN}$$

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

5. Final Step

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

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

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

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

$$\epsilon \leq \widehat{V}_0^n(s_0) - V_0^{\pi^n}(s_0) \leq \sum_{h=0}^{H-1} \mathbb{E}_{s,a\sim d_h^{\pi^n}} \left[b_h^n(s,a) + \left(\widehat{P}_h^n(\cdot \mid s,a) - P_h(\cdot \mid s,a) \right) \cdot \widehat{V}_{h+1}^n \right]$$

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