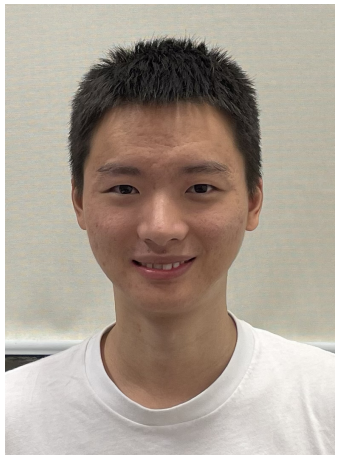
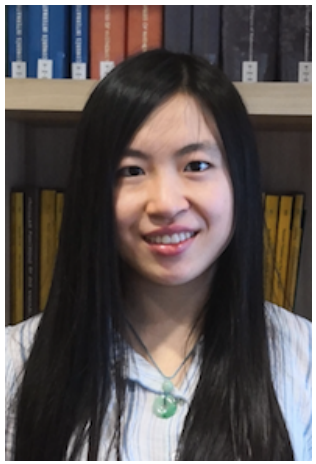
# Almost Optimal Variance-Constrained Best Arm Identification

Yunlong Hou Zixin Zhong **Vincent Y. F. Tan**





National University of Singapore

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IORA, NUS

# Introduction to Stochastic Multi-Armed Bandits in BAI

Efficacies: $\mu_1 = 0.8$ $\mu_2 = 0.9$ $\mu_3 = 0.2$ $\mu_4 = 0.5$

- 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.

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

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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 $\delta$, 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

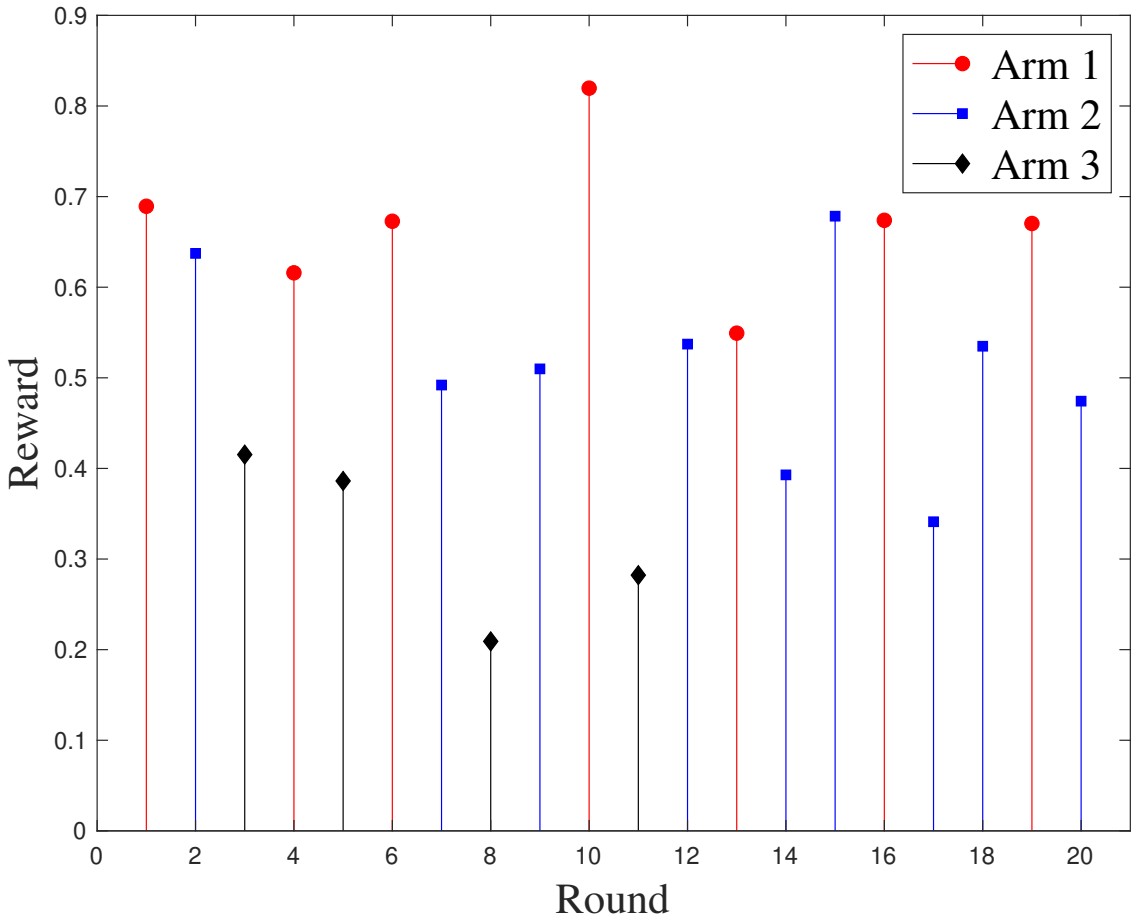



Figure 1: An illustration of a 3-arm BAI problem. At each round, only one arm is sampled and the reward is observed.

# Motivation of Risk-Aware BAI

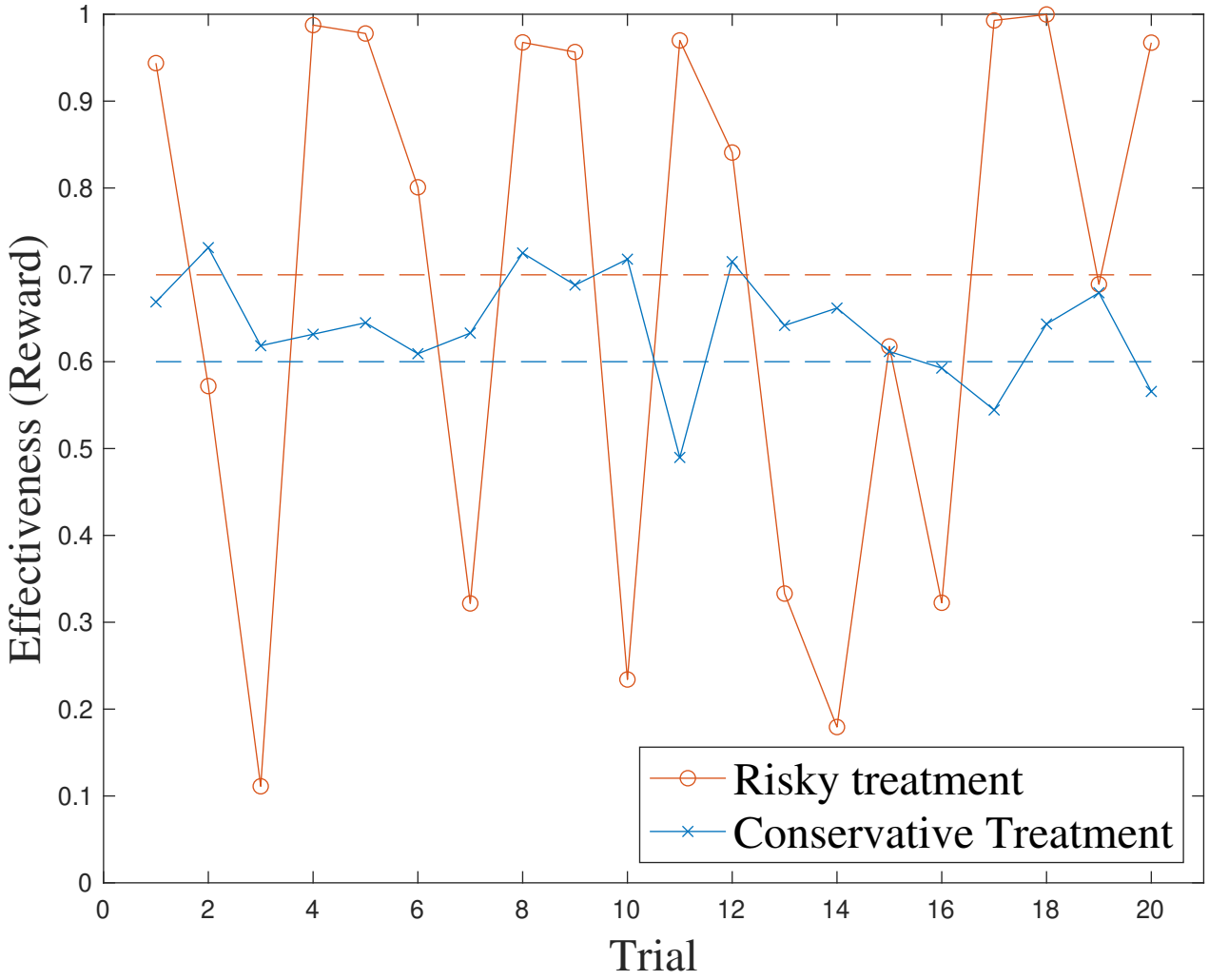


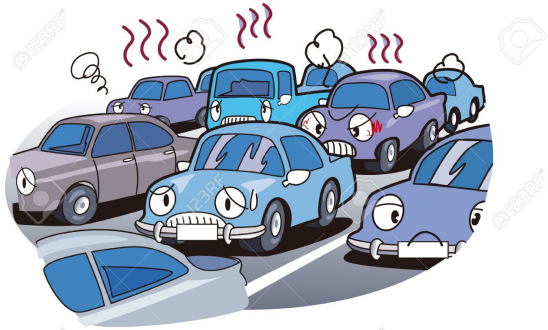

Figure 2: An example of risk-aware BAI: Clinical trials

# 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?



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

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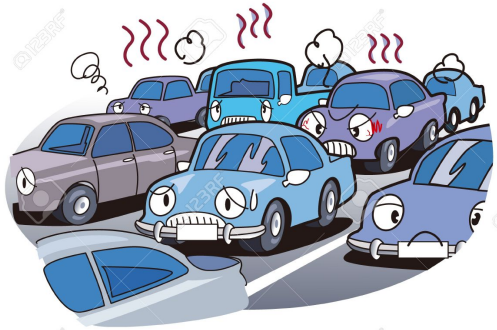

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- Delays are stochastic.
- In choosing between routes, we need not necessarily want to minimize expected delay.
- Two route scenario: Average delay of Route 1 slightly below that of Route 2.
- Route 1 has a small chance of very high delay, e.g., jams.
- 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 $\alpha$-quantile: David and Shimkin (2016)
  - Conditional Value-at-risk (CVaR): Kagrecha et al. (2020) and Baudry et al. (2021)

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- Risk-constrained problem, i.e., conventional BAI with constraints
  - Variance
  - $\alpha$-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 $\nu_i$ with expectation $\mu_i$ and variance $\sigma_i^2$.
- permissible upper bound on the variance: $\bar{\sigma}^2$.

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- Mean gap $\Delta_i = \mu_{i^\star} - \mu_i \geq 0$

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- Mean gap $\Delta_i = \mu_{i^\star} - \mu_i \geq 0$
- Variance gap $\Delta_i^{\mathrm{v}} = |\sigma_i^2 - \bar{\sigma}^2|$

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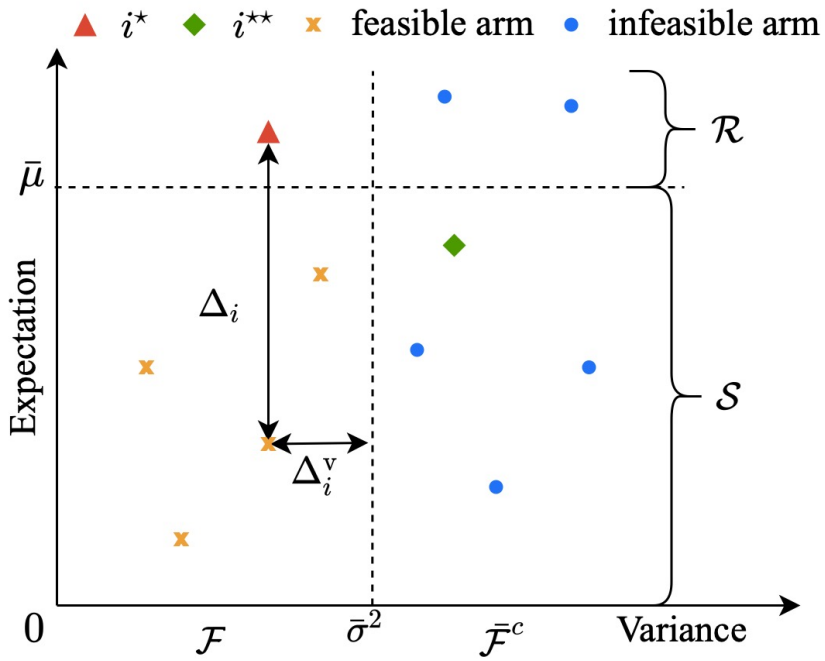


Figure 3: An illustration of an instance

# Introduction to Variance-Constrained BAI

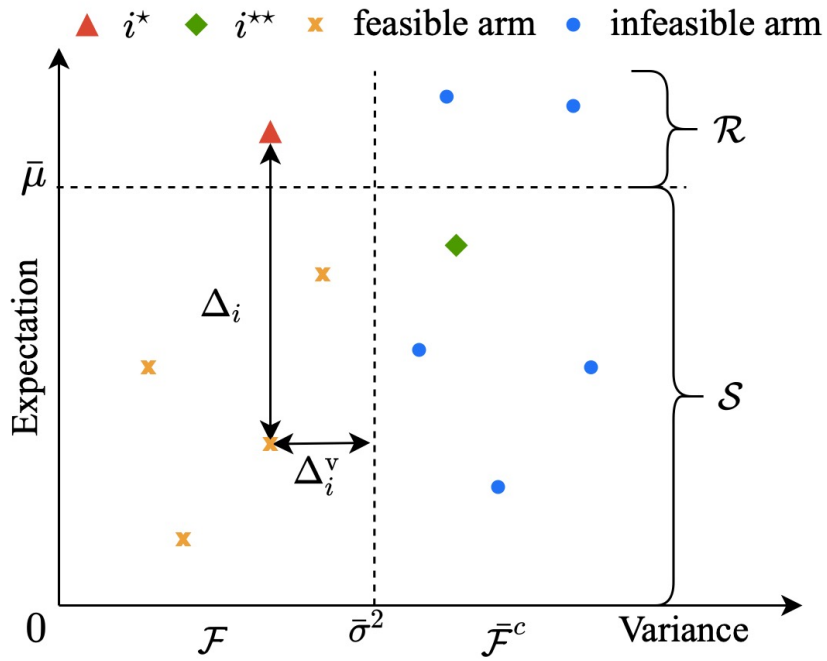


Figure 3: An illustration of an instance

**Goal: Minimize the number of arm pulls needed for**

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

with probability $\geq 1 - \delta$

# Main Result: Upper Bound

## Theorem 1 (Upper bound)

*Define the hardness parameter*

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

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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*

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

*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* $\tau_\delta^\star$ *satisfies*

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

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## Corollary 3 (Almost optimality of VA-LUCB)

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

$$\tau_\delta^\star = \widetilde{\Theta}\Big(H_{\mathrm{VA}} \ln \frac{1}{\delta}\Big),$$

*which is achieved by* VA-LUCB*.*

# Interpretation of Hardness Parameter I

Hardness parameter:

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

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- Ascertain optimality and feasibility of $i^\star$;
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- 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

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

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

where

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

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*

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

*and*

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

*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,

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

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- Define good event

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

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

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

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

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

# VA-LUCB: Confidence Bounds

- With high probability,

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

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

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

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

# VA-LUCB: Possibly Feasible Set

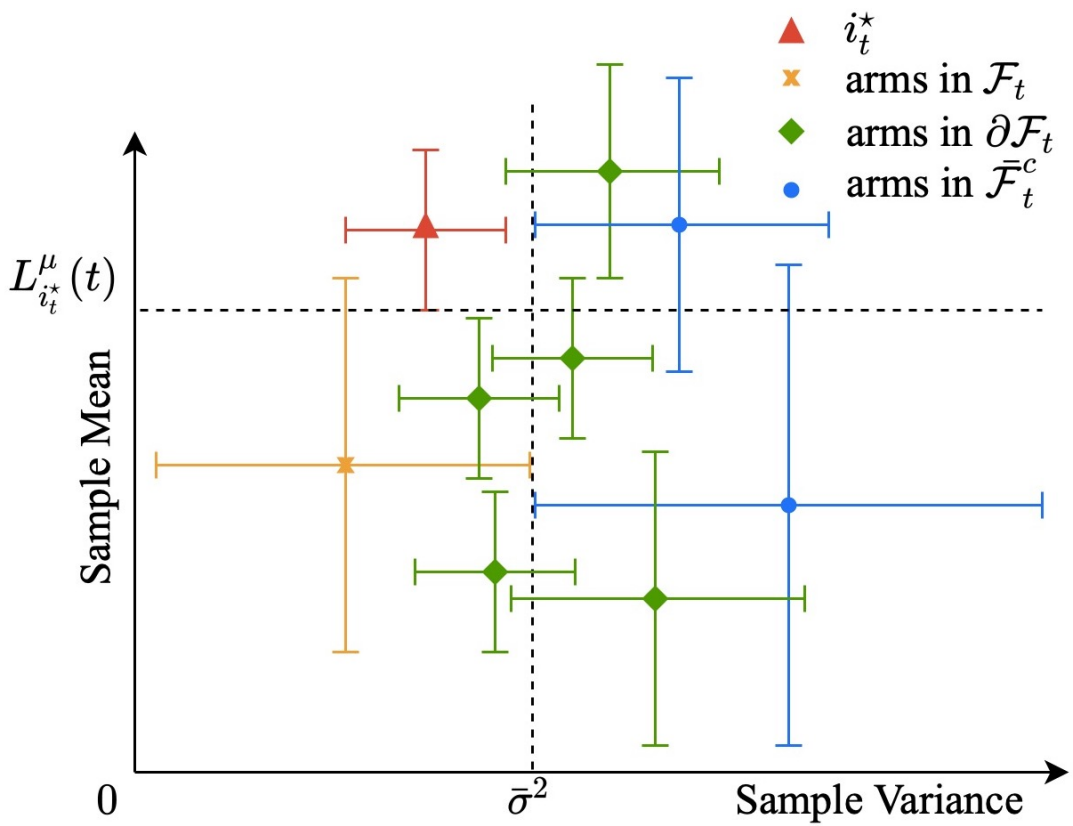



Figure 4: Illustration of the empirical sets. Each dot represents the sample mean and sample variance of each arm at time step $t$.

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

# VA-LUCB: Sampling Strategy

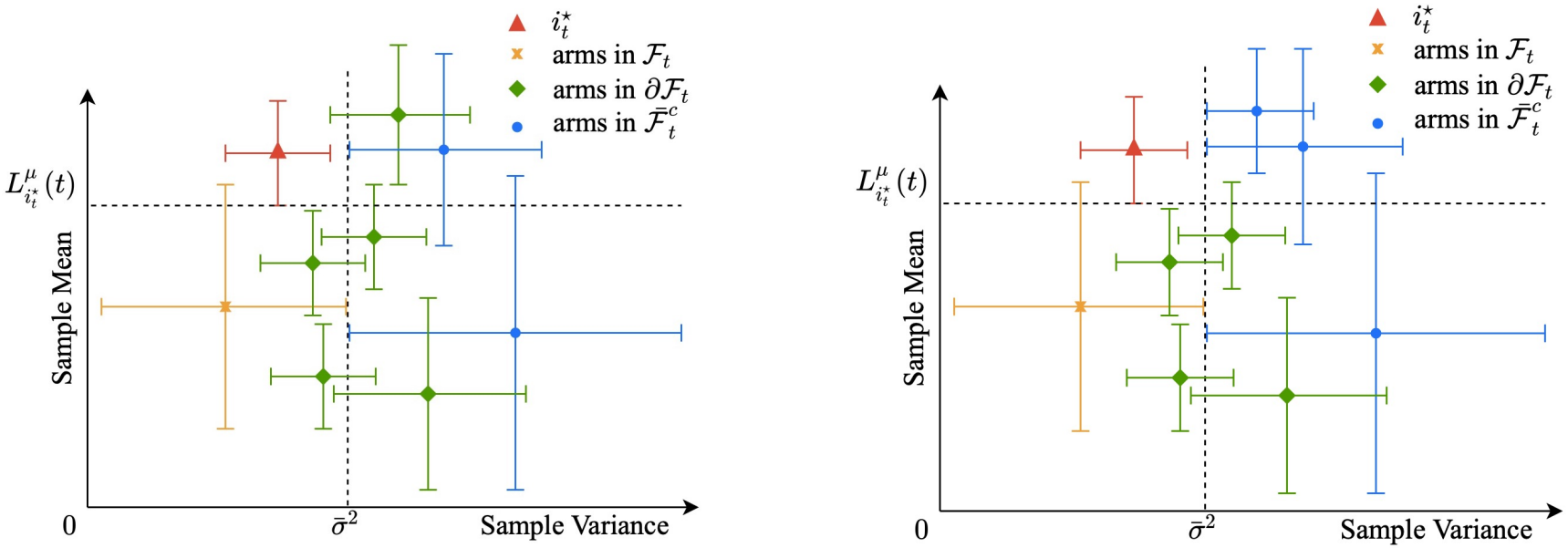
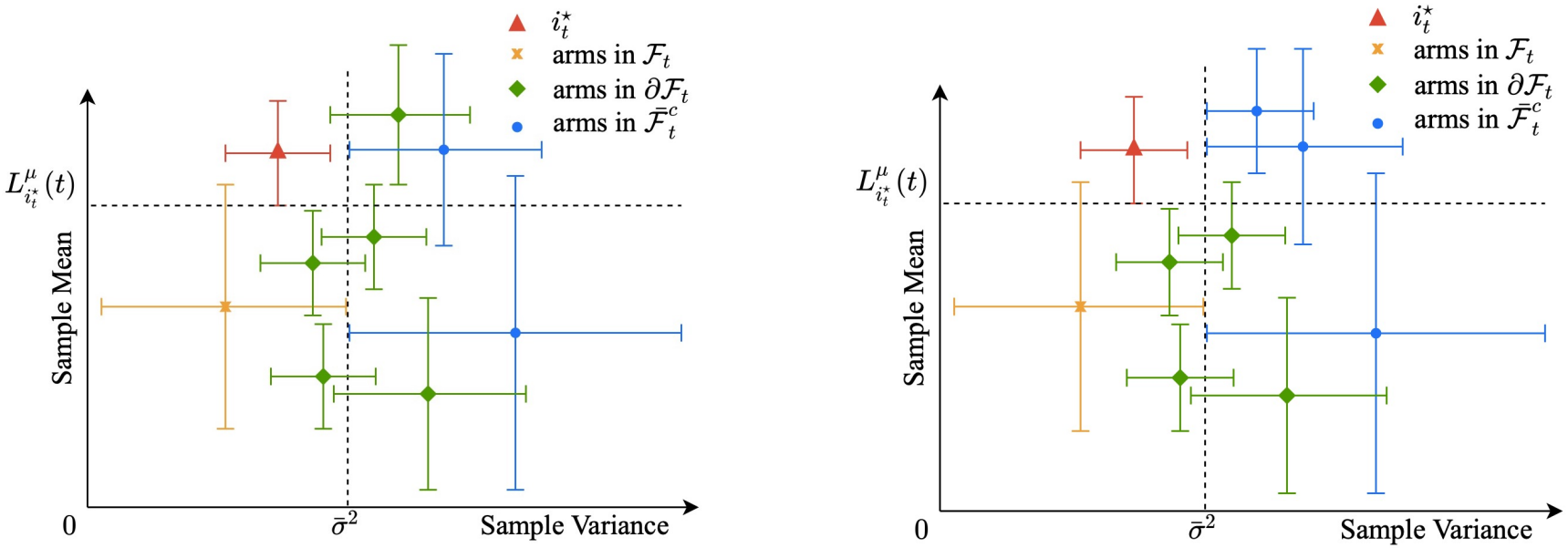



Figure 5: Illustration of the empirical sets.

# VA-LUCB: Sampling Strategy

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

# VA-LUCB: Sampling Strategy

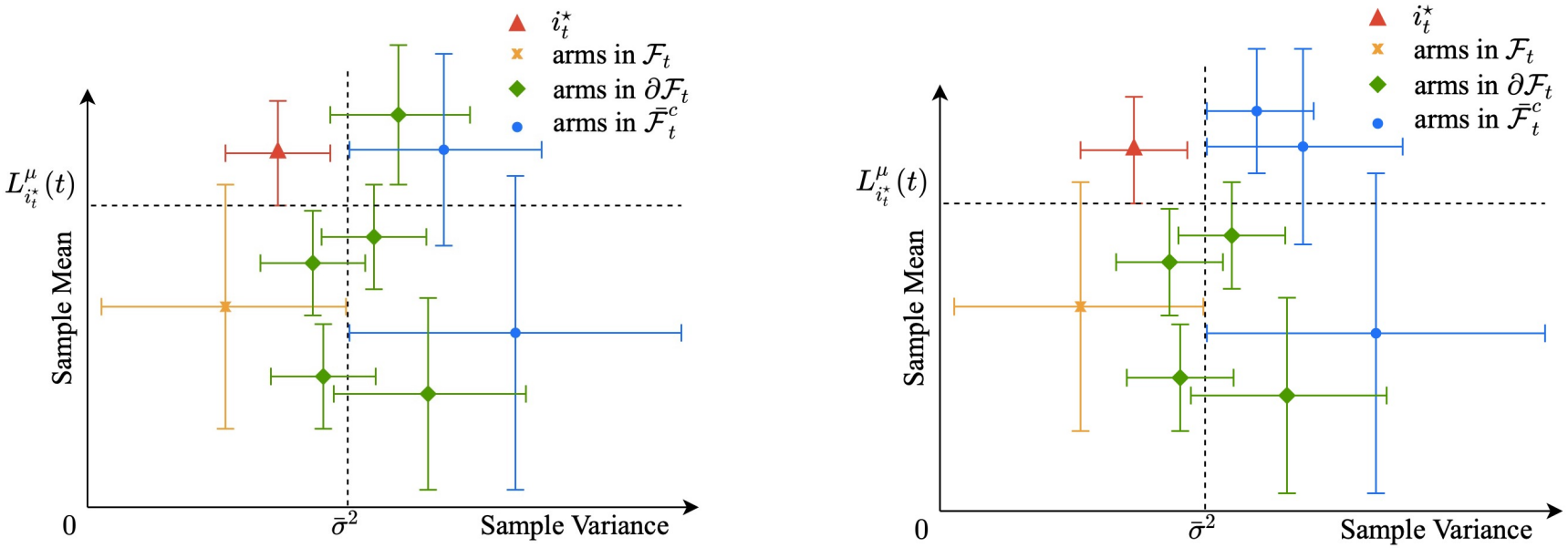


Figure 5: Illustration of the empirical sets.

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

# VA-LUCB: Stopping Strategy

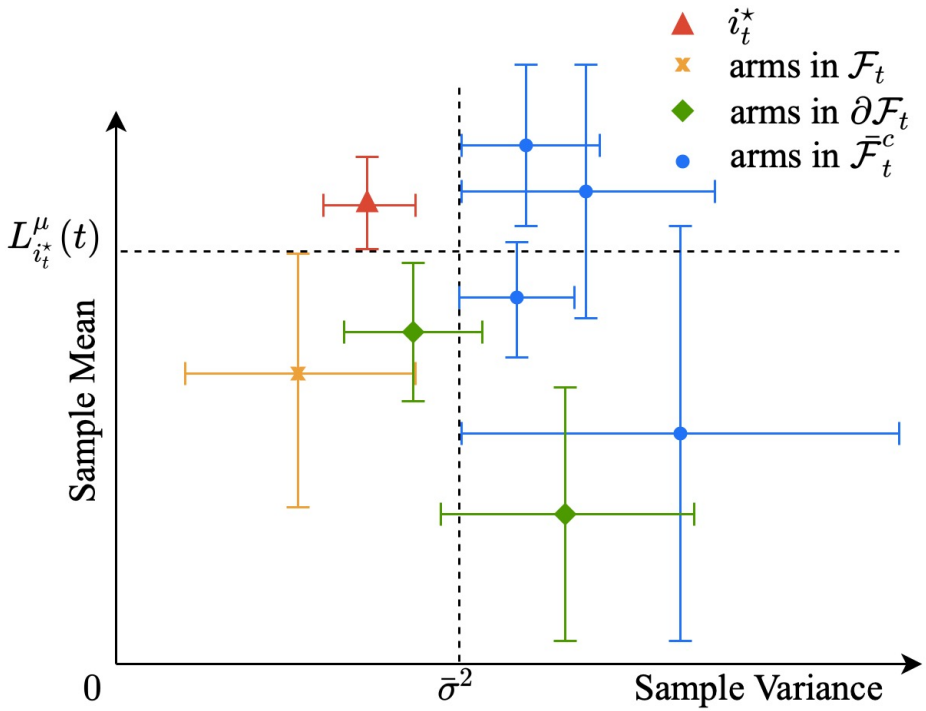


Figure 6: Illustration of the empirical sets.

# VA-LUCB: Stopping Strategy

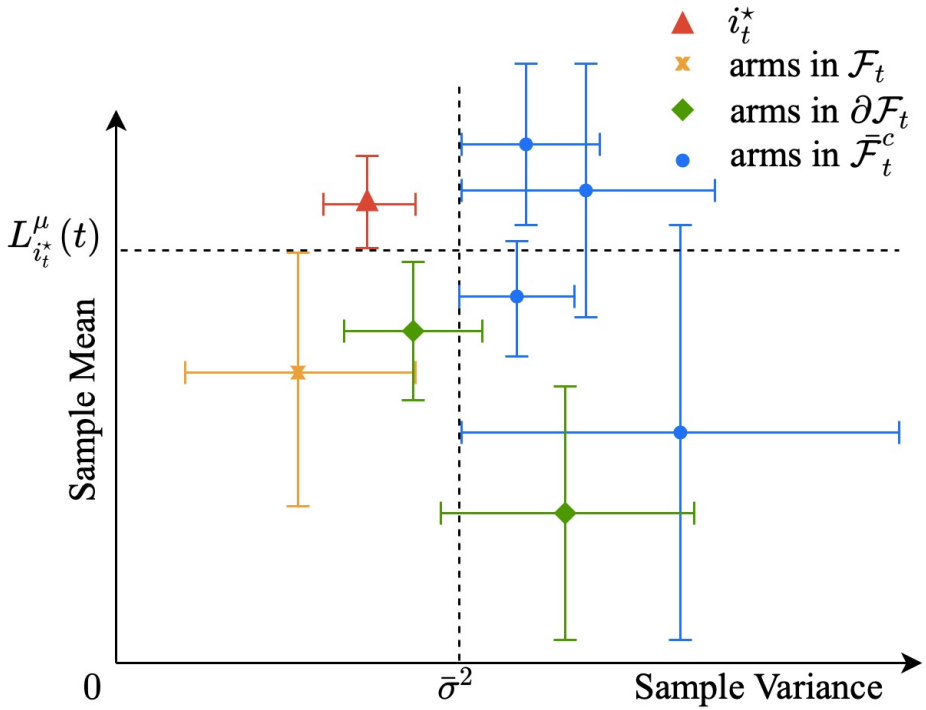


Figure 6: Illustration of the empirical sets.

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

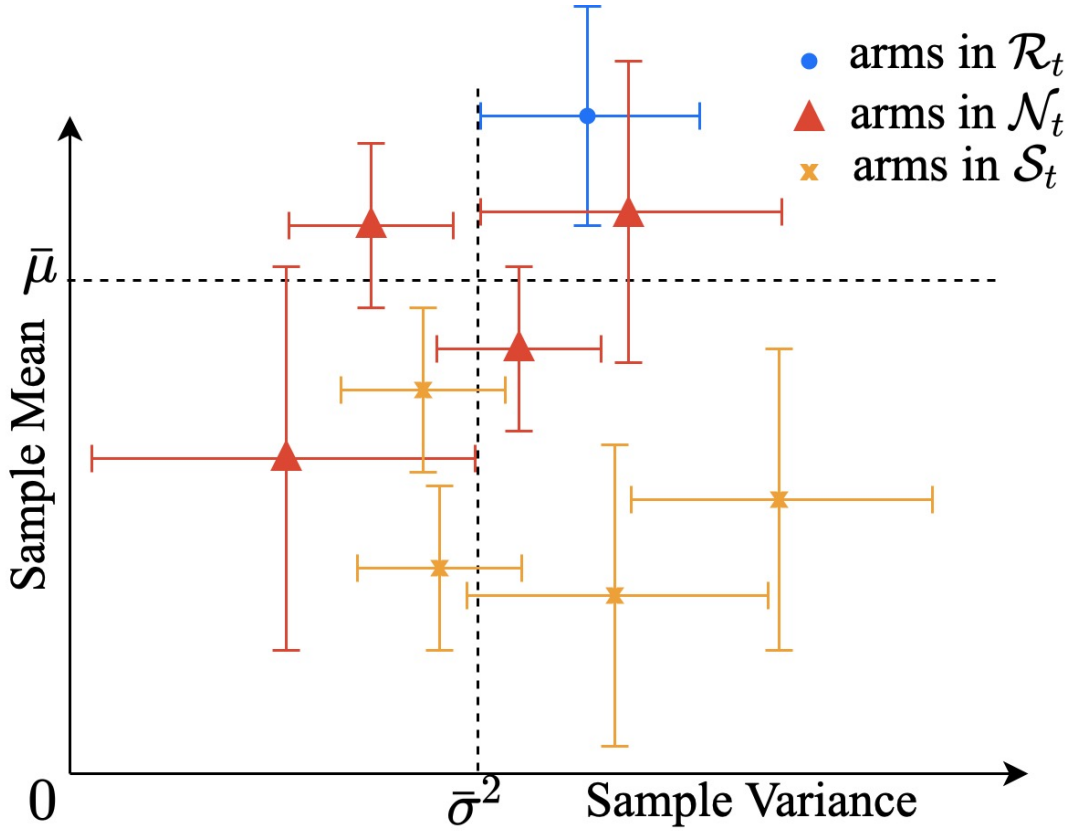


Figure 7: An illustration of the suboptimal and risky set.

# Time/Sample Complexity of VA-LUCB

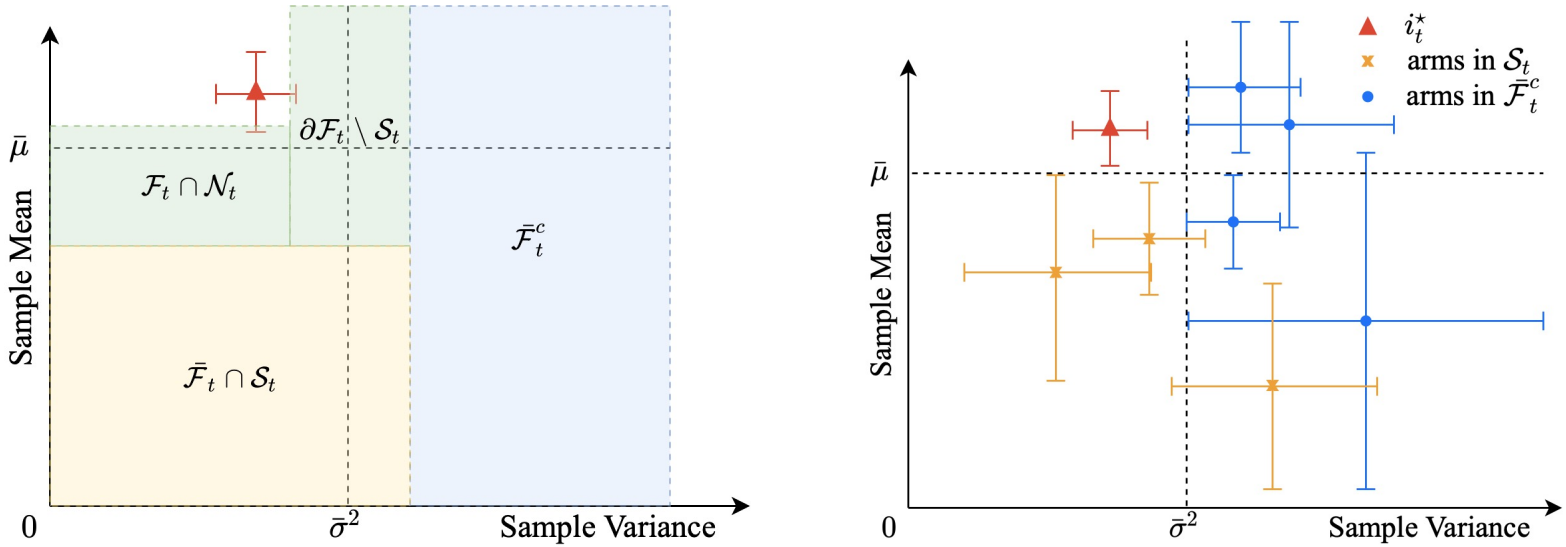


Figure 8: A scenario where all arms have been pulled sufficiently many times.

# Time/Sample Complexity of VA-LUCB

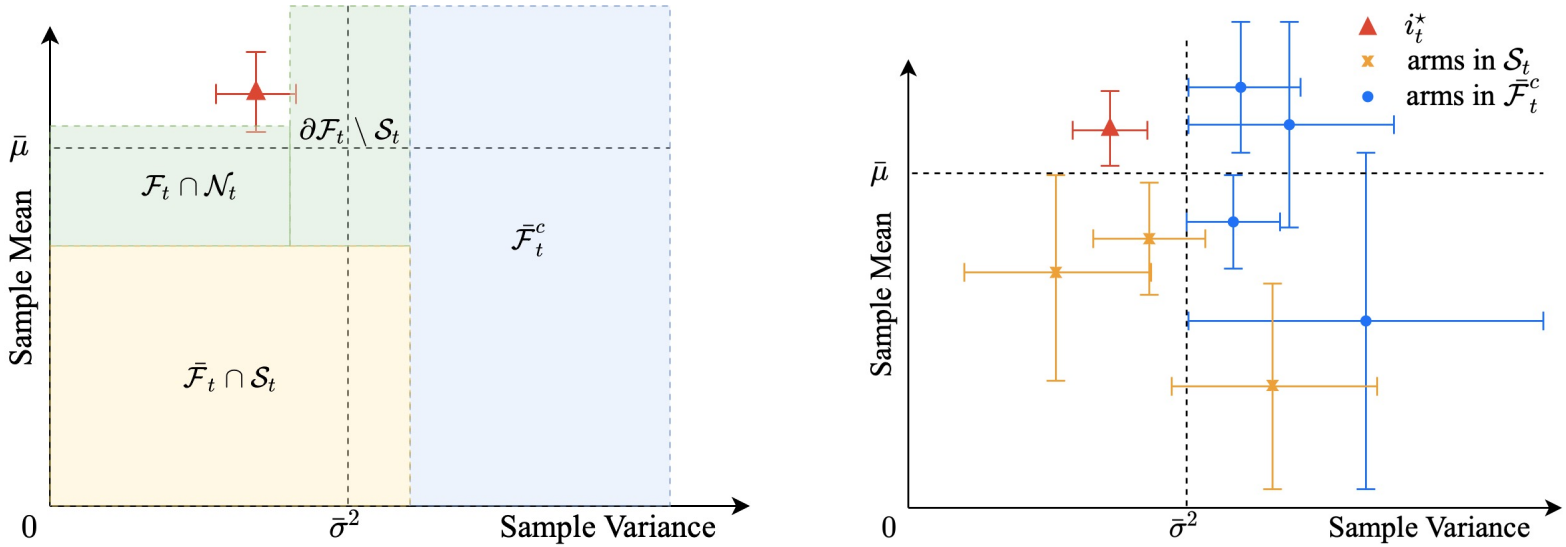


Figure 8: A scenario where all arms have been pulled sufficiently many times.

When **empirically potential best feasible arm set**

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

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:

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

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

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

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## Lemma: Small Non-Termination Probability

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

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

# Experiment: VA-LUCB

- Recall the upper bound on $\tau_\delta^\star$ is $O\left(H_{\mathrm{VA}} \ln \frac{H_{\mathrm{VA}}}{\delta}\right)$ where

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

- Test the four terms individually

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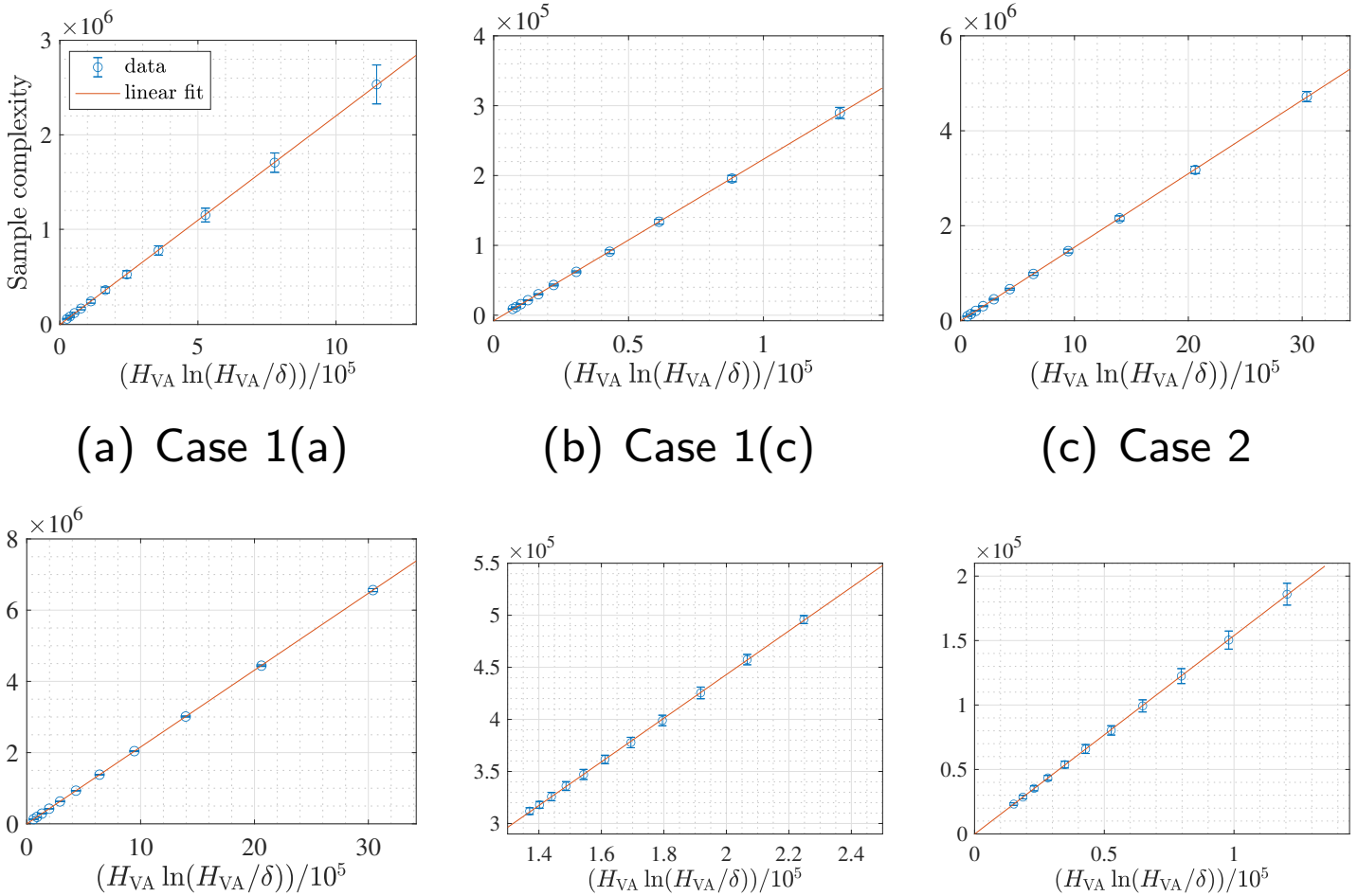
- Test the four terms individually
- For example, change $\Delta_{i^\star}$ and observe how sample complexity changes as a function of $H_{\mathrm{VA}}$ or $H_{\mathrm{VA}} \ln \frac{H_{\mathrm{VA}}}{\delta}$.

# VA-LUCB: Exploring Effects of the Terms in $H_{\mathrm{VA}}$




(a) Case 1(a) (b) Case 1(c) (c) Case 2

(d) Case 3 (e) Case 4(b) (f) Case 4(c)

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

# Experiment: Comparison to Competing Algorithms

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

# Experiment: Comparison to Competing Algorithms

- VA-UNIFORM: Randomly and uniformly sample two different arms at each time step.
- RISKAVERSE-UCB-BAI: A variant of the algorithm proposed in David et al. (2018):
  - Sample $i_t = \operatorname{argmax}\left\{U_i^{\mu}(t) : i \in \bar{\mathcal{F}}_t\right\}$ (UCB type).
  - Terminate at time $t$ when the confidence radius of the mean of $i_t$ is smaller than $\epsilon_{\mathrm{v}}$.

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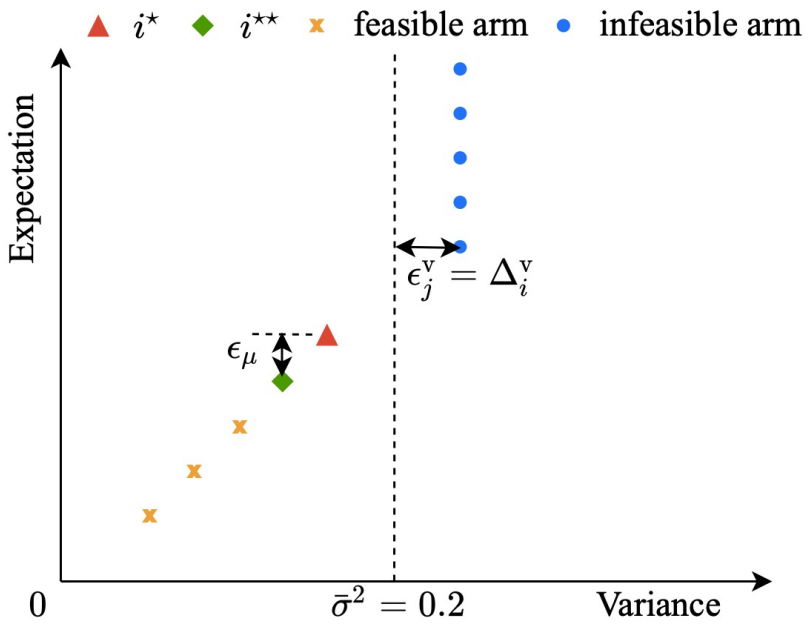
  - Terminate at time $t$ when the confidence radius of the mean of $i_t$ is smaller than $\epsilon_{\mathrm{v}}$.
  - Not parameter free: find the $\epsilon_{\mathrm{v}}$-approximately feasible and $\epsilon_{\mu}$-approximately optimal arm; the confidence radius involves $H$, the hardness parameter in 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



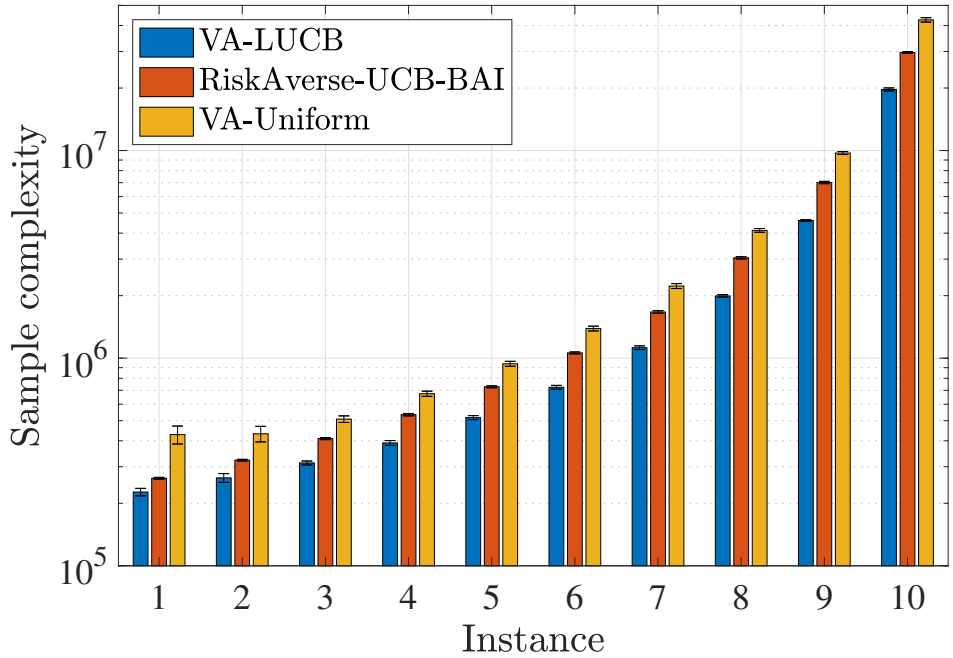




Figure 10: Parameter settings for instance $j \in [10]$. The variance gaps for the infeasible arms $\Delta_i^{\mathrm{v}} = \epsilon_j^{\mathrm{v}} = 0.233 - 0.003 \cdot j$ in instance $j \in [10]$.

# Conclusion and Extensions

- Proposed a framework for risk-constrained best arm identification
- Developed an algorithm $\mathrm{VA\text{-}LUCB}$ 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 $\mathrm{VA\text{-}LUCB}$ 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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