

Minimax Optimal Fixed-Budget Best Arm Identification in Linear Bandits

Junwen Yang¹, and Vincent Y. F. Tan¹²³

¹Institute of Operations Research and Analytics, ²Department of Mathematics, and ³Department of ECE, National University of Singapore, Singapore

Linear Bandits

- An arm set $\mathcal{A} = [K]$, which corresponds to arm vectors $\{a(1), a(2), \dots, a(K)\} \subset \mathbb{R}^d$.
- ullet At each time t, the agent chooses an arm A_t from the arm set \mathcal{A} and then observes a noisy reward

$$X_t = \langle \theta^*, a(A_t) \rangle + \eta_t,$$

where $\theta^* \in \mathbb{R}^d$ is the unknown parameter vector and η_t is independent zero-mean 1-subgaussian random noise.

Best Arm Identification in the Fixed-Budget Setting

- To maximize the probability of identifying the best arm with no more than T arm pulls.
- ullet The agent uses an online algorithm π to decide the arm A_t to pull at each time step t, and the arm $i_{\mathrm{out}} \in \mathcal{A}$ to output as the identified best arm by time T.
- We seek to minimize the error probability

$$\Pr\left[i_{\text{out}} \neq \underset{j \in \mathcal{A}}{\operatorname{arg\,max}} \langle \theta^*, a(j) \rangle\right].$$

Notations

- For any arm $i \in \mathcal{A}$, let $p(i) = \langle \theta^*, a(i) \rangle$ denote the expected reward.
- Assume that $p(1) > p(2) \ge \cdots \ge p(K)$.
- For any suboptimal arm i, we denote $\Delta_i = p(1) p(i)$ as the optimality gap. Also set $\Delta_1 = \Delta_2$.

Hardness Quantities

$H_1 = \sum_{1 \le i \le K} \Delta_i^{-2}$	$H_2 = \max_{2 \le i \le K} \frac{i}{\Delta_i^2}$	$1 \le \frac{H_1}{H_2} \le \log(2K)$
$H_{1,\text{lin}} = \sum_{1 \le i \le d} \Delta_i^{-2}$	$H_{2,\text{lin}} = \max_{2 \le i \le d} \frac{i}{\Delta_i^2}$	$1 \le \frac{H_{1,\text{lin}}}{H_{2,\text{lin}}} \le \log(2d)$
$1 \le \frac{H_1}{H_{1,\text{lin}}} \le \frac{K}{d}$	$1 \le \frac{H_2}{H_{2,\text{lin}}} \le \frac{K}{d}$	

Algorithm: Optimal Design-based Linear Best Arm Identification (OD-LinBAI)

Input: time budget T, arm set $\mathcal{A} = [K]$ and arm vectors $\{a(1), a(2), \ldots, a(K)\} \subset \mathbb{R}^d$.

- Initialize $t_0 = 1$, $A_0 \leftarrow A$ and $d_0 = d$.
- 2: For each arm $i \in \mathcal{A}_0$, set $a_0(i) = a(i)$.
- 3: Calculate $m = \Theta(T/\log_2 d)$.
- 4: **for** r=1 **to** $\lceil \log_2 d \rceil$ **do**
- Set $d_r = \dim (\operatorname{span} (\{a_{r-1}(i) : i \in \mathcal{A}_{r-1}\})).$
- if $d_r = d_{r-1}$ then
- For each arm $i \in \mathcal{A}_{r-1}$, set $a_r(i) = a_{r-1}(i)$.
 - else
- Find matrix $B_r \in \mathbb{R}^{d_{r-1} \times d_r}$ whose columns form a orthonormal basis of the subspace spanned by $\{a_{r-1}(i): i \in \mathcal{A}_{r-1}\}$.
- For each arm $i \in \mathcal{A}_{r-1}$, set $a_r(i) =$ $B_r^{\top}a_{r-1}(i)$.
- end if
- if r=1 then
- Find a G-optimal design $\pi_r:\{a_r(i):i\in$ A_{r-1} \rightarrow [0, 1] with $| \text{Supp}(\pi_r) | \le \frac{d(d+1)}{2}$.

else

- Find a G-optimal design $\pi_r: \{a_r(i): i \in \mathcal{A}_{r-1}\} \rightarrow$
- end if Set

$$T_r(i) = \lceil \pi_r(a_r(i)) \cdot m \rceil$$
 and $T_r = \sum_{i \in \mathcal{A}_{r-1}} T_r(i)$.

- Choose each arm $i \in \mathcal{A}_{r-1}$ exactly $T_r(i)$ times.
- Calculate the OLS estimator:

$$\hat{\theta}_r = V_r^{-1} \sum_{t=t_r}^{t_r + T_r - 1} a_r(A_t) X_t \text{ with } V_r = \sum_{i \in \mathcal{A}_{r-1}} T_r(i) a_r(i) a_r(i)^\top.$$

- For each arm $i \in \mathcal{A}_{r-1}$, estimate the expected reward: $\hat{p}_r(i) = \langle \hat{\theta}_r, a_r(i) \rangle$.
- Let \mathcal{A}_r be the set of $\lceil d/2^r \rceil$ arms in \mathcal{A}_{r-1} with the largest estimates of the expected rewards.
- Set $t_{r+1} = t_r + T_r$.
- 23: end for

Output: the only arm i_{out} in $\mathcal{A}_{\lceil \log_2 d \rceil}$.

First Phase r^{th} Phase (1 $< r \le \lceil \log_2 d \rceil$) Beain with K >> d arms Dimensionality Reduction Dimensionality Reduction Find G-opt Design π_1 Find G-opt Design π_r Pull arms according to π_1 Pull arms according to π_r Retain best $\lceil d/2 \rceil$ arms Retain best $\lceil d/2^r \rceil$ arms

Error Probability of OD-LinBAI

Let $\mathcal{E}(a)$ denote the set of linear bandit instances whose $H_{1,\mathrm{lin}}$ is bounded by a>0, i.e.,

Minimax Lower Bound

$$\mathcal{E}(a) = \{ \nu : H_{1, \text{lin}}(\nu) \le a \}.$$

If $T \ge a^2 \log(6Td)/900$, then

$$\min_{\pi} \max_{\nu \in \mathcal{E}(a)} \Pr\left[i_{\text{out}}^{\pi} \neq 1\right] \ge \frac{1}{6} \exp\left(-\frac{240T}{a}\right).$$

Further if $a \geq 15d^2$, then

 ${\cal A}_1$

$$\min_{\pi} \max_{\nu \in \mathcal{E}(a)} \left(\Pr\left[i_{\text{out}}^{\pi} \neq 1 \right] \cdot \exp\left(\frac{2700T}{H_{1,\text{lin}}(\nu) \log_2 d} \right) \right) \geq \frac{1}{6}.$$
• Upper bound: $\exp\left(-\Omega\left(\frac{T}{H_{2,\text{lin}} \log_2 d} \right) \right)$
• Lower bound: $\exp\left(-O\left(\frac{T}{H_{1,\text{lin}} \log_2 d} \right) \right)$

For any linear bandit instance ν , OD-LinBAI outputs an arm $i_{
m out}$ satisfying

$$\Pr\left[i_{\text{out}} \neq 1\right] \le \left(\frac{4K}{d} + 3\log_2 d\right) \exp\left(-\frac{m}{32H_{2,\text{lin}}}\right).$$

Minimax Optimality

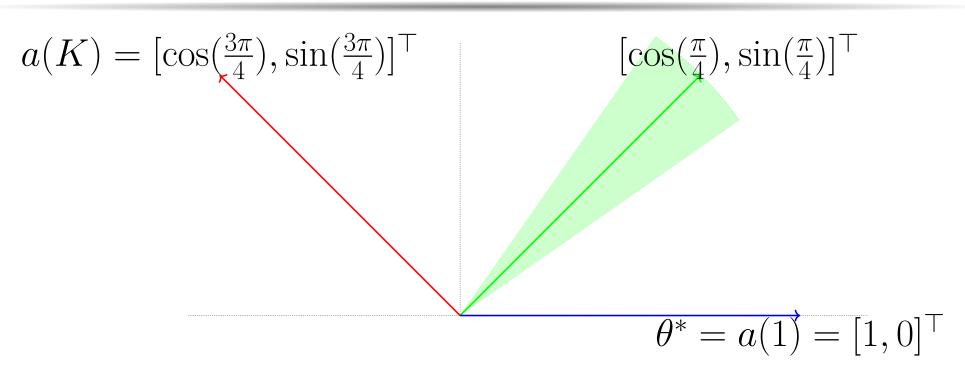
As the time budget T tends to infinity,

- Lower bound: $\exp\left(-O\left(\frac{T}{H_{1,\ln\log_2 d}}\right)\right)$

Comparison to Existing Art

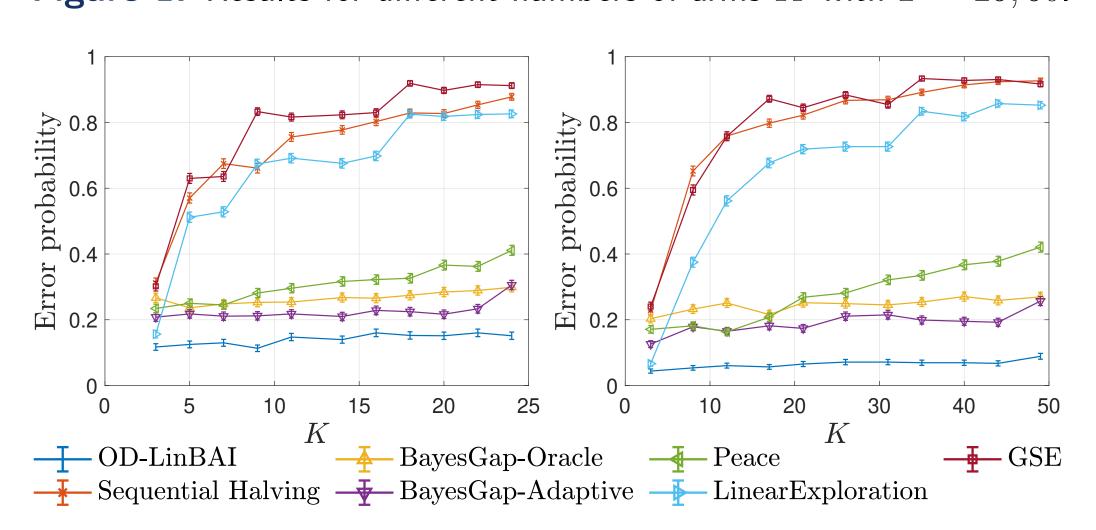
- BayesGap [1]:
- Not parameter-free (require the knowledge of the instance)
- Error probability: $\exp\left(-\Omega\left(\frac{T}{H_1}\right)\right)$
- Peace [2]:
 - Not parameter-free (require the knowledge of the instance)
 - Not minimax optimal
- LinearExploration [3]:
- Error probability: $\exp\left(-\Omega(\frac{T}{\tilde{H}_2\log_2 K})\right)$
- GSE [4]:
- Error probability: $\exp\left(-\Omega(\frac{T\Delta_1^2}{d\log_2 K})\right)$

Numerical Experiments



- One best arm, one worst arm and K-2 almost second best arms.
- $a(i) = [\cos(\pi/4 + \phi_i), \sin(\pi/4 + \phi_i)]^{\top}$ with $\phi_i \sim \mathcal{N}(0, 0.09^2)$ for $i = 2, 3, \dots, K - 1$

Figure 1: Results for different numbers of arms K with T=25,50.



References

- [1] M. Hoffman, B. Shahriari, and N. Freitas, "On correlation and budget constraints in model-based bandit optimization with application to automatic machine learning," in AISTATS, 2014.
- [2] J. Katz-Samuels, L. P. Jain, Z. S. Karnin, and K. G. Jamieson, "An empirical process approach to the union bound: Practical algorithms for combinatorial and linear bandits." NeurIPS, 2020.
- [3] A. Alieva, A. Cutkosky, and A. Das, "Robust pure exploration in linear bandits with limited budget," in ICML, 2021.
- [4] M. Azizi, B. Kveton, and M. Ghavamzadeh, "Fixed-budget best-arm identification in structured bandits," in IJCAI, 2022.

Full Paper is Available at:



https://arxiv.org/abs/2105.13017

