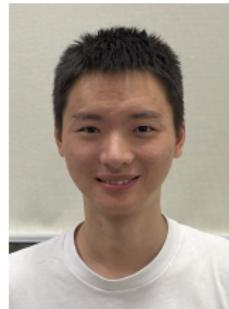


Almost Optimal Variance-Constrained Best Arm Identification

Yunlong Hou



Zixin Zhong

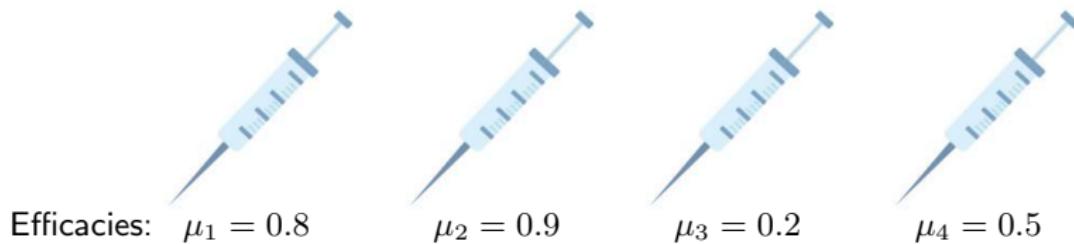


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National University of Singapore

S3 Optimization Day July 2022
IORA, NUS

Introduction to Stochastic Multi-Armed Bandits in BAI



- In clinical trials, there are N potential treatments for a disease.
- At each time, the scientist prescribes one of them to each lab animal and the efficacies of the treatments can be observed.
- Goal: Find the best treatment using the smallest number of trials.

Formulation of Stochastic Multi-Armed Bandits in BAI

- N arms: $[N] = \{1, 2, \dots, N\}$ with **unknown distributions** $\{\nu_i\}_{i=1}^N$

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$$\mathcal{H}_r = ((i_1, X_{1,i_1}), \dots, (i_{r-1}, X_{r-1,i_{r-1}}))$$

and observe the **reward** $X_{r,i_r} \sim \nu_{i_r}$

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- Goal: Design a policy to find the arm with the **highest expectation** (best arm) in the **smallest number of rounds**.
- **Probably approximately correct (PAC)** framework (Even-Dar et al., 2006). Given a fixed confidence parameter δ , find any $i \in [N]$ s.t.

$$\mathbb{P}\left[i \in \arg \max_{j \in [N]} \mu_j\right] \geq 1 - \delta.$$

Introduction to BAI

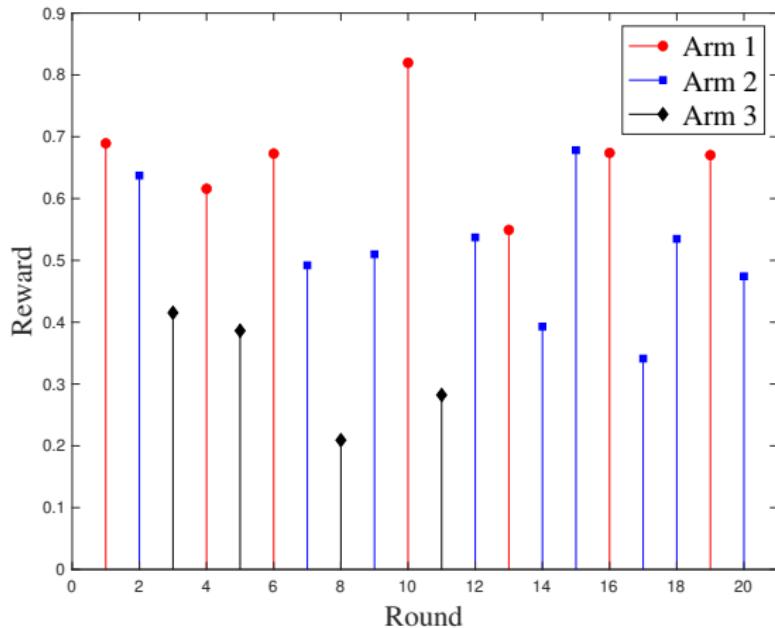


Figure 1: An illustration of a 3-arm BAI problem. At each round, only one arm is sampled and the reward is observed.

Motivation of Risk-Aware BAI

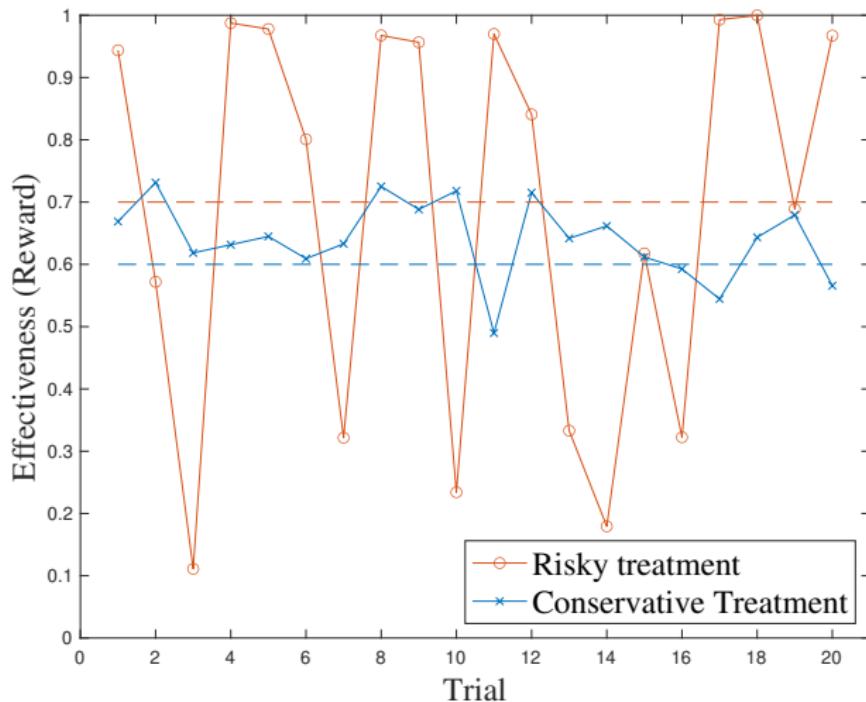
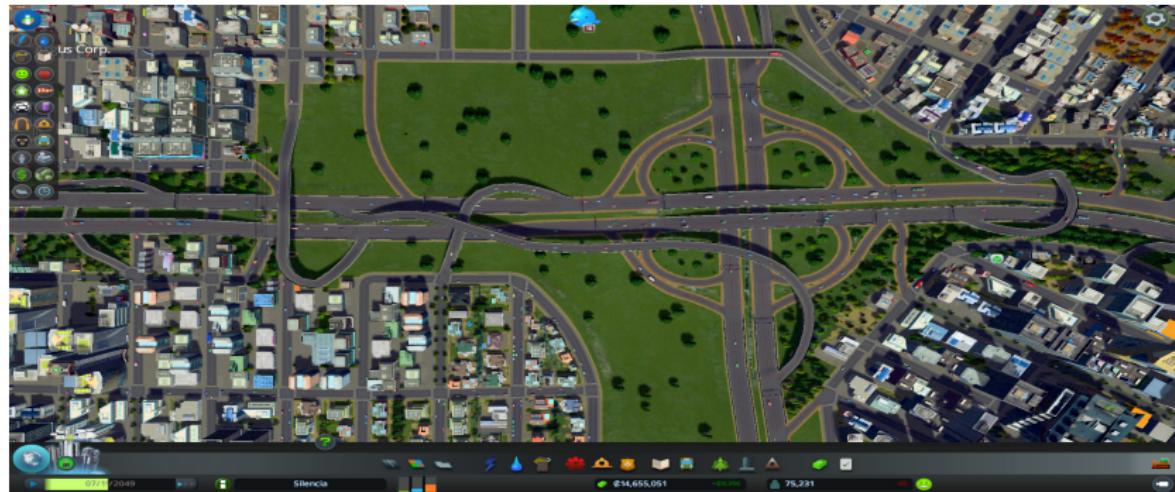


Figure 2: An example of risk-aware BAI: Clinical trials

Another motivation: Going to office bandit style



On every day

- ① Pick a route to office
- ② Reach office and record (suffered) delay



Why consider risk?



$\mathbb{E}[\text{time}] = 10 \text{ mins}, \text{Var}(\text{time}) = 10$

$\mathbb{E}[\text{time}] = 11 \text{ mins}, \text{Var}(\text{time}) = 0.1$

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$$\mathbb{E}[\text{time}] = 10 \text{ mins}, \text{Var}(\text{time}) = 10 \quad \mathbb{E}[\text{time}] = 11 \text{ mins}, \text{Var}(\text{time}) = 0.1$$

- Delays are stochastic.
- In choosing between routes, we **need not necessarily** want to minimize expected delay.
- Two route scenario: Average delay of Route 1 slightly below that of Route 2.
- Route 1 has a **small** chance of **very** high delay, e.g., jams.
- I might prefer Route 2.

Introduction to Risk-Aware Bandits

- Incorporate the risk into the quality measure:
 - ▶ Mean-variance: Sani et al. (2012), Vakili and Zhao (2016), and Zhu and Tan (2020).
 - ▶ Value-at-Risk or α -quantile: David and Shimkin (2016)
 - ▶ Conditional Value-at-risk (CVaR): Kagrecha et al. (2020) and Baudry et al. (2021)

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 - ▶ Conditional Value-at-risk (CVaR): Kagrecha et al. (2020) and Baudry et al. (2021)
- Risk-constrained problem, i.e., conventional BAI with constraints
 - ▶ Variance
 - ▶ α -quantile: David et al. (2018)
 - ▶ Safe bandits: Wu et al. (2016); Amani et al. (2019)

Introduction to Variance-Constrained BAI

An **instance** ($\nu = \{\nu_i\}_{i=1}^N, \bar{\sigma}^2$) consists of

- N arms with associated with **unknown reward distributions** $\{\nu_i\}_{i=1}^N$, where arm i follows ν_i with **expectation** μ_i and **variance** σ_i^2 .
- permissible **upper bound on the variance**: $\bar{\sigma}^2$.

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- Variance gap $\Delta_i^v = |\sigma_i^2 - \bar{\sigma}^2|$

Introduction to Variance-Constrained BAI

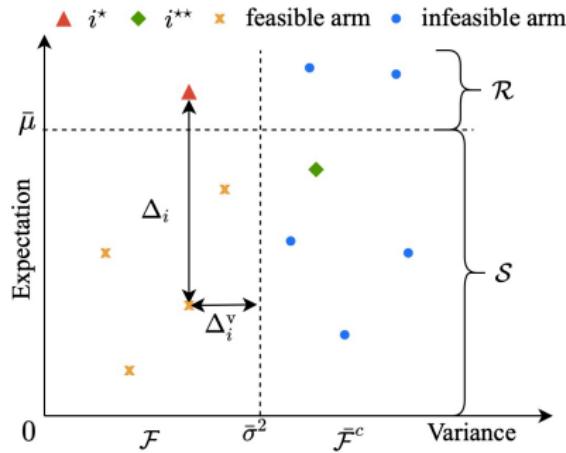


Figure 3: An illustration of an instance

Introduction to Variance-Constrained BAI

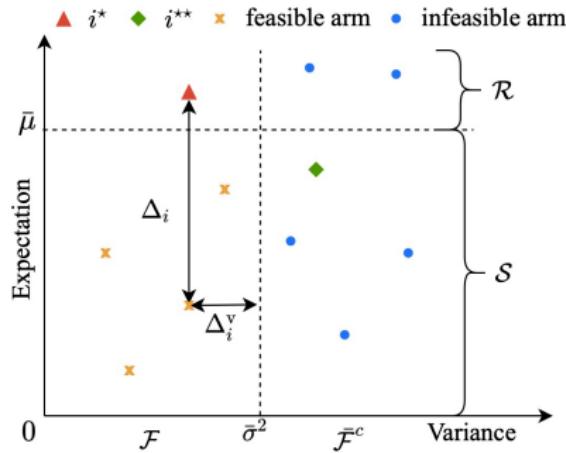


Figure 3: An illustration of an instance

Goal: Minimize the number of arm pulls needed for

- Ascertaining the feasibility of the instance $(\nu, \bar{\sigma}^2)$;
- Finding the best feasible arm i^* if $\mathcal{F} \neq \emptyset$

with probability $\geq 1 - \delta$

Main Result: Upper Bound

Theorem 1 (Upper bound)

Define the hardness parameter

$$H_{\text{VA}} := \frac{1}{\min\left\{\frac{\Delta_{i^*}}{2}, \Delta_{i^*}^v\right\}^2} + \sum_{i \in \mathcal{F} \cap \mathcal{S}} \frac{1}{\left(\frac{\Delta_i}{2}\right)^2} \\ + \sum_{i \in \bar{\mathcal{F}}^c \cap \mathcal{R}} \frac{1}{(\Delta_i^v)^2} + \sum_{i \in \bar{\mathcal{F}}^c \cap \mathcal{S}} \frac{1}{\max\left\{\frac{\Delta_i}{2}, \Delta_i^v\right\}^2}.$$

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Given an instance $(\nu, \bar{\sigma}^2)$ with probability at least $1 - \delta$, our proposed algorithm **VA-LUCB** succeeds and terminates in

$$O\left(H_{\text{VA}} \ln \frac{H_{\text{VA}}}{\delta}\right)$$

time steps.

Main Result: Lower Bound and Almost-Tightness

Theorem 2 (Lower bound)

Given any instance $(\nu, \bar{\sigma}^2)$ with $\bar{\sigma}^2 \in (0, 1/4)$, the optimal expected time complexity τ_δ^* satisfies

$$\tau_\delta^* = \Omega \left(H_{\text{VA}} \ln \frac{1}{\delta} \right).$$

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Corollary 3 (Almost optimality of VA-LUCB)

Given any instance $(\nu, \bar{\sigma}^2)$ and variance threshold $\bar{\sigma}^2 \in (0, \frac{1}{4})$,

$$\tau_\delta^* = \tilde{\Theta}\left(H_{\text{VA}} \ln \frac{1}{\delta}\right),$$

which is achieved by VA-LUCB.

Interpretation of Hardness Parameter I

Hardness parameter:

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- Ascertain **optimality** and **feasibility** of i^* ;
- Ascertain **suboptimality** of arms in the feasible and suboptimal set;
- Ascertain **infeasibility** of risky and infeasible arms;
- Ascertain either **infeasibility** or **suboptimality** of arms in infeasible and suboptimal set.

Interpretation of Hardness Parameter II

Hardness Parameter

$$H_{VA} := \frac{1}{\min\{\frac{\Delta_{i^*}}{2}, \Delta_{i^*}^v\}^2} + \sum_{i \in \mathcal{F} \cap \mathcal{S}} \frac{1}{(\frac{\Delta_i}{2})^2} \\ + \sum_{i \in \bar{\mathcal{F}}^c \cap \mathcal{R}} \frac{1}{(\Delta_i^v)^2} + \sum_{i \in \bar{\mathcal{F}}^c \cap \mathcal{S}} \frac{1}{\max\{\frac{\Delta_i}{2}, \Delta_i^v\}^2}.$$

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$$H_{VA} := \frac{1}{\min\left\{\frac{\Delta_i^*}{2}, \cancel{\Delta_i^y}\right\}^2} + \sum_{i \in \mathcal{F} \cap \mathcal{S}} \frac{1}{\left(\frac{\Delta_i}{2}\right)^2}$$
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As $\bar{\sigma}^2 \rightarrow \infty$,

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As $\bar{\sigma}^2 \rightarrow \infty$,

$$H_{\text{VA}} = H_{\text{VA}}(\bar{\sigma}^2) \longrightarrow \tilde{H}_1 = \sum_{i \in [N]} \frac{4}{\Delta_i^2} \quad \text{and} \quad 4 H_1 \leq \tilde{H}_1 \leq 8 H_1$$

where

$$H_1 := \sum_{i \neq i^*} \frac{1}{\Delta_i^2}.$$

Particularizes to classical **unconstrained result** (Even-Dar et al., 2006).

VA-LUCB

Concentration inequalities (for distributions bounded on $[0, 1]$):

Lemma 4 (Implication of Hoeffding's and McDiarmid's Inequalities)

Given an instance $(\nu, \bar{\sigma}^2)$, for any arm i with $T_i(t) \geq 2$ and $\varepsilon > 0$ we have

$$\mathbb{P}[|\hat{\mu}_i(t) - \mu_i| \geq \varepsilon] \leq 2 \exp(-2T_i(t)\varepsilon^2)$$

and

$$\mathbb{P}[|\hat{\sigma}_i^2(t) - \sigma_i^2| \geq \varepsilon] \leq 2 \exp(-2T_i(t)\varepsilon^2)$$

where

- $T_i(t)$ is the number of times arm i is sampled before time t ;
- $\hat{\mu}_i(t)$ is the **sample mean** of arm i at time t ;
- $\hat{\sigma}_i^2(t)$ is the **unbiased sample variance** of arm i at time t .

VA-LUCB: Confidence Bounds

- With high probability,

$$\mu_i \in [\hat{\mu}_i(t) - \varepsilon, \hat{\mu}_i(t) + \varepsilon] =: [L_i^\mu(t), U_i^\mu(t)]$$

$$\sigma_i^2 \in [\hat{\sigma}_i^2(t) - \varepsilon, \hat{\sigma}_i^2(t) + \varepsilon] =: [L_i^\text{v}(t), U_i^\text{v}(t)]$$

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- Define good event

$$E = \bigcap_{t \in \mathbb{N}} \bigcap_{i \in [N]} \left\{ \mu_i \in [L_i^\mu(t), U_i^\mu(t)], \sigma_i^2 \in [L_i^\nu(t), U_i^\nu(t)] \right\}$$

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- At time step $t \in \mathbb{N}$ and for arm $i \in [N]$, take

$$\varepsilon = \sqrt{\frac{1}{2T_i(t)} \ln \left(\frac{2Nt^4}{\delta} \right)}$$

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- Event E occurs with probability at least $1 - \frac{\delta}{2}$.

VA-LUCB: Possibly Feasible Set

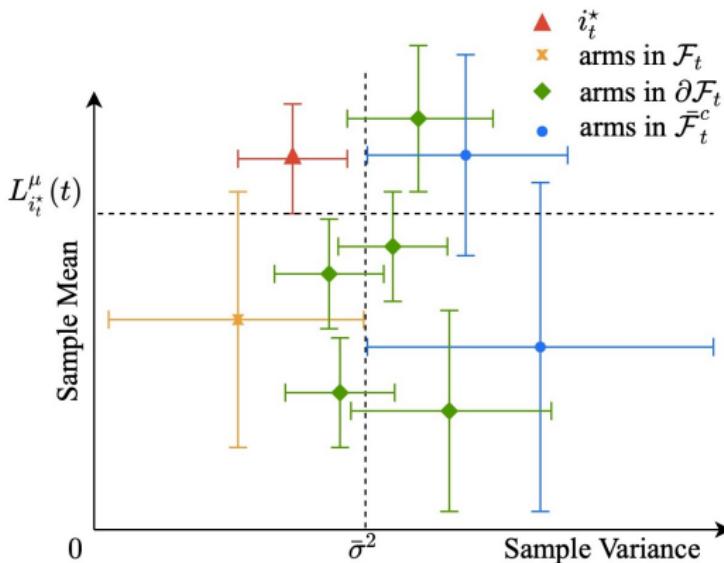


Figure 4: Illustration of the empirical sets. Each dot represents the sample mean and sample variance of each arm at time step t .

Possibly feasible set at time t is $\bar{\mathcal{F}}_t := \mathcal{F}_t \cup \partial\mathcal{F}_t$.

VA-LUCB: Sampling Strategy

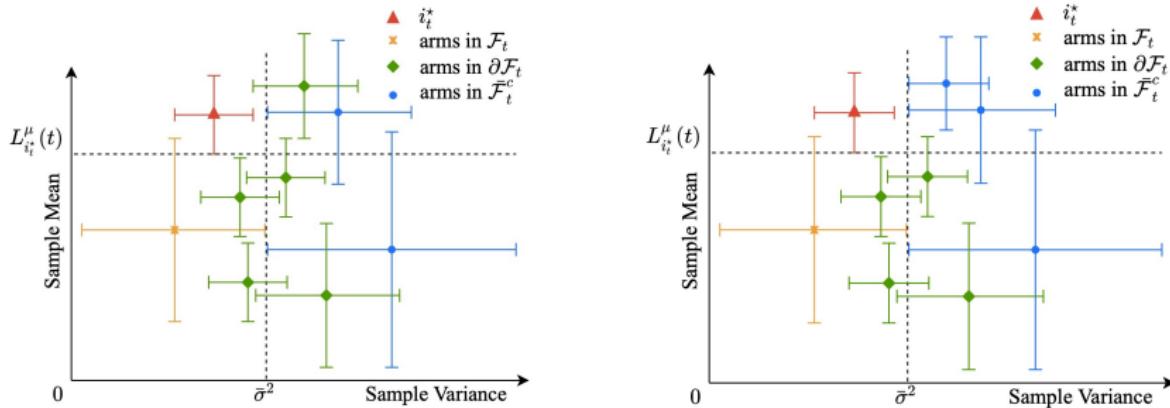


Figure 5: Illustration of the empirical sets.

VA-LUCB: Sampling Strategy

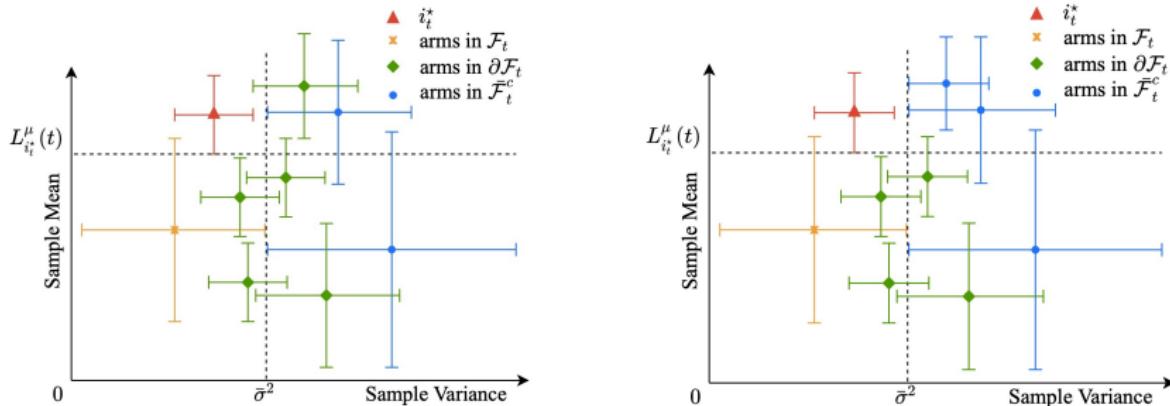


Figure 5: Illustration of the empirical sets.

- Empirical Leader $i_t := \operatorname{argmax} \{\hat{\mu}_i(t) : i \in \bar{\mathcal{F}}_t\}$

VA-LUCB: Sampling Strategy

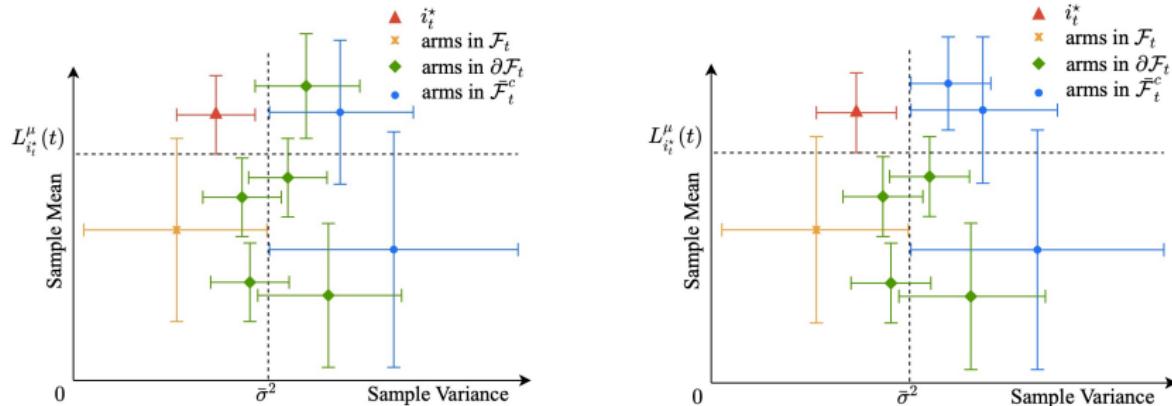


Figure 5: Illustration of the empirical sets.

- Empirical **Leader** $i_t := \operatorname{argmax} \{\hat{\mu}_i(t) : i \in \bar{\mathcal{F}}_t\}$
- Empirical **Challenger** $c_t := \operatorname{argmax} \{U_i^\mu(t) : i \in \bar{\mathcal{F}}_t \setminus \{i_t\}\}$.

VA-LUCB: Stopping Strategy

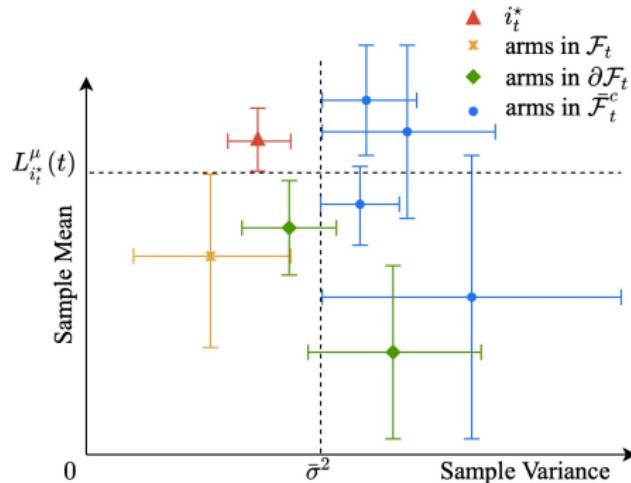


Figure 6: Illustration of the empirical sets.

VA-LUCB: Stopping Strategy

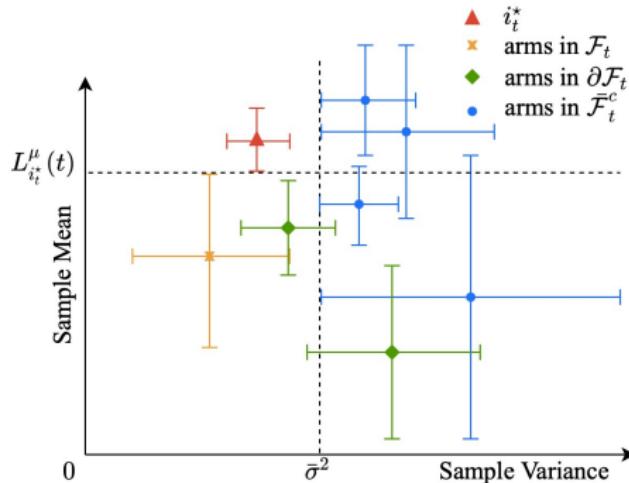


Figure 6: Illustration of the empirical sets.

- Potential set $\mathcal{P}_t := \begin{cases} \{i : L_{i_t^*}^{\mu}(t) \leq U_i^{\mu}(t), i \neq i_t^*\}, & \mathcal{F}_t \neq \emptyset \\ [N], & \mathcal{F}_t = \emptyset \end{cases}$
- Termination condition: $\bar{\mathcal{F}}_t \cap \mathcal{P}_t = \emptyset$.

Time/Sample Complexity of VA-LUCB

Enhance deployment and analysis of LUCB (Kalyanakrishnan et al., 2012)

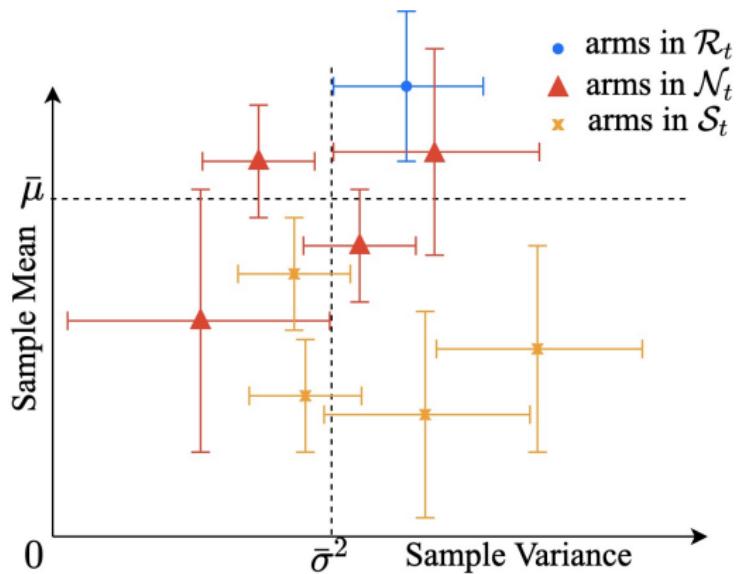


Figure 7: An illustration of the suboptimal and risky set.

Time/Sample Complexity of VA-LUCB

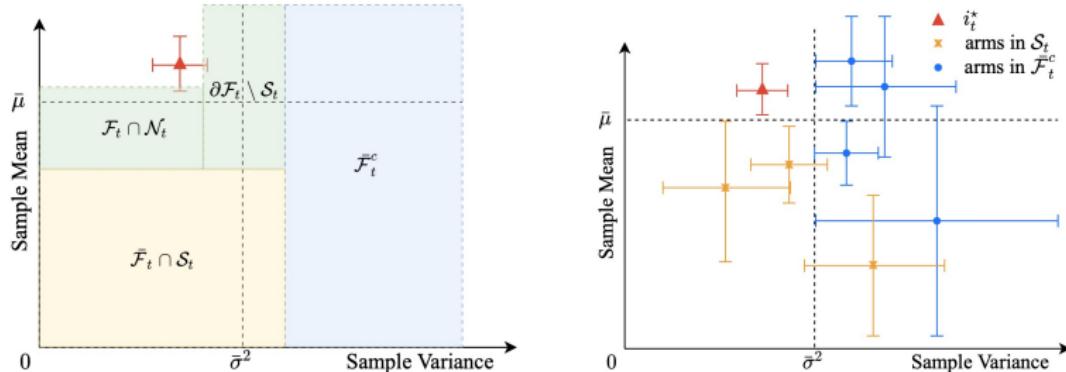


Figure 8: A scenario where all arms have been pulled sufficiently many times.

Time/Sample Complexity of VA-LUCB

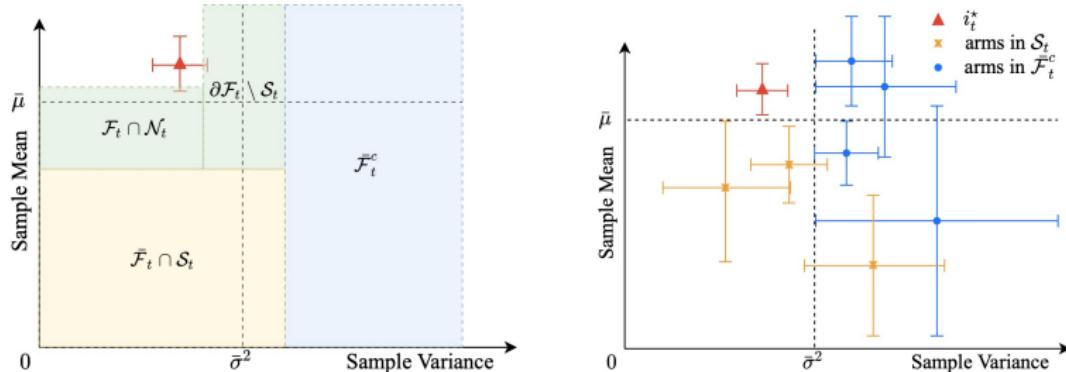


Figure 8: A scenario where all arms have been pulled sufficiently many times.

When **empirically potential best feasible arm set**

$$(\partial\mathcal{F}_t \setminus \mathcal{S}_t) \cup (\mathcal{F}_t \cap \mathcal{N}_t) = \emptyset,$$

VA-LUCB must stop.

Time/Sample Complexity of VA-LUCB

Lemma: Existence of Arms to Pull

On the event E , if VA-LUCB does not terminate, then at least one of the following statements holds:

- $i_t \in (\partial\mathcal{F}_t \setminus \mathcal{S}_t) \cup (\mathcal{F}_t \cap \mathcal{N}_t)$.
- $c_t \in (\partial\mathcal{F}_t \setminus \mathcal{S}_t) \cup (\mathcal{F}_t \cap \mathcal{N}_t)$.

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Need to compute the number of pulls needed for each arm i such that

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Lemma: Small Non-Termination Probability

Let $t^* := 152 H_{\text{VA}} \ln \frac{H_{\text{VA}}}{\delta}$. For any $t > t^*$,

$$\mathbb{P}\left[\text{VA-LUCB does not terminate} \mid E\right] \leq \frac{2\delta}{t^2}.$$

Experiment: VA-LUCB

- Recall the upper bound on τ_δ^* is $O\left(H_{\text{VA}} \ln \frac{H_{\text{VA}}}{\delta}\right)$ where

$$H_{\text{VA}} := \frac{1}{\min\{\frac{\Delta_{i^*}}{2}, \Delta_{i^*}^v\}^2} + \sum_{i \in \mathcal{F} \cap \mathcal{S}} \frac{1}{(\frac{\Delta_i}{2})^2} \\ + \sum_{i \in \bar{\mathcal{F}}^c \cap \mathcal{R}} \frac{1}{(\Delta_i^v)^2} + \sum_{i \in \bar{\mathcal{F}}^c \cap \mathcal{S}} \frac{1}{\max\{\frac{\Delta_i}{2}, \Delta_i^v\}^2}.$$

- Test the four terms individually

Experiment: VA-LUCB

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$$\begin{aligned} H_{\text{VA}} := & \frac{1}{\min\left\{\frac{\Delta_{i^*}}{2}, \Delta_{i^*}^v\right\}^2} + \sum_{i \in \mathcal{F} \cap \mathcal{S}} \frac{1}{(\frac{\Delta_i}{2})^2} \\ & + \sum_{i \in \bar{\mathcal{F}}^c \cap \mathcal{R}} \frac{1}{(\Delta_i^v)^2} + \sum_{i \in \bar{\mathcal{F}}^c \cap \mathcal{S}} \frac{1}{\max\left\{\frac{\Delta_i}{2}, \Delta_i^v\right\}^2}. \end{aligned}$$

- Test the four terms individually
- For example, change Δ_{i^*} and observe how sample complexity changes as a function of H_{VA} or $H_{\text{VA}} \ln \frac{H_{\text{VA}}}{\delta}$.

VA-LUCB: Exploring Effects of the Terms in H_{VA}

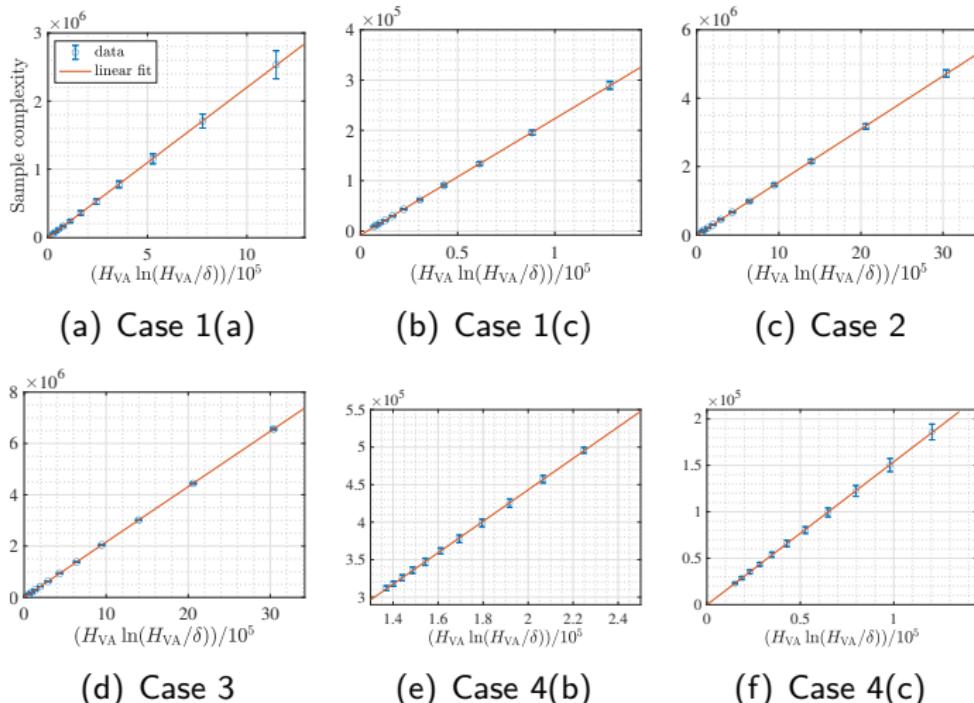


Figure 9: Time complexities with respect to $H_{VA} \ln(H_{VA}/\delta)$ with $\delta = 0.05$.

Experiment: Comparison to Competing Algorithms

- VA-UNIFORM: Randomly and uniformly sample two different arms at each time step.

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- RISKAVERSE-UCB-BAI: A variant of the algorithm proposed in David et al. (2018):
 - ▶ Sample $i_t = \operatorname{argmax} \{U_i^\mu(t) : i \in \bar{\mathcal{F}}_t\}$ (UCB type).
 - ▶ Terminate at time t when the confidence radius of the mean of i_t is smaller than ϵ_v .

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 - ▶ Terminate at time t when the confidence radius of the mean of i_t is smaller than ϵ_v .
 - ▶ Not parameter free: find the ϵ_v -approximately feasible and ϵ_μ -approximately optimal arm; the confidence radius involves H , the hardness parameter in David et al. (2018).
 - ▶ The upper bound is greater than that of VA-LUCB in sample complexity.
 - ▶ The lower bound is looser than ours for almost all instances.

Experiment: Comparison to Competing Algorithms

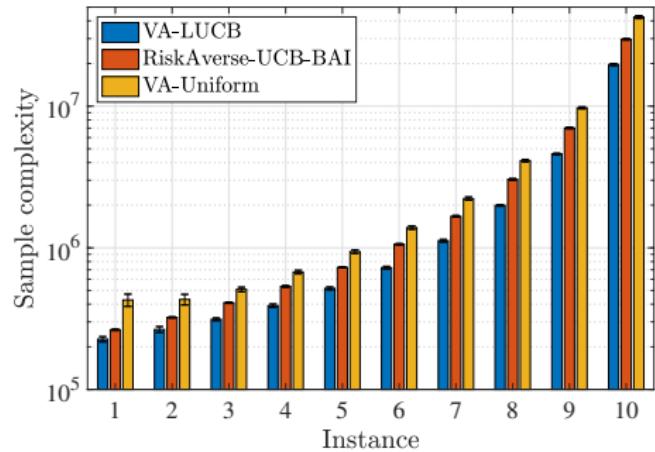
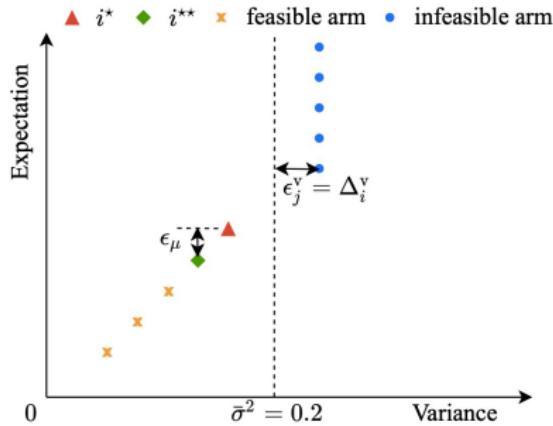


Figure 10: Parameter settings for instance $j \in [10]$. The variance gaps for the infeasible arms $\Delta_i^v = \epsilon_j^v = 0.233 - 0.003 \cdot j$ in instance $j \in [10]$.

Conclusion and Extensions

- Proposed a framework for risk-constrained best arm identification
- Developed an algorithm VA-LUCB whose time/sample complexity matches the information-theoretic lower bound (up to constants and log terms)

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- Proposed a framework for risk-constrained best arm identification
- Developed an algorithm VA-LUCB whose time/sample complexity matches the information-theoretic lower bound (up to constants and log terms)
- Future work 1: Development of tracking-based risk-constrained BAI algorithms that can nail down constants
- Future work 2: Other bandit feedback models, e.g., dueling bandits.

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