STATS 701 – Theory of Reinforcement Learning
Stochastic Bandit Problems

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Slide Credits: Alan Malek @ DeepMind

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Protocol

Protocol: Stochastic Bandits

Given: game length T, number of arms K, reward distributions $\nu_1, \ldots, \nu_K$

For $t = 1, 2, \ldots, T$,

- The learner picks action $I_t \in \{1, \ldots, K\}$
- The learner observes and receives reward $X_t \sim \nu_{I_t}$

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- Stochastic bandits is an old problem [Thompson, 1933]
- We will use the following notation
  - Reward of arm i is sampled from ν_i with $\mu_i := \mathbb{E}_{X \sim \nu_i}[X]$
  - $i^* = \arg\max_i \mu_i$ is the best arm
  - Gaps $\Delta_i := \mu_{i^*} - \mu_i \geq 0$,
  - Number of pulls $N_{i,t} := \sum_{s=1}^{t} \mathbb{1}_{\{I_s = i\}}$
  - Empirical mean $\hat{\mu}_{i,t} := \frac{\sum_{s=1}^{t} X_s \mathbb{1}_{\{I_s = i\}}}{N_{i,t}}$

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- We still want to minimize the expected regret, which has the useful decomposition

$$\mathbb{E}[\mathcal{R}_T] = T\mu_{i^*} - \sum_{t=1}^{T} \mathbb{E}[X_t] = \sum_i \Delta_i \mathbb{E}[N_{i,T}]$$

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Assumption: 1-sub-Gaussian reward distributions

For all stochastic bandit problems, we will assume that all arms are 1-sub-Gaussian, i.e. $\mathbb{E}_{X\sim\mu}[e^{\lambda(X-\mu)^2-\lambda^2/2}] \leq 1$. For $X_1, \ldots, X_t$, This implies the Hoeffding bound

$$P\left(\frac{1}{t}\sum_{s=1}^{t} X_s - \mu_i \geq \epsilon\right) \leq e^{-\frac{\epsilon^2 t}{2}}.$$

Warm-up: Explore-Then-Commit

Algorithm: Explore-Then-Commit

Given: Game length T, exploration parameter M

For $t = 1, 2, \ldots, MK$:

- Choose $i_t = (t \mod K)$, see $X_t \sim \nu_{i_t}$

Compute empirical means $\hat{\mu}_{i,mK}$

For $t = MK + 1, MK + 2, \ldots, T$:

- Pull arm $i = \arg\max_i \hat{\mu}_{i,mK}$

- The first strategy you might try
- A proof idea that we will return to: bound regret by first bounding $\mathbb{E}[N_{i,T}]$.
- In this simple algorithm,

$$\mathbb{E}[N_{i,T}] = M + (T - MK) P\left(i = \arg\max_j \hat{\mu}_{j,MK}\right)$$

Explore-Then-Commit Upper Bound

Using the sub-Gaussian concentration bound,

$$
\begin{aligned}
P\left(i = \arg\max_j \hat{\mu}_{j,MK}\right) &\le P\left(\hat{\mu}_{i,MK} \ge \hat{\mu}_{i^*,MK}\right) \\
&= P\left((\hat{\mu}_{i,MK} - \mu_i) \ge (\hat{\mu}_{i^*,MK} - \mu_{i^*}) + \Delta_i\right) \\
&\le e^{-\frac{M\Delta_i^2}{4}} \text{ (the difference is } \sqrt{2/M}\text{-sub-Gaussian)}
\end{aligned}
$$

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\end{aligned}
$$

Theorem (Explore-Then-Commit upper bound)

$$
\mathbb{E}[\mathcal{R}_T] = \sum_i \Delta_i \mathbb{E}[N_{i,T}] \leq \sum_{i=1}^{K} \Delta_i \left(M + (T - MK)e^{-\frac{M\Delta_i^2}{4}}\right)
$$

- For the two arm case, if we know Δ, then $m = \frac{4}{\Delta_1^2} \log \frac{T\Delta_1^2}{4}$, results in $\mathbb{E}[\mathcal{R}_T] \leq \sum_{i=1}^{K} \frac{4}{\Delta_1} \log \frac{T\Delta_1^2}{4} + T\frac{4}{T\Delta_1^2} = O\left(\frac{K\log(T)}{\Delta_1}\right)$
- But we don't know Δ...can we be adaptive?

Algorithm Design Principle: OFU

- OFU: Optimism in the Face of Uncertainty
- We establish some confidence set for the problem instance (e.g. means) to within some confidence set
- We then assume the most favorable instance in the confidence set and act greedily

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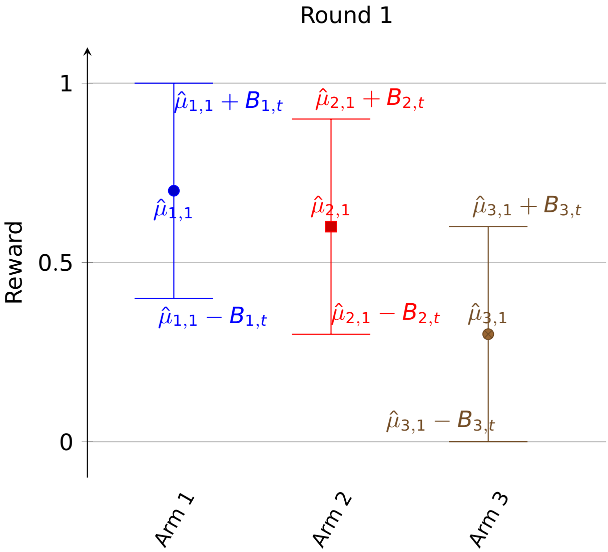
Algorithm: UCB1 [Auer et al., 2002]

Given: Game length T
Initialize: play every arm once
For $t = K+1, 2, \ldots, T$:

- Compute upper confidence bounds $B_{i,t-1} = \sqrt{\frac{6\log(t)}{N_{i,t-1}}}$
- Choose $I_t = \arg\max_i \hat{\mu}_{i,t-1} + B_{i,t-1}$, observe $X_t \sim \nu_{I_t}$
- Update $N_{i,t} = N_{i,t-1} + \mathbb{1}_{\{I_t=i\}}$ and $\hat{\mu}_{i,t} = \frac{\sum_{s=1}^{t} \mathbb{1}_{\{I_s=i\}} X_s}{N_{i,t}}$

UCB Illustration



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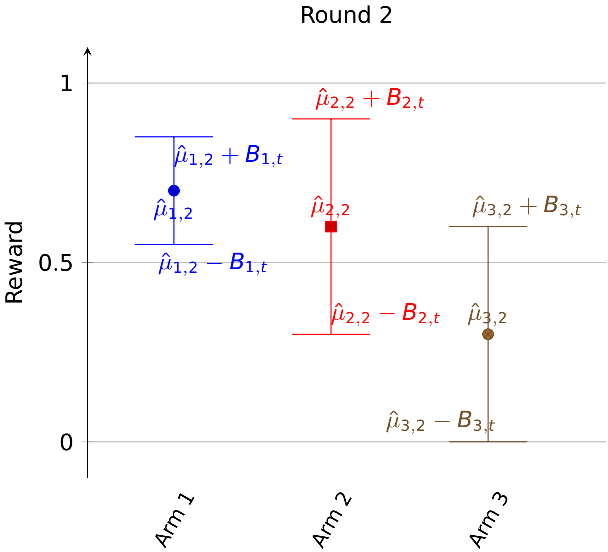

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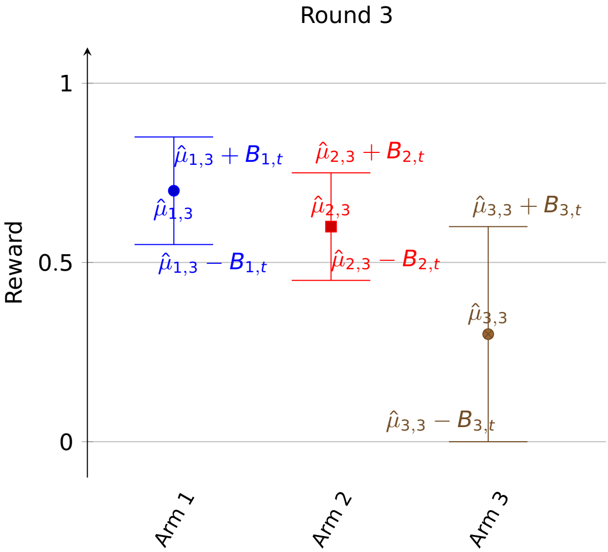


UCB: Intuition

- Naturally balances exploration and exploitation: an arm has a high UCB if
  - It has a high $\hat{\mu}_{i,t}$, or
  - $B_{i,t}$ is large because $N_{i,t-1}$ is small
- Optimistic because we pretend the rewards are the plausibly best and then do the greedy thing

UCB: Analysis

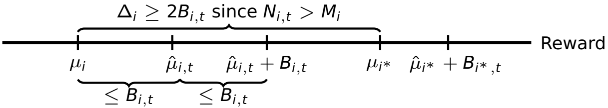
- Define $M_i = \left\lceil \frac{12\log(T)}{\Delta_i^2} \right\rceil$, the number of pulls of arm i such that $B_{i,t} = \sqrt{\frac{6\log(t)}{N_{i,t}}} \leq \sqrt{\frac{6\log(T)}{N_{i,t}}} \leq \frac{\Delta_i}{2}$
- The intuition of the proof is
  1. Since $\overline{\mathcal{R}_T} = \sum_i \Delta_i \mathbb{E}[N_{i,T}]$, we bound $\mathbb{E}[N_{i,t}]$ first.
  2. With high probability, we will never pull arm i more than M_i times, so

$$\mathbb{E}[N_{i,T}] = \mathbb{E}\sum_{t=1}^{T} \mathbb{1}_{\{I_t=i\}} \leq M_i + \sum_{t=M_i}^{T} \underbrace{\mathbb{E}\mathbb{1}_{\{I_t=i, N_{i,t}>M_i\}}}_{\text{we will bound this}}$$

  3. If $\{I_t = i, N_{i,t} > M_i\}$ occurs, then the UCB for i^* or for i must be wrong (next slide)

UCB: Analysis

Claim: if $\{I_t = i, N_{i,t} > M_i\}$ occurs, then either $\hat{\mu}_{i,t}$ must be too high or $\hat{\mu}_{i^*,t}$ must be too low. In a picture:



In an equation: suppose that $N_{i,t} > M_i$, $\hat{\mu}_{i,t} - B_{i,t} < \mu_i$, and $\hat{\mu}_{i^*,t} + B_{i^*,t} > \mu_{i^*}$. Then

$$\hat{\mu}_{i^*,t} + B_{i^*,t} > \mu_{i^*} = \mu_i + \Delta_i \geq \mu_i + \underbrace{2B_{i,t}}_{\text{by choice of } B_{i,t}} > \hat{\mu}_{i,t} + B_{i,t},$$

so the algorithm will not choose $I_t = i$.
If $I_t = i$, at least one of the bounds must be wrong, implying

$$P(I_t = i, N_{i,t} > M_i) \leq P\left(\hat{\mu}_{i,t} \geq \mu_i + B_{i,t}\right) + P\left(\hat{\mu}_{i^*,t} + B_{i^*,t} \leq \mu_{i^*}\right).$$

UCB: Analysis

Using the Hoeffding bound,

$$P\left(\hat{\mu}_{i,t} - \mu_i \leq B_{i,t}\right) \leq P\Bigg(\underbrace{\exists s \leq t}_{\text{we don't know } N_{i,t-1}} : \hat{\mu}_{i,s} - \mu_i \leq \sqrt{\frac{6\log(t)}{s}}\Bigg)$$

$$\leq \sum_{s=1}^{t} P\left(\hat{\mu}_{i,s} - \mu_i \leq \sqrt{\frac{6\log(t)}{s}}\right)$$

$$\leq \sum_{s=1}^{t} \exp\left\{-\frac{3\log(t)}{s}\right\} \leq \sum_{s=1}^{t} t^{-3} = t^{-2}.$$

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The same inequality holds for i^*, so

$$\overline{\mathcal{R}_T} = \sum_i \Delta_i \mathbb{E}[N_{i,T}] \le \sum_i \Delta_i \left(\frac{12\log(T)}{\Delta_i^2} + 2\sum_{t=M_i+1}^{T} t^{-2}\right).$$

UCB: Analysis

Theorem (UCB upper bound [Auer, 2002])

The UCB1 algorithm on 1-sub-Gaussian data has

$$\overline{\mathcal{R}_T} \leq \sum_i \frac{12 \log(T)}{\Delta_j} + o(1).$$

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Theorem (Lower Bound [Lai and Robbins, 1985])

Suppose we have a parametric family P_θ and $\theta_1, \ldots, \theta_k$. For any "admissible" algorithm,

$$\liminf_{T\to\infty} \frac{\overline{R_T}}{\log(T)} \geq \sum_{i\neq i^*} \frac{\Delta_i}{KL(P_{\theta_i}, P_{\theta_{i^*}})} \approx O\left(\sum_{i\neq i^*} \frac{1}{\Delta_i}\right)$$

E.g. if P_θ is Bernoulli, then $\frac{(\theta_i-\theta_{i^*})^2}{\theta_{i^*}(1-\theta_{i^*})} \geq KL(P_{\theta_i}, P_{\theta_{i^*}}) \geq 2(\theta_i - \theta_{i^*})^2$.

Algorithm Design Principle: Probability Matching

- We put a prior π over means μ_i and a likelihood $\nu_i = P(\cdot|\mu_i)$ over rewards
- Choose $P(I_t = i) = P(\mu_i = \mu_{i^*}|\mathit{history})$ (the matching)
- We usually pick conjugate models (e.g. $\mu_i \sim N(0,1)$, $X_t \sim N(\mu_i, 1)$)

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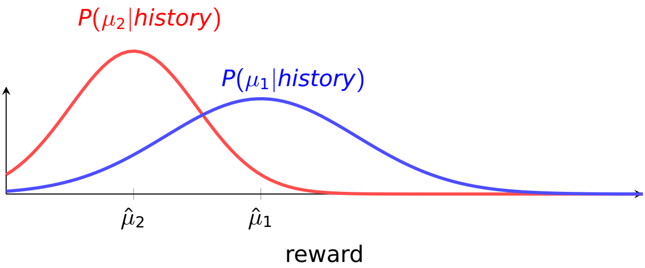
Algorithm: Thompson Sampling

Given: game length T, prior $\pi(\mu)$, likelihoods $p(\cdot|\mu)$
Initialize posteriors $p_{i,0}(\mu) = \pi(\mu)$

For $t = 1, 2, \ldots, T$:

- Draw $\theta_{i,t} \sim p_{i,t-1}$ for all i
- Choose $I_t = \arg\max_i \theta_{i,t}$ (implements the matching)
- Receive and observe $X_t \sim \nu_{I_t}$
- Update the posterior $p_{I_T,t}(\mu) = p(X_t|\mu) p_{I_t,t-1}(\mu)$

Thompson Sampling: Overview



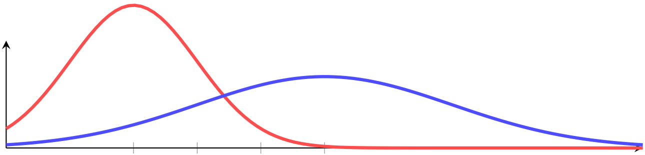
- *Not* Bayesian: a Bayesian method would maximize the Bayes regret (the expectation under the probability model)
- The regret bound is frequentist
- Arms with small $N_{i,t}$ implies a wide posterior, hence a good probability of being selected
- Generally performs empirically better that UCB (it is much more aggressive)
- Analysis is difficult

Thompson Sampling: Upper Bound

Theorem (Agrawal and Goyal [2013])

For binary rewards, Gamma-Beta Thompson sampling has
$\mathbb{E}[R_T] \leq (1+\epsilon)\sum_{i\neq i^*} \Delta_i \frac{\log(T)}{KL(\mu_i,\mu_{i^*})} + O\left(\frac{N}{\epsilon^2}\right)$.

- The proof is much more technical that UCB's
- We cannot rely on the upper bounds being correct w.h.p.



For some to-be-tuned $\mu_i \leq x_i \leq y_i \leq \mu_{i^*}$, we have

$$\begin{aligned}
\mathbb{E}[N_{i,T}] &\leq \sum_{t=1}^{T} P(I_t = i) \\
&\leq \sum_{t=1}^{T} P(I_t = i, \hat{\mu}_{i,t-1} \leq x_i, \theta_{i,t} \geq y_i) && \left(O\left(\frac{\log(T)}{kl(x_j, y_j)}\right)\right) \\
&\quad + \sum_{t=1}^{T} P(I_t = i, \hat{\mu}_{i,t-1} \leq x_i, \theta_{i,t} \leq y_i) && \text{(the tricky case)} \\
&\quad + \sum_{t=1}^{T} P(I_t = i, \hat{\mu}_{i,t-1} \geq x_i) && \text{(Small by concentration)}
\end{aligned}$$

Thompson Sampling: Proof Outline

- The tricky case is $\sum_{t=1}^{T} P(I_t = i, \hat{\mu}_{i,t-1} \leq x_i, \theta_{i,t} \leq y_i)$
- This happens when we have enough samples of i but not many of i^*
- A key lemma argues that, on $\hat{\mu}_{i,t-1} \leq x_i, \theta_{i,t} \leq y_i$, the probability of picking i is a constant less than of picking i^*:

$$\sum_{t=1}^{T} P(I_t = i, \hat{\mu}_{i,t-1} \leq x_i, \theta_{i,t} \leq y_i)$$
$$\leq \sum_{t=1}^{T} \underbrace{\frac{P(\theta_{i^*,t} \leq y_i)}{P(\theta_{i^*,t} > y_i)}}_{\text{exponentially small}} P(I_t = i^*, \hat{\mu}_{i,t-1} \leq x_i, \theta_{i,t} \leq y_i) = O(1)$$

- Hence, we will quickly get enough samples of i^*

Best of Both Worlds

- The stochastic and adversarial algorithms are quite different
- A natural question: is there an algorithm that
  - gets $\mathcal{R}_T = O(\sqrt{TK})$ regret for adversarial
  - gets $\mathcal{R}_t = O(\sum_i \log(T)/\Delta_i)$ regret for stochastic
  - without knowing the setting?

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    - without knowing the setting?
- Bubeck and Slivkins [2012] proposed an algorithm that assumes stochastic but falls back to UCB once adversarial data is detected
- Zimmert and Seldin [2019] showed that (for pseudo-regret), it is possible
    - Their algorithm: online mirror descent with $\frac{1}{2}$-Tsallis entropy
    - $\Psi(w) = -\sum_i 4(\sqrt{w_i} - \frac{1}{2} w_i)$

A New Problem

- What if we only wanted to identify the best arm i^* without caring about loss along the way?
- Intuitively, we would explore more; we are happy to accrue less reward if we get more useful samples.
- More similar to hypothesis testing; useful for selecting treatments
- Known as “Best Arm Identification” or “Pure Exploration”

Two Settings

Protocol: Best-arm Identification

Given:number of arms K, arm distributions $\nu_1, \ldots, \nu_K$

For $t = 1, 2, \ldots,$

- The learner picks arm $I_t \in \{1, \ldots, K\}$
- The learner observes $X_t \sim \nu_{I_t}$
- The learner decides whether to stop

The learner returns arm A

Two settings:

	fixed-confidence	*fixed-budget*
Input	$\delta > 0$,	T
Goal	$P(A = i^*) \geq 1 - \delta$	maximize $P(A = i^*)$
Stopping	once learner is confident	after T rounds

- Standard stochastic bandit algorithms under explore (they fail to meet lower bounds on this problem)
- Many can be adapted
  - LUCB [Kalyanakrishnan et al., 2012]
  - Top-Two Thompson Samping [Russo, 2016]
- Instead, we will describe a new algorithm design principle

Algorithm Design Principle: Action Elimination

Algorithm: Successive Elimination

Given: confidence $\delta > 0$
Initialize plausibly-best set $S = \{1, \ldots, K\}$

For $t = 1, 2, \ldots$:

- Pull all arms in S and update $\hat{\mu}_{i,t}$
- Calculate $B_t = \sqrt{2t^{-1} \log(4Kt^2/\delta)}$
- Remove i from S if $\underbrace{\max_{j \in S} \hat{\mu}_{j,t} - B_t}_{\text{Lowest } \mu_i^* \text{ could be}} \geq \underbrace{\hat{\mu}_{i,t} + B_t}_{\text{highest } \mu_i \text{ could be}}$
- If $|S| = 1$, stop and return $A = S$.

- S is a list of plausibly-best arms
- Each epoch, all arms that cannot be the best (if the bounds hold) are removed

Successive Elimination Analysis

- Define the "bad event" $\mathcal{E} = \bigcup_{i,t}\{|\hat{\mu}_{i,t} - \mu_i| \geq B_t(\delta)\}$: we have

$$P(\mathcal{E}) \leq \sum_{i,t} P\left(|\hat{\mu}_{i,t} - \mu_i| \geq \sqrt{2t^{-1}\log(4Kt^2/\delta)}\right) \leq \sum_{i,t} 2e^{-\log\left(\frac{4Kt^2}{\delta}\right)}$$

$$\leq \sum_{i,t} \frac{2\delta}{4Kt^2} = \frac{2\pi^2}{24}\delta \leq \delta$$

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- (Correctness) If $\mathcal{E}$ does not happen,
  - $|\hat{\mu}_{i^*} - \mu_{i^*}| \leq B_t$ and $|\mu_j - \hat{\mu}_j| \leq B_t$ for all j. Thus, for all j $\hat{\mu}_j - \hat{\mu}_{i^*} \leq (\mu_{i^*} - \hat{\mu}_{i^*}) + (\mu_j - \mu_{i^*}) + (\hat{\mu}_j - \mu_j) \leq 2B_t$
  - i is removed if $\max_{j \in S} \hat{\mu}_{j,t} - \hat{\mu}_{i,t} \geq 2B_t \Rightarrow i^*$ is never removed
  - $\lim_{t\to\infty} B_t(\delta) \to 0$: every arm will eventually be removed
  - Successive Elimination is correct with probability $1 - \delta$

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  - i is removed if $\max_{j\in S}\hat{\mu}_{j,t} - \hat{\mu}_{i,t} \geq 2B_t \Rightarrow i^*$ is never removed
  - $\lim_{t\to\infty} B_t(\delta) \to 0$: every arm will eventually be removed
  - Successive Elimination is correct with probability $1 - \delta$
- (Sample Complexity): arm i will be eliminated once $\Delta_i \leq 2B_t$
  - We can verify that $N_i = O\left(\Delta_i^{-2}\log(K/\delta\Delta_i)\right)$ is sufficient
  - Total sample complexity of $\sum_i \Delta_i^{-2}\log(K/\delta\Delta_i)$

Theorem

Successive Elimination is $(0, \delta)$-PAC with sample complexity

$$O\left(\sum_i \Delta_i^{-2} \log(K/\delta\Delta_i)\right)$$

Theorem

For any best-arm identification algorithm, there is a problem instance that requires

$$\Omega\left(\sum_i \Delta_i^{-2} \log\log\left(\frac{1}{\delta\Delta_i^2}\right)\right)$$

samples.

Review

- Setting: adversarial bandits
  - Exp3 (exponential weights)
- Setting: stochastic bandits
  - ETC (Explore-Then-Commit)
  - UCB (optimism)
  - Thompson Sampling (probability matching)
- Setting: pure exploration
  - Successive Elimination (action-elimination)

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