Towards Minimax Optimal Best Arm Identification in Linear Bandits

Junwen Yang
Institute of Operations Research and Analytics
National University of Singapore
junwen_yang@u.nus.edu

Vincent Y. F. Tan
Department of Electrical and Computer Engineering
Department of Mathematics
National University of Singapore
vtan@nus.edu.sg

Abstract

We study the problem of best arm identification in linear bandits in the fixed-budget setting. By leveraging properties of the G-optimal design and incorporating it into the arm allocation rule, we design a parameter-free algorithm, Optimal Design-based Linear Best Arm Identification (OD-LinBAI). We provide a theoretical analysis of the failure probability of OD-LinBAI. While the performances of existing methods (e.g., BayesGap) depend on all the optimality gaps, OD-LinBAI depends on the gaps of the top \(d\) arms, where \(d\) is the effective dimension of the linear bandit instance. Furthermore, we present a minimax lower bound for this problem. The upper and lower bounds show that OD-LinBAI is minimax optimal up to multiplicative factors in the exponent. Finally, numerical experiments corroborate our theoretical findings.

1 Introduction

The multi-armed bandit problem is a model that exemplifies the exploration-exploitation tradeoff in online decision making. It has various applications in drug design, online advertising, recommender systems, and so on. In stochastic multi-armed bandit problems, the agent sequentially chooses an arm from the given arm set at each time step and then observes a random reward drawn from the unknown distribution associated with the chosen arm.

The standard multi-armed bandit problem, where the arms are not correlated with one another, has been studied extensively in literature. While the regret minimization problem aims at maximizing the cumulative rewards by the trade-off between exploration and exploitation [1–4], the pure exploration problem focuses on efficient exploration with specific goals, e.g., to identify the best arm [5–10].

There are two complementary settings for the problem of best arm identification: (i) Given \(T \in \mathbb{N}\), the agent aims to maximize the probability of finding the best arm in at most \(T\) time steps; (ii) Given \(\delta > 0\), the agent aims to find the best arm with the probability of at least \(1 - \delta\) in the smallest number of steps. These settings are respectively known as the fixed-budget and fixed-confidence settings.

In this paper, we consider the problem of best arm identification in linear bandits in the fixed-budget setting. In linear bandits, the arms are correlated through an unknown global regression parameter vector \(\theta^* \in \mathbb{R}^d\). In particular, each arm \(i\) from the arm set \(\mathcal{A}\) is associated with an arm vector \(a(i) \in \mathbb{R}^d\); and the expected reward of arm \(i\) is given by the inner product between \(\theta^*\) and \(a(i)\). Hence, the standard multi-armed bandits and linear bandits are fundamentally different due to the
fact that for the latter, pulling one arm can indirectly reveal information about the other arms but in the former, the arms are independent.

A wide range of applications in practice can be modeled by linear bandits. For example, Tao et al. \cite{11} considered online advertising, where the goal is to select an advertisement from a pool to maximize the probability of clicking for web users with different features. Empirically, the probability of clicking can be approximated by a linear combination of various attributes associated with the user and the advertisements (such as age, gender, the domain, keywords, advertising genres, etc.). Moreover, Hoffman et al. \cite{12} applied the linear bandit model into the traffic sensor network problem and the problem of automatic model selection and algorithm configuration.

Main contributions. Our main contributions are as follows:

(i) We design an algorithm named Optimal Design-based Linear Best Arm Identification (OD-LinBAI). This parameter-free algorithm utilizes a phased elimination-based strategy in which the number of times each arm is pulled in each phase depends on G-optimal designs \cite{13}.

(ii) We derive an upper bound on the failure probability of OD-LinBAI. In particular, we show that the exponent depends on a hardness quantity $H_{2,\text{lin}}$. This quantity is a function of only the first $d - 1$ optimality gaps, where $d$ is the dimension of the arm vectors. This is a significant improvement over the upper bound of the failure probability of BayesGap in Hoffman et al. \cite{12} which depends on a hardness quantity that depends on all the gaps. Furthermore, OD-LinBAI is parameter-free, whereas BayesGap requires the knowledge of the hardness quantity (which is usually not known).

(iii) Finally, using ideas from Carpentier and Locatelli \cite{8}, we prove a minimax lower bound which involves another hardness quantity $H_{1,\text{lin}}$. By comparing $H_{1,\text{lin}}$ to $H_{2,\text{lin}}$, we show that OD-LinBAI is minimax optimal up to constants in the exponent. Experiments firmly corroborate the efficacy of OD-LinBAI vis-à-vis BayesGap \cite{12} and its variants, especially on hard instances.

Related work. The problem of regret minimization in linear bandits was first studied by Abe and Long \cite{14}, and has attracted extensive interest in the development of various algorithms (e.g., UCB-style algorithms \cite{15,19}, Thompson sampling \cite{20,21}). In particular, in the book of Lattimore and Szepesvári \cite{22}, a regret minimization algorithm based on the G-optimal design was proposed for linear bandits with finitely many arms. Although both this algorithm and our algorithm OD-LinBAI utilize the G-optimal design technique, they differ in numerous aspects including the manner of elimination and arm allocation, which emanates from the two different objectives.

For the problem of best arm identification in linear bandits, the fixed-confidence setting has previously studied in \cite{11,23,28}. In particular, Soare et al. \cite{23} introduced the optimal G-allocation problem and proposed a static algorithm $X^\gamma$-Oracle as well as a semi-adaptive algorithm $X^\gamma$-Adaptive; see Remark 2 for more discussions to Soare et al. \cite{23}. Degenne et al. \cite{28} treated the problem as a two-player zero-sum game between the agent and the nature, and thus designed an asymptotically optimal algorithm for the fixed-confidence setting.

To the best of our knowledge, Hoffman et al. \cite{12} is the only previous work on the problem of best arm identification in linear bandits in the fixed-budget setting. They introduced a gap-based exploration algorithm BayesGap, which is a Bayesian treatment of UGapEb \cite{9}. However, BayesGap is computationally expensive and not parameter-free. See Section 4 and Section 5 for more comparisons.

2 Problem setup and preliminaries

Best arm identification in linear bandits. We consider the standard linear bandit problem with an unknown global regression parameter. In a linear bandit instance $\nu$, the agent is given an arm set $A = [K]$, which corresponds to arm vectors $\{a(1), a(2), \ldots, a(K)\} \subset \mathbb{R}^d$. At each time $t$, the agent chooses an arm $A_t$ from the arm set $A$ 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 $\eta_t$ is independent zero-mean 1-subgaussian random noise.
In the fixed-budget setting, given a time budget $T \in \mathbb{N}$, the agent aims at maximizing the probability of identifying the best arm, i.e., the arm with the largest expected reward, with no more than $T$ arm pulls. More formally, the agent uses an online algorithm $\pi$ to decide the arm $A_t^\pi$ to pull at each time step $t$, and the arm $i_{\text{out}}^t \in A$ to output as the identified best arm by time $T$. We abbreviate $A_t^\pi$ as $A_t$ and $i_{\text{out}}^t$ as $i_{\text{out}}$ when there is no ambiguity.

For any arm $i \in A$, let $p(i) = \langle \theta^*, a(i) \rangle$ denote the expected reward. For convenience, we assume that the expected rewards of the arms are in descending order and the best arm is unique. That is to say, $p(1) > p(2) \geq \cdots \geq p(K)$. For any suboptimal arm $i$, we denote $\Delta_i = p(1) - p(i)$ as the optimality gap. For ease of notation, we also set $\Delta_1 = \Delta_2$. Furthermore, let $E$ denote the set of all the linear bandit instances defined above.

**Dimensionality-reduced arm vectors.** For any linear bandit instance, if the corresponding arm vectors do not span $\mathbb{R}^d$, i.e., $\text{span} \{a(1), a(2), \ldots, a(K)\} \nsubseteq \mathbb{R}^d$, the agent can work with a set of dimensionality-reduced arm vectors $\{a'(1), a'(2), \ldots, a'(K)\} \subset \mathbb{R}^{d'}$, that spans $\mathbb{R}^{d'}$, with little consequence. Specifically, let $B \in \mathbb{R}^{d \times d'}$ be a matrix whose columns form an orthonormal basis of the subspace spanned by $a(1), a(2), \ldots, a(K)$. Then the agent can simply set $a'(i) = B^\top a(i)$ for each arm $i$.

To verify this, notice that $BB^\top$ is a projection matrix onto the subspace spanned by $\{a(1), a(2), \ldots, a(K)\}$ and consequently

$$p(i) = \langle \theta^*, a(i) \rangle = \langle \theta^*, BB^\top a(i) \rangle = \langle B^\top \theta^*, B^\top a(i) \rangle = \langle \theta'^*, a'(i) \rangle.$$  

Note that $\theta'^*$ is the unknown parameter vector for original arm vectors while $\theta'^* = B^\top \theta^*$ is the corresponding unknown parameter vector for the dimensionality-reduced arm vectors. In the problem of linear bandits, what we really care about is not the original unknown parameter $\theta^*$ itself but the inner products between $\theta^*$ and the arm vectors $a(i)$, which establishes the equivalence of original arm vectors and dimensionality-reduced arm vectors.

In our work, without loss of generality, we assume that the entire set of original arm vectors $\{a(1), a(2), \ldots, a(K)\}$ span $\mathbb{R}^d$ and $d \geq 2$. However, this idea of transforming into dimensionality-reduced arm vectors is often used in our elimination-based algorithm. See Section[3] for details.

**Least squares estimators.** Let $A_1, A_2, \ldots, A_n$ be the sequence of arms pulled by the agent and $X_1, X_2, \ldots, X_n$ be the corresponding noisy rewards. Suppose that the corresponding arm vectors $\{a(A_1), a(A_2), \ldots, a(A_n)\}$ span $\mathbb{R}^d$, then the ordinary least squares (OLS) estimator of $\theta^*$ is given by

$$\hat{\theta} = V^{-1} \sum_{t=1}^n a(A_t)X_t$$

where $V = \sum_{t=1}^n a(A_t)a(A_t)^\top \in \mathbb{R}^{d \times d}$ is invertible. By applying the properties of subgaussian random variables, a confidence bound for the OLS estimator can be derived as follows.

**Proposition 1** (Lattimore and Szepesvári[22, Chapter 20]). If $A_1, A_2, \ldots, A_n$ are deterministically chosen without knowing the realizations of $X_1, X_2, \ldots, X_n$, then for any $x \in \mathbb{R}^d$ and $\delta > 0$,

$$\Pr \left( \langle \hat{\theta} - \theta^*, x \rangle \geq \sqrt{2\|x\|^2_{V^{-1}} \log \left( \frac{1}{\delta} \right)} \right) \leq \delta.$$  

**Remark 1.** When the arm pulls are not adaptively chosen according to the random rewards, Proposition[4] no longer applies and an extra factor $\sqrt{d}$ has to be paid for adaptive arm pulls[18]. Our algorithm avoids this issue by deciding the arm pulls at the beginning of each phase, and designing the OLS estimator based on information from current phase. See Section[3] for details.

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[1] Such an orthonormal basis can be calculated efficiently with the reduced singular value decomposition, Gram–Schmidt process, etc.

[2] The situation that $d = 1$ is trivial: each arm vector is a scalar multiple of one another.
**G-optimal design.** The confidence interval in Proposition 1 shows the strong connection between the arm allocation in linear bandits and experimental design theory [29]. To control the confidence bounds, we first introduce the G-optimal design technique into the problem of best arm identification in linear bandits in the fixed-budget setting. Formally, the G-optimal design problem aims at finding a probability distribution $\pi : \{a(i) : i \in A\} \rightarrow [0, 1]$ that minimises

$$g(\pi) = \max_{i \in A} \|a(i)\|_{V(\pi)^{-1}}^{2}$$

where $V(\pi) = \sum_{i \in A} \pi(a(i))a(i)a(i)^{T}$. Theorem 1 states the existence of a small-support G-optimal design and the minimum value of $g$.

**Theorem 1 (Kiefer and Wolfowitz [13]).** If the arm vectors $\{a(i) : i \in A\}$ span $\mathbb{R}^{d}$, the following statements are equivalent:

1. $\pi^{*}$ is a minimiser of $g$.
2. $\pi^{*}$ is a maximiser of $f(\pi) = \log \det V(\pi)$.
3. $g(\pi^{*}) = d$.

Furthermore, there exists a minimiser $\pi^{*}$ of $g$ such that $|\text{Supp}(\pi^{*})| \leq d(d + 1)/2$.

**Remark 2.** It is worth mentioning that the G-optimal design problem for finite arm vectors is a convex optimization problem while the G-allocation problem in Soare et al. [23] for the fixed-confidence best arm identification in linear bandits is an NP-hard discrete optimization problem. A classical algorithm to solve the G-optimal design problem is the Frank-Wolfe algorithm [30], whose modified version guarantees linear convergence [31]. For our work, it is sufficient to compute an $\epsilon$-approximate optimal design with minimal impact on performance. Recently, a near-optimal design with smaller support was proposed in Lattimore et al. [32], which might be helpful in some scenarios. See Appendix A for more discussions on the above issues. To reduce clutter and ease the reading, henceforward in the main text, we assume that a G-optimal design for finite arm vectors can be found accurately and efficiently.

### 3 Algorithm

Our algorithm Optimal Design-based Linear Best Arm Identification (OD-LinBAI) is presented in Algorithm 1.

The algorithm partitions the whole horizon into $\lceil \log_{2} d \rceil$ phases, and maintains an active arm set $A_{r}$ in each phase $r$. The length of each phase is roughly equal to $m$, which will be formally defined later.

Motivated by the equivalence of the original arm vectors and the dimensionality-reduced arm vectors, at the beginning of each phase $r$, the algorithm computes a set of dimensionality-reduced arm vectors $\{a_{r}(i) : i \in A_{r-1}\} \subset \mathbb{R}^{d_{r}}$ which spans the $d_{r}$-dimensional Euclidean space $\mathbb{R}^{d_{r}}$. This can be implemented based on the dimensionality-reduced arm vectors of the last phase $\{a_{r-1}(i) : i \in A_{r-1}\}$ in an iterative manner (Lines 5 – 11).

After that, Algorithm 1 finds a G-optimal design $\pi_{r}$ for the current dimensionality-reduced arm vectors, with a restriction on the cardinality of the support when $r = 1$. OD-LinBAI then pulls each arm in $A_{r-1}$ according to the proportions specified by the optimal design $\pi_{r}$. Specifically, the algorithm chooses each arm $i \in A_{r-1}$ exactly $T_{r}(i) = \lceil \pi_{r}(a_{r}(i)) \rceil m$ times, where the parameter $m$ is fixed among different phases and defined as

$$m = \frac{T - \min(K, \frac{d(d+1)}{2}) - \sum_{r=1}^{\lceil \log_{2} d \rceil - 1} \lceil \frac{d}{2^{r}} \rceil}{\lceil \log_{2} d \rceil}.$$  \hspace{1cm} (1)

Note that $m = \Theta(T/ \log_{2} d)$ as $T \rightarrow \infty$ with $K$ fixed. Lemma 1 in Appendix B shows with such choice of $m$, the total time budget consumed by the agent is no more than $T$. It turns out that the

\footnote{For an $\epsilon$-approximate optimal design $\pi$, $g(\pi) \leq (1 + \epsilon)d$.}
Algorithm 1: Optimal Design-based Linear Best Arm Identification (OD-LinBAI)

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

1: Initialize $t_0 = 1$, $A_0 \leftarrow \mathcal{A}$ and $d_0 = d$.
2: For each arm $i \in A_0$, set $a_0(i) = a(i)$.
3: Solve $m$ by Equation (1).
4: for $r = 1$ to $\left\lfloor \log_2 d \right\rfloor$ do
5:  Set $d_r = \dim (\text{span} (\{a_{r-1}(i) : i \in \mathcal{A}_{r-1}\}))$.
6:  if $d_r = d_{r-1}$ then
7:      For each arm $i \in \mathcal{A}_r$, set $a_r(i) = a_{r-1}(i)$.
8:  else
9:      Find matrix $B_r \in \mathbb{R}^{d_{r-1} \times d_r}$ whose columns form a orthonormal basis of the subspace spanned by $\{a_{r-1}(i) : i \in \mathcal{A}_{r-1}\}$.
10:     For each arm $i \in \mathcal{A}_{r-1}$, set $a_r(i) = B_r^T a_{r-1}(i)$.
11: end if
12: if $r = 1$ then
13:     Find a G-optimal design $\pi_r : \{a_r(i) : i \in \mathcal{A}_{r-1}\} \to [0, 1]$ with $|\text{Supp} (\pi_r)| \leq d(d + 1)/2$.
14: else
15:     Find a G-optimal design $\pi_r : \{a_r(i) : i \in \mathcal{A}_{r-1}\} \to [0, 1]$.
16: end if
17: Set $T_r(i) = \lfloor \pi_r(a_r(i)) \cdot m \rfloor$ and $T_r = \sum_{i \in \mathcal{A}_{r-1}} T_r(i)$.
18: Choose each arm $i \in \mathcal{A}_{r-1}$ exactly $T_r(i)$ times.
19: Calculate the OLS estimator:
20: \[ \hat{\theta}_r = V_r^{-1} \sum_{t = t_r}^{t_r + T_r - 1} a_r(A_t)X_t \quad \text{with} \quad V_r = \sum_{i \in \mathcal{A}_{r-1}} T_r(i)a_r(i)a_r(i)^T \]
21: For each arm $i \in \mathcal{A}_{r-1}$, estimate the expected reward:
22: \[ \hat{p}_r(i) = \langle \hat{\theta}_r, a_r(i) \rangle. \]
23: end for

**Output:** the only arm $i_{\text{out}}$ in $\mathcal{A}_{(\log_2 d)}$.

Parameter $m$ plays a significant role in the implementation as well as the theoretical analysis of Algorithm 1.

Since the support of the G-optimal design $\pi_r$ must span $\mathbb{R}^{d_r}$, the OLS estimator can be directly applied (Line 19). Then for each arm $i \in \mathcal{A}_{r-1}$, an estimate of the expected reward is derived. Note that Algorithm 1 decouples the estimates of different phases and only utilizes the information obtained in the current phase $r$.

At the end of each phase $r$, Algorithm 1 eliminates a subset of possibly suboptimal arms. In particular, $K - \left\lfloor d/2^r \right\rfloor$ arms are eliminated in the first phase and about half of the active arms are eliminated in each of the following phases. Eventually, there is only single arm $i_{\text{out}}$ in the active set, which is the output of Algorithm 1.

Remark 3. It is worth considering the case of standard multi-armed bandits, which can be modeled as a special case of linear bandits. In particular, for any arm $i \in \mathcal{A} = [K]$, the corresponding arm vector is chosen to be $e_i$, which is the $i$th standard basis of $\mathbb{R}^K$. It follows that $d = K$, $\theta^* = [p(1), p(2), \ldots, p(K)]^T \in \mathbb{R}^K$ and arms are not correlated with one another. A simple mathematical derivation shows that we can always use a set of standard basis vectors of $\mathbb{R}^d$ to represent the arm vectors regardless of which arms remain active during phase $r$. Also, the G-optimal design for a set of standard basis vectors is the uniform distribution on all of the active arms. Since pulling one arm is not able to give information about the other arms, the empirical estimates
based on the OLS estimator are exactly the empirical means. Altogether, for standard multi-armed bandits, OD-LinBAI reduces to the procedure of Sequential Halving [7], which is a state-of-the-art algorithm for best arm identification in standard multi-armed bandits.

4 Main results

4.1 Upper bound

We first state an upper bound on the error probability of OD-LinBAI (Algorithm 1). The proof of Theorem 2 is deferred to Appendix B.

**Theorem 2.** For any linear bandit instance $\nu \in \mathcal{E}$, OD-LinBAI outputs an arm $i_{out}$ satisfying

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

where $m$ is defined in Equation (1) and

$$H_{2, \text{lin}} = \max_{2 \leq i \leq d} \frac{i}{\Delta_i^2}.$$

Theorem 2 shows the error probability of OD-LinBAI is upper bounded by

$$\exp \left( -\Omega \left( \frac{T}{H_{2, \text{lin}} \log_2 d} \right) \right)$$

which depends on $T$, $d$ and $H_{2, \text{lin}}$. We remark that none of the three terms is avoidable in view of our lower bounds (see Section 4.2).

In particular, $T$ is the time budget of the problem and $d$ is the effective dimension of the arm vectors. Given $T$ and $d$, $H_{2, \text{lin}}$ quantifies the difficulty of identifying the best arm in the linear bandit instance. The parameter $H_{2, \text{lin}}$ generalizes its analogue $H_2$ proposed by Audibert et al. [33] for standard multi-armed bandits. However, $H_{2, \text{lin}}$ is not larger than $H_2$ since $H_{2, \text{lin}}$ is only a function of the first $d - 1$ optimality gaps while $H_2$ considers all of the $K - 1$ optimality gaps. In the extreme case that all of the suboptimal arms have the same optimality gaps, i.e., $\Delta_2 = \Delta_3 = \cdots = \Delta_K$, the two terms $H_2$ and $H_{2, \text{lin}}$ can differ significantly. In general, we have

$$H_{2, \text{lin}} \leq H_2 \leq \frac{K}{d}H_{2, \text{lin}}$$

and both inequalities are essentially sharp, i.e., can be achieved by some linear bandit instances. This highlights a major difference between best arm identification in the fixed-budget setting for linear bandits and standard multi-armed bandits. Due to the linear structure, arms are correlated and we can estimate the mean reward of one arm with the help of the other arms. Thus, the hardness quantity $H_{2, \text{lin}}$ is only a function of the top $d$ arms and not all the arms.

Comparisons with BayesGap [12]. To the best of our knowledge, the only previous algorithm in the same setting of best arm identification in linear bandits with a fixed budget with our work is BayesGap, which is adapted from UGapEb [9] for standard multi-armed bandits. We compare BayesGap and OD-LinBAI with respect to the algorithm design as well as the theoretical guarantees in the following.

(i) The model of BayesGap is Bayesian linear bandits, in which the unknown parameter vector $\theta^*$ is drawn from a known prior distribution $N(0, \eta^2 I)$ and the additive noise is required to be strictly Gaussian. However, OD-LinBAI does not require these assumptions and the upper bound holds for any $\theta^* \in \mathbb{R}^d$.

4Recall that we assume the entire set of original arm vectors $\{a(1), a(2), \ldots, a(K)\}$ span $\mathbb{R}^d$. 

6
Theorem 3. If $d > 0$, this parameter is also associated with the top $d$ arms similarly to $H_{2,\text{lin}}$. The proof of Theorem 3 is deferred to Appendix C, which is built on the lower bound for standard multi-armed bandits [8].

Before stating the lower bound formally, we introduce a generalization of $H_1$ that characterizes the difficulty of a linear bandit instance:

$$H_{1,\text{lin}} = \sum_{1 \leq i \leq d} \Delta_i^{-2}.$$  

This parameter is also associated with the top $d$ arms similarly to $H_{2,\text{lin}}$. See Table 1 for a thorough comparison on different hardness quantities.

For any linear bandit instance $\nu \in \mathcal{E}$, we denote the hardness quantity $H_{1,\text{lin}}$ of $\nu$ as $H_{1,\text{lin}}(\nu)$.

In addition, let $\mathcal{E}(a)$ denote the set of linear bandit instances in $\mathcal{E}$ whose $H_{1,\text{lin}}$ is bounded by $a$ ($a > 0$), i.e., $\mathcal{E}(a) = \{\nu \in \mathcal{E} : H_{1,\text{lin}}(\nu) \leq a\}$.

Here we give a minimax lower bound for the problem of best arm identification in linear bandits in the fixed-budget setting. The proof of Theorem 3 is deferred to Appendix C, which is built on the connection between linear bandits and standard multi-armed bandits and then utilizes the minimax lower bound for standard multi-armed bandits [8].

### Theorem 3

If $T \geq a^2 \log (6T/d)/900$, then

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

Table 1: Comparisons of different hardness quantities: $H_1$, $H_2$, $H_{1,\text{lin}}$ and $H_{2,\text{lin}}$

| $H_1$ | $H_2$ | $H_{1,\text{lin}}$ | $H_{2,\text{lin}}$ |
|-------|-------|-------------------|-------------------|
| $\sum_{1 \leq i \leq K} \Delta_i^{-2}$ | $\max_{2 \leq i \leq K} i \cdot \Delta_i^{-2}$ | $1 \leq H_1/H_2 \leq \log(2K)$ [33] | $1 \leq H_{1,\text{lin}}/H_{2,\text{lin}} \leq \log(2d)$ |
| $1 \leq H_1/H_{1,\text{lin}} \leq K/d$ | $1 \leq H_2/H_{2,\text{lin}} \leq K/d$ |

(ii) The algorithm and theoretical guarantee of BayesGap explicitly require the knowledge of a hardness quantity

$$H_1 = \sum_{1 \leq i \leq K} \Delta_i^{-2}$$

to control the confidence region and then allocate exploration. However, this hardness quantity $H_1$ is almost always unknown to the agent in practice. In most practical applications, BayesGap has to estimate $H_1$ in an adaptive way, which works reasonably well in numerical experiments but lacks guarantees. On the contrary, OD-LinBAI is fully parameter-free.

(iii) The error probability of BayesGap is upper bounded by

$$\exp \left( -\Omega \left( \frac{T}{H_1} \right) \right)$$

which depends on $T$ and $H_1$.

Compared with (3), the upper bound of OD-LinBAI in (2) has an extra $\log_2 d$ term. This is an interesting phenomena which also occurs in standard multi-armed bandits [33, 8]. For best arm identification in standard multi-armed bandits, without the knowledge of the hardness quantity $H_1$, the agent has to pay a price of $\log_2 K$ for the adaptation to the problem complexity. In Theorem 3 we prove a similar result for linear bandits, in which the price for the adaptation is $\log_2 d$.

The upper bound (3) involves $H_1$, which is a function of all the optimality gaps. It holds that $H_1 \geq H_2 \geq H_{2,\text{lin}}$. Thus, the upper bound of OD-LinBAI is better with regard to the problem complexity parameter. BayesGap, at least in the theoretical analysis, does not fully utilize the linear structure of the bandit problem. See Section 4.2 for a more detailed comparison on different hardness quantities.

### 4.2 Lower bound

Before stating the lower bound formally, we introduce a generalization of $H_1$ that characterizes the difficulty of a linear bandit instance:

$$H_{1,\text{lin}} = \sum_{1 \leq i \leq d} \Delta_i^{-2}.$$
Further if \( a \geq 15d^2 \), then
\[
\min_{\pi} \max_{\nu \in E(\alpha)} \Pr [ i_{\text{out}} \neq 1] \cdot \exp \left( \frac{2700T}{H_{1,\text{lin}}(\nu) \log_2 d} \right) \geq \frac{1}{6}.
\]

Theorem 3 first shows that for any best arm identification algorithm \( \pi \), even with the knowledge of an upper bound \( a \) on the hardness quantity \( H_{1,\text{lin}} \), there exists a linear bandit instance such that the error probability is at least
\[
\exp \left( -O \left( \frac{T}{a} \right) \right).
\]
Furthermore, for any best arm identification algorithm \( \pi \), without the knowledge of an upper bound \( a \) on the hardness quantity \( H_{1,\text{lin}} \), there exists a linear bandit instance \( \nu \) such that the error probability is at least
\[
\exp \left( -O \left( \frac{T}{H_{1,\text{lin}}(\nu) \log_2 d} \right) \right).
\]

Comparing the lower bounds (4) and (5) in two different settings, we show that the agent has to pay a price of \( \log_2 d \) in the absence of the knowledge about the problem complexity. Finding a best arm identification algorithm that matching the lower bound (4) remains an open problem since the upper bound of BayesGap (3) involves \( H_1 \) but not \( H_{1,\text{lin}} \). However, notice that the knowledge about the complexity quantity which is required for BayesGap is usually unavailable in real-life applications.

Now we compare the upper bound on the error probability of OD-LinBAI in (2) with the lower bound (5). Table 1 shows that \( H_{1,\text{lin}} \geq H_{2,\text{lin}} \) always holds. Therefore, the upper bound (2) is not larger than the lower bound (5) order-wise in the exponent. However, the upper bound holds for all instances, while the lower bound is a minimax result which holds for specific instances. This shows OD-LinBAI (Algorithm 1) is minimax optimal up to multiplicative factors in the exponent. At the same time, since an upper bound can never be smaller than a lower bound, we know that the hard instances for the problem of best arm identification in linear bandits in the fixed-budget setting are those whose \( H_{1,\text{lin}} \) and \( H_{2,\text{lin}} \) are of the same order.

5 Numerical experiments

In this section, we evaluate the performance of our algorithm OD-LinBAI and compare it with Sequential Halving and BayesGap. We present the results of two synthetic datasets here and the results of a real-world dataset, the Abalone dataset [34], in Appendix D.3 in the supplementary. Sequential Halving [7] is a state-of-the-art algorithm for best arm identification in standard multi-armed bandits. For BayesGap [12], there are two versions: one is BayesGap-Oracle, which is given the exact information of the required hardness quantity \( H_1 \); the other is BayesGap-Adaptive, which adaptively estimates the hardness quantity by the three-sigma rule. Throughout in the synthetic datasets we assume that the additive random noise follows the standard Gaussian distribution \( \mathcal{N}(0, 1) \). In each setting, the reported error probabilities of different algorithms are averaged over 1024 independent trials. Additional implementation details and numerical results are provided in Appendix D.

5.1 Synthetic dataset 1: a hard instance

This dataset, where there are numerous competitors for the second best arm, was considered for the problem of best arm identification in linear bandits in the fixed-confidence setting [23, 20]. Similarly, we consider the situation that \( d = 2 \) and \( K \geq 3 \). For simplicity, we set the unknown parameter vector \( \theta^* = [1, 0]^T \). There is one best arm and one worst arm, which correspond to the arm vectors \( a(1) = [1, 0]^T \) and \( a(K) = [\cos(3\pi/4), \sin(3\pi/4)]^T \) respectively. For any arm \( i \in \{2, 3, \ldots, K-1\} \), the corresponding arm vector is chosen to be \( a(i) = [\cos((\pi/4 + \phi_i)), \sin((\pi/4 + \phi_i))]^T \) with \( \phi_i \) drawn independently from \( \mathcal{N}(0, 0.09) \) independently. Therefore, there are \( K - 2 \) almost second best arms. Considering the definitions of four hardness quantities, it holds that
\[
H_1 \approx H_2 \approx \frac{K}{d} H_{1,\text{lin}} \approx \frac{K}{d} H_{2,\text{lin}}.
\]

Hence this is a hard instance in the sense that the linear structure is extremely strong. A good algorithm needs to fully utilize the correlations of the arms induced by the linear structure to pull arms as efficiently as possible.
Figure 1: Error probabilities for different numbers of arms $K$ with $T = 25, 50, 100$ from left to right.

Figure 2: Error probabilities for different time budgets $T$ with $K = 25, 50, 100$ from left to right.

The experimental results with fixed $T$ and $K$ are presented in Figure 1 and Figure 2 respectively. In terms of this hard linear bandit instance, OD-LinBAI is clearly superior compared to its competitors. In fact, OD-LinBAI consistently pulls only one arm from the $K - 2$ almost second best arms and thus suffers minimal impact from the increase in $K$.

5.2 Synthetic dataset 2: random arm vectors

In this experiment, the $K$ arm vectors are uniformly sampled from the unit $d$-dimensional sphere $S^{d-1}$. Without loss of generality, we assume that $a(1), a(2)$ are the two closest arm vectors and then set $\theta^* = a(1) + 0.01(a(1) - a(2))$. Thus the best arm is arm 1 while the second best arm is arm 2. Differently from previous works [11, 25, 26, 28], we set the number of arms to be $K = c^d$ with a integer constant $c$. According to Theorem 8 in Cai et al. [35], the minimum optimality gap $\Delta_1$ will converge in probability to a positive number as $d$ tends to infinity so that the random linear bandit instances which we perform our experiments on are neither too hard nor too easy.

Figure 3: Error probabilities for different $d$ with $c = 2$ on the left and $c = 3$ on the right.

Figure 3 shows the error probabilities of the 4 different algorithms for this dataset with $c = 2$ or 3 when the time budget $T = 2K$. In most situations, OD-LinBAI outperforms the other algorithms. Moreover, Table 4 and Table 5 in the supplementary show that OD-LinBAI is computationally ef-
cient compared to BayesGap, which involves matrix inverse updates to calculate the confidence widths at each time step. See Appendix D.2 for additional results and discussion on this dataset.

6 Conclusion

In this paper, we introduce the G-optimal design technique into the problem of best arm identification in linear bandits in the fixed-budget setting. We design a parameter-free algorithm OD-LinBAI. To characterize the difficulty of a linear bandit instance, we introduce two hardness quantities $H_{1,\text{lin}}$ and $H_{2,\text{lin}}$. The upper bound of the error probability of OD-LinBAI and the minimax lower bound of this problem are respectively characterized by $H_{1,\text{lin}}$ and $H_{2,\text{lin}}$ instead of their analogues $H_1$ and $H_2$ in standard multi-armed bandits. Moreover, OD-LinBAI is minimax optimal up to multiplicative factors in the exponent, which is also supported by the considerable improvement of the performance in the numerical experiments over existing algorithms.

An potential direction for future work is to design an instance-dependent asymptotically optimal algorithm for this problem. However, finding a such algorithm or even an instance-dependent lower bound for the problem of best arm identification in standard multi-armed bandits in the fixed-budget setting remains open.
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A More discussions on the G-optimal design

c-approximate G-optimal design. For the problem of best arm identification in linear bandits in the fixed-budget setting, it is sufficient to compute an c-approximate G-optimal design with minimal impact on performance. For an c-approximate optimal design \(\pi\), \(g(\pi) \leq (1 + \epsilon)d\). Todd [36] shows that such a design can be computed within \(4d(\log \log d + 7/2) + 28d/\epsilon\) iterations by the Frank-Wolfe algorithm with a specific initialization. If we only compute c-approximate optimal designs in OD-LinBAI (Algorithm\([\Pi]\)), the upper bound on the error probability will only deteriorate by a factor of \((1 + \epsilon)\) as follows.

**Theorem 4.** For any linear bandit instance \(\nu \in \mathcal{E}\), OD-LinBAI, using c-approximate G-optimal designs, outputs an arm \(i_{\text{out}}\) satisfying

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

where \(m\) is defined in Equation \((7)\).

Near-optimal design with smaller support. Recently, a near-optimal design with smaller support was proposed in Lattimore et al. [32]. In detail, there exists a design \(\pi : \{a(i) : i \in \mathcal{A}\} \rightarrow [0, 1]\) such that \(g(\pi) \leq 2d\) and \(|\text{Supp}(\pi)| \leq 4d(\log \log d + 11)\). Todd [36] shows that such a design can be computed within \(4d(\log \log d + 21/2)\) iterations by the Frank-Wolfe algorithm with a specific initialization. Since the support of the design is smaller when \(d\) is large, we can choose a larger \(m\) in OD-LinBAI while the total budget consumed by the agent is still bounded by \(T\). In particular, we can choose the parameter \(m\) as

\[
m = \frac{T - \min(K, 4d(\log \log d + 11)) - \sum_{r=1}^{\lceil \log_2 d \rceil - 1} \left\lfloor \frac{d}{\pi_r^*} \right\rfloor}{\lceil \log_2 d \rceil}.
\]

(6)

The error probability can be bounded as follows.

**Theorem 5.** For any linear bandit instance \(\nu \in \mathcal{E}\), OD-LinBAI, using near-optimal designs with smaller support, outputs an arm \(i_{\text{out}}\) satisfying

\[
\text{Pr}[i_{\text{out}} \neq 1] \leq \left(\frac{4K}{d} + 3\log_2 d\right) \exp\left(-\frac{m}{64H_{2,\text{lin}}}\right)
\]

where \(m\) is defined in Equation \((6)\).

B Proof of Theorem[2]

Before going to the proof of Theorem[2] we first introduce some useful lemmas. Lemma[1] shows Algorithm\([\Pi]\) is feasible in the sense that the total budget consumed by the agent is no more than \(T\), and \(i_{\text{out}}\) is well-defined.

**Lemma 1.** With parameter \(m\) defined as Equation \((7)\), Algorithm\([\Pi]\) terminates in phase \([\log_2 d]\) with no more than a total of \(T\) arm pulls.

**Proof.** When \(d = 2\), Algorithm\([\Pi]\) terminates in one phase. When \(d > 2\), by the property of ceiling function, we have \(\frac{d}{2^{\lceil \log_2 d \rceil - 1}} \leq 1\). Thus, the number of arms in \(\mathcal{A}_{\lceil \log_2 d \rceil - 1}\) is \(\left\lfloor \frac{d}{2^{\lceil \log_2 d \rceil - 1}} \right\rfloor = 2\), while the number of arms in \(\mathcal{A}_{\lceil \log_2 d \rceil}\) is \(\left\lfloor \frac{d}{2^{\lceil \log_2 d \rceil}} \right\rfloor = 1\). As a result, Algorithm\([\Pi]\) always terminates in phase \([\log_2 d]\).

Now we bound the number of arm pulls. For any phase \(r\), \(|\text{Supp}(\pi_r)|\) is always bounded by the cardinality of the active set \(\mathcal{A}_{r-1}\). In particular, for the first phase, according to Theorem[1] there exists a G-optimal design \(\pi_0\) with \(|\text{Supp}(\pi_0)| \leq d(d + 1)/2\). Altogether, we have

\[
|\text{Supp}(\pi_r)| \leq \begin{cases} 
\min(K, \frac{d(d+1)}{2}) & \text{when } r = 1 \\
\frac{d}{2^{r-1}} & \text{when } r > 1.
\end{cases}
\]
Then the number of total arm pulls is bounded as

\[
\sum_{r=1}^{\lceil \log_2 d \rceil} T_r = \sum_{r=1}^{\lceil \log_2 d \rceil} \sum_{i \in \mathcal{A}_r} T_r(i)
= \sum_{r=1}^{\lceil \log_2 d \rceil} \sum_{i \in \mathcal{A}_r} [\pi_r(a_r(i)) \cdot m]
\leq \sum_{r=1}^{\lceil \log_2 d \rceil} \left( |\text{Supp}(\pi_r)| + \sum_{i \in \mathcal{A}_r} \pi_r(a_r(i)) \cdot m \right)
\leq \min \left( K, \frac{d(d+1)}{2} \right) + \sum_{r=2}^{\lceil \log_2 d \rceil} \left[ \frac{d}{2^{r-1}} \right] + \lceil \log_2 d \rceil \cdot m
= T
\]

where line (7) follows from the property of ceiling function and line (8) follows from the definition of \(m\).

Lemma 2 bounds the probability that a certain arm has its estimate of the expected reward larger than that of the best arm in single phase \(r\).

**Lemma 2.** Assume that the best arm is not eliminated prior to phase \(r\), i.e., \(1 \in \mathcal{A}_{r-1}\). Then for any arm \(i \in \mathcal{A}_{r-1}\),

\[
\Pr[\hat{\theta}_r(1) < \hat{\theta}_r(i) \mid 1 \in \mathcal{A}_{r-1}, i \in \mathcal{A}_{r-1}] \leq \exp \left( -\frac{m\Delta^2}{8\ceil{\frac{d}{2^{r-1}}}} \right).
\]

**Proof.** Let \(\theta^*_r\) denote the corresponding unknown parameter vector for the dimensionality-reduced arm vectors \(\{a_r(i) : i \in \mathcal{A}_{r-1}\}\). Also we set

\[
V_r(\pi_r) = \sum_{i \in \mathcal{A}_{r-1}} \pi_r(a_r(i))a_r(i)\top.
\]

Then we have

\[
\Pr[\hat{\theta}_r(1) < \hat{\theta}_r(i) \mid 1 \in \mathcal{A}_{r-1}, i \in \mathcal{A}_{r-1}]
= \Pr[\langle \hat{\theta}_r - \theta^*_r, a_r(1) - a_r(i) \rangle < -\Delta i \mid 1 \in \mathcal{A}_{r-1}, i \in \mathcal{A}_{r-1}]
\leq \exp \left( -\frac{\Delta^2}{2\|a_r(1) - a_r(i)\|_{V_r^{-1}}^2} \right)
\leq \exp \left( -\frac{\Delta^2}{8 \max_{i \in \mathcal{A}_r} \|a_r(i)\|_{V_r^{-1}}^2} \right)
\leq \exp \left( -\frac{\Delta^2 \cdot m}{8 \max_{i \in \mathcal{A}_r} \|a_r(i)\|_{V_r(\pi_r)\top}^2} \right)
\leq \exp \left( -\frac{m\Delta^2}{8d_r} \right)
\leq \exp \left( -\frac{m\Delta^2}{8\ceil{\frac{d}{2^{r-1}}}} \right).
\]

Line (9) follows from

\[
\begin{align*}
\hat{\theta}_r(1) &= \langle \hat{\theta}_r, a_r(1) \rangle \\
\hat{\theta}_r(i) &= \langle \hat{\theta}_r, a_r(i) \rangle \\
\Delta_i &= \langle \theta^*_r, a_r(1) - a_r(i) \rangle = \langle \theta^*, a(1) - a(i) \rangle.
\end{align*}
\]
Line (10) follows from Proposition 1, the confidence bound for the OLS estimator. Line (11) follows from the triangle inequality for \( \| \cdot \|_{V_{r^{-1}}} \) norm. Line (12) follows from

\[
\| a_r(i) \|^2_{V_{r^{-1}}} = a_r(i)^T V_{r^{-1}} a_r(i)
\]

\[
= a_r(i)^T \left( \sum_{i \in A_{r^{-1}}} T_r(i) a_r(i) a_r(i)^T \right)^{-1} a_r(i)
\]

\[
\leq a_r(i)^T \left( \sum_{i \in A_{r^{-1}}} m \pi_r(a_r(i)) a_r(i) a_r(i)^T \right)^{-1} a_r(i)
\]

\[
= \frac{1}{m} a_r(i)^T \left( \sum_{i \in A_{r^{-1}}} \pi_r(a_r(i)) a_r(i) a_r(i)^T \right)^{-1} a_r(i)
\]

\[
= \frac{1}{m} a_r(i)^T V_r(\pi_r)^{-1} a_r(i)
\]

\[
= \frac{1}{m} \| a_r(i) \|^2_{V_r(\pi_r)^{-1}}.
\]

Line (13) follows from Theorem 1, the property of G-optimal design. Line (14) follows from the fact that the dimension of the space spanned by the corresponding arm vectors of the active arm set \( A_{r^{-1}} \) is not larger than the cardinality of \( A_{r^{-1}} \).

Armed with Lemma 2 then we bound the error probability of single phase \( r \) in Lemma 3.

**Lemma 3.** Assume that the best arm is not eliminated prior to phase \( r \), i.e., \( 1 \in A_{r^{-1}} \). Then the probability that the best arm is eliminated in phase \( r \) is at most

\[
\begin{aligned}
& \frac{4K}{d} \exp \left( -\frac{m \Delta^2}{32i_r^2} \right) \quad \text{when } r = 1 \\
& 3 \exp \left( -\frac{m \Delta^2}{32i_r^2} \right) \quad \text{when } r > 1
\end{aligned}
\]

where \( i_r = \left\lceil \frac{d}{2^r} \right\rceil + 1 \).

**Proof.** Define \( \mathcal{B}_r \) as the set of arms in \( A_{r^{-1}} \) excluding the best arm and \( \left\lceil \frac{d}{2^r} \right\rceil - 1 \) suboptimal arms with the largest expected rewards. Therefore, we have \( |\mathcal{B}_r| = |A_{r^{-1}}| - \left\lceil \frac{d}{2^r} \right\rceil \) and \( \min_{\mathcal{I} \in \mathcal{B}_r} \Delta_i \geq \Delta \left\lceil \frac{d}{2^r} \right\rceil + 1 \).

If the best arm is eliminated in phase \( r \), then at least \( \left\lceil \frac{d}{2^r} \right\rceil - \left\lceil \frac{d}{2^r} \right\rceil + 1 \) arms of \( \mathcal{B}_r \) have their estimates of the expected rewards larger than that of the best arm.
Let $N_r$ denote the number of arms in $B_r$ whose estimates of the expected rewards larger than that of the best arm. By Lemma 2, we have

$$
\mathbb{E} [N_r | 1 \in A_{r-1}] = \sum_{i \in B_r} \Pr [\hat{\beta}_r(i) < \beta_r \mid 1 \in A_{r-1}]
$$

$$
\leq \sum_{i \in B_r} \exp \left( -\frac{m \Delta_i^2}{8 \left(\frac{d}{2^r + 1}\right)} \right)
$$

$$
\leq |B_r| \max_{i \in B_r} \exp \left( -\frac{m \Delta_i^2}{8 \left(\frac{d}{2^r + 1}\right)} \right)
$$

$$
\leq \left( |A_{r-1}| - \left\lceil \frac{d}{2^{r+1}} \right\rceil \right) \exp \left( \frac{- m \Delta_i^2}{8 \left(\frac{d}{2^r + 1}\right)} \right) + 1
$$

$$
\leq \left( |A_{r-1}| - \left\lceil \frac{d}{2^{r+1}} \right\rceil \right) \exp \left( \frac{- m \Delta_i^2}{8 \left(\frac{d}{2^{r+1}} \right)} + 1 \right).
$$

Then, together with Markov’s inequality, we can get

$$
\Pr [1 \notin A_r \mid 1 \in A_{r-1}] \leq \Pr [N_r \geq \left\lceil \frac{d}{2^r} \right\rceil - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1 \mid 1 \in A_{r-1}]
$$

$$
\leq \mathbb{E} [N_r \mid 1 \in A_{r-1}]
$$

$$
\leq \left| A_{r-1} \right| - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1 \exp \left( \frac{- m \Delta_i^2}{8 \left(\frac{d}{2^{r+1}} \right)} + 1 \right).
$$

When $r = 1$, we have $|A_{r-1}| = K$. Thus,

$$
\frac{|A_{r-1}| - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1}{\left\lceil \frac{d}{2^r} \right\rceil - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1} = \frac{K - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1}{\left\lceil \frac{d}{2^r} \right\rceil - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1}
$$

$$
\leq \frac{K}{2 - \frac{d}{2^r}}
$$

$$
= \frac{4K}{d}.
$$

When $r > 1$, we have $|A_{r-1}| = \left\lceil \frac{d}{2^{r+1}} \right\rceil$. Thus,

$$
\frac{|A_{r-1}| - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1}{\left\lceil \frac{d}{2^r} \right\rceil - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1} = \frac{\left\lceil \frac{d}{2^r} \right\rceil - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1}{\left\lceil \frac{d}{2^r} \right\rceil - \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1}
$$

$$
\leq \frac{\frac{d}{2^r} + 1 - \frac{d}{2^{r+1}}}{\frac{d}{2^r} - \frac{d}{2^{r+1}} + 1}
$$

$$
\leq \frac{3 \cdot \frac{d}{2^{r+1}} + \frac{d}{2^{r+1}} + 1 - \frac{d}{2^{r+1}}}{\frac{d}{2^{r+1}} + \frac{d}{2^{r+1}} + 1 - \frac{d}{2^{r+1}}}
$$

$$
\leq 3
$$

where the last inequality results from the fact that for any $x, y > 0$, $\frac{3x+y}{x+y} < 3$.

Eventually, the error probability of phase $r$ can be bounded as

$$
\Pr [1 \notin A_r \mid 1 \in A_{r-1}] \leq \begin{cases} 
\frac{4K}{d} \exp \left( -\frac{m \Delta_i^2}{32r} \right) & \text{when } r = 1 \\
3 \exp \left( -\frac{m \Delta_i^2}{32r} \right) & \text{when } r > 1
\end{cases}
$$

where $i_r = \left\lceil \frac{d}{2^{r+1}} \right\rceil + 1$.  \qed
Now we return to the proof of Theorem 2.

Proof of Theorem 2 By applying Lemma 1 and Lemma 3 we have
\[
\Pr \left[ i_{out} \neq 1 \right] = \Pr \left[ 1 \notin \mathcal{A}_{\log_2 d} \right]
= \sum_{r=1}^{K} \Pr \left[ 1 \notin \mathcal{A}_r \mid 1 \in \mathcal{A}_{r-1} \right]
\leq \frac{4K}{d} \exp \left( -\frac{m \Delta_i^2}{32r} \right) + \sum_{r=2}^{\log_2 d} \exp \left( -\frac{m \Delta_i^2}{32r} \right)
\leq \left( \frac{4K}{d} + 3 (\lceil \log_2 d \rceil - 1) \right) \exp \left( -\frac{m}{32} \frac{1}{\max_{2 \leq i \leq d} \Delta_i^2} \right)
< \left( \frac{4K}{d} + 3 \log_2 d \right) \exp \left( -\frac{m}{32H_{2,lin}} \right)
\]
where \( H_{2,lin} \) is defined as
\[
H_{2,lin} = \max_{2 \leq i \leq d} \frac{i}{\Delta_i^2}.
\]
\hfill \Box

C Proof of Theorem 3

The proof of Theorem 3 is built on the connection between linear bandits and standard multi-armed bandits [8]. Therefore, we first introduce the setting of best arm identification in standard multi-armed bandits.

In a standard multi-armed bandit instance \( \tilde{\nu} \), the agent is given an arm set \( \mathcal{A} = [K] \). Each arm \( i \in \mathcal{A} \) is associated with a reward distribution \( P_i \) supported in \([0, 1]\), which is unknown to the agent. At each time \( t \), the agent chooses an arm \( A_t \) from the arm set \( \mathcal{A} \) and then observes a stochastic reward \( X_t \in [0, 1] \) drawn from \( P_{A_t} \).

In the fixed-budget setting, given a time budget \( T \in \mathbb{N} \), the agent also aims at maximizing the probability of identifying the best arm with no more than \( T \) arm pulls. More formally, the agent uses an online algorithm \( \tilde{\pi} \) to decide the arm \( A_t^{\tilde{\pi}} \) to pull at each time step \( t \), and the arm \( i_{out}^{\tilde{\pi}} \in \mathcal{A} \) to output as the identified best arm by time \( T \).

As in linear bandits, we assume that the expected rewards of the arms are in descending order and the best arm is unique. Let \( \mathcal{E} \) denote the set of all the linear bandit instances defined above. For any arm \( i \in \mathcal{A} \), let \( p(i) \) denote the expected reward under \( P_i \). Similarly, for any suboptimal arm \( i \), we denote \( \Delta_i = p(1) - p(i) \) as the optimality gap. For ease of notation, we also set \( \Delta_1 = \Delta_2 \).

Moreover, the two hardness quantities \( H_1 \) and \( H_2 \) are also applicable to standard multi-armed bandits. For any standard multi-armed bandit instance \( \tilde{\nu} \in \mathcal{E} \), we denote the hardness quantity \( H_1 \) of \( \tilde{\nu} \) as \( H_1(\tilde{\nu}) \). In addition, let \( \mathcal{E}(a) \) denote the set of standard multi-armed bandit instances in \( \mathcal{E} \) whose \( H_1 \) is bounded by \( a \) (a > 0), i.e., \( \mathcal{E}(a) = \{ \tilde{\nu} \in \mathcal{E} : H_1(\tilde{\nu}) \leq a \} \).

A minimax lower bound for the problem of best arm identification in standard multi-armed bandits in the fixed-budget setting is provided in Theorem 6.

**Theorem 6** (Adapted from [8], Theorem 1). If \( T \geq a^2 \log(6TK) / 900 \), then
\[
\min_{\tilde{\pi}} \max_{\nu \in \mathcal{E}(a)} \Pr \left[ i_{out}^{\tilde{\pi}} \neq 1 \right] \geq \frac{1}{6} \exp \left( -\frac{240T}{a} \right).
\]

Further if \( a \geq 15K^2 \), then
\[
\min_{\tilde{\pi}} \max_{\nu \in \mathcal{E}(a)} \left( \Pr \left[ i_{out}^{\tilde{\pi}} \neq 1 \right] \cdot \exp \left( \frac{2700T}{H_1(\nu) \log_2 K} \right) \right) \geq \frac{1}{6}.
\]
We construct a special linear bandit instance $\nu$ as follows. Recall that we assume the entire set of original arm vectors \{a(1), a(2), \ldots, a(K)\} span $\mathbb{R}^d$, so it holds that $K \geq d$. For any arm $i \in \{1, 2, \ldots, d\}$, the corresponding arm vector is chosen to be $e_i$, the $i$th standard basis of $\mathbb{R}^d$. It follows that $\theta^* = [p(1), p(2), \ldots, p(d)]^\top \in \mathbb{R}^d$. For all the remaining arms $i \in \{d + 1, d + 2, \ldots, K\}$, the corresponding arm vector $a(i)$ is chosen to be zero vector, i.e., a vector with all entries equal to 0. Furthermore, we require the expected rewards of all the arms to be nonnegative. That is to say, $p(i) \geq 0$ for all $i \in [K]$ and in particular $p(i) = 0$ for all $i \in \{d + 1, d + 2, \ldots, K\}$.

If the agent is given the above extra information that the expected rewards of all the arms are nonnegative (which can only help the agent improve the identification probability), then the agent knows immediately that the best arm must be among the arms $\{1, 2, \ldots, d\}$ since $p(1), p(2), \ldots, p(K) \geq 0$. In addition, pulling the remaining arms cannot provide any useful information since the corresponding arm vectors are vectors of all zeros. Thus, the best strategy that the agent can follow is to only pull the first $d$ arms. Consequently, this linear bandit instance $\nu$ is reduced to a standard bandit instance $\tilde{\nu}$ with $d$ independent arms.

Therefore, Theorem 6 gives a minimax lower bound on the probability of misidentifying the best arm in the standard bandit instance $\tilde{\nu}$, due to the fact that any bounded random variable on $[0, 1]$ is $1$-subgaussian. Also, following the above construction, it holds that

$$H_{1, \text{lin}}(\nu) = H_1(\tilde{\nu}).$$

Notice that the agent cannot do better in the absence of the extra information in the linear bandit instance $\nu$. The minimax lower bound derived from Theorem 6 is also a minimax lower bound for the problem of best arm identification in linear bandits in the fixed-budget setting.

**Proof of Theorem 3** The idea of the proof is to reduce the linear bandit problem to the standard multi-armed bandit problem.

We construct a special linear bandit instance $\nu$ as follows. Recall that we assume the entire set of original arm vectors \{a(1), a(2), \ldots, a(K)\} span $\mathbb{R}^d$, so it holds that $K \geq d$. For any arm $i \in \{1, 2, \ldots, d\}$, the corresponding arm vector is chosen to be $e_i$, the $i$th standard basis of $\mathbb{R}^d$. It follows that $\theta^* = [p(1), p(2), \ldots, p(d)]^\top \in \mathbb{R}^d$. For all the remaining arms $i \in \{d + 1, d + 2, \ldots, K\}$, the corresponding arm vector $a(i)$ is chosen to be zero vector, i.e., a vector with all entries equal to 0. Furthermore, we require the expected rewards of all the arms to be nonnegative. That is to say, $p(i) \geq 0$ for all $i \in [K]$ and in particular $p(i) = 0$ for all $i \in \{d + 1, d + 2, \ldots, K\}$.

If the agent is given the above extra information that the expected rewards of all the arms are nonnegative (which can only help the agent improve the identification probability), then the agent knows immediately that the best arm must be among the arms $\{1, 2, \ldots, d\}$ since $p(1), p(2), \ldots, p(K) \geq 0$. In addition, pulling the remaining arms cannot provide any useful information since the corresponding arm vectors are vectors of all zeros. Thus, the best strategy that the agent can follow is to only pull the first $d$ arms. Consequently, this linear bandit instance $\nu$ is reduced to a standard bandit instance $\tilde{\nu}$ with $d$ independent arms.

Therefore, Theorem 6 gives a minimax lower bound on the probability of misidentifying the best arm in the standard bandit instance $\tilde{\nu}$, due to the fact that any bounded random variable on $[0, 1]$ is $1$-subgaussian. Also, following the above construction, it holds that

$$H_{1, \text{lin}}(\nu) = H_1(\tilde{\nu}).$$

Notice that the agent cannot do better in the absence of the extra information in the linear bandit instance $\nu$. The minimax lower bound derived from Theorem 6 is also a minimax lower bound for the problem of best arm identification in linear bandits in the fixed-budget setting. \hfill \Box

**D Additional implementation details and numerical results**

**D.1 Additional implementation details**

**OD-LinBAI.** In each phase, we compute an $\epsilon$-approximate G-optimal design, where $\epsilon = 10^{-7}$. As noted in Appendix A, this causes minimal impact on performance. Moreover, we follow the Wolfe-Atwood Algorithm with the Kumar-Yildirim start introduced in Todd [36].

**Sequential Halving.** In any linear bandit instance, we treat the $K$ arms as being independent and then apply Sequential Halving [7].

**BayesGap.** For unknown parameter vector $\theta^*$, we use an uninformative prior with $\eta = 10^6$, a very large variance, for a fair comparison. In fact, through testing we find that this parameter has limited influence on the performance. With respect to the parameter $\epsilon$ that controls the tolerance of output, although it suffices to set $\epsilon$ to be the minimum optimality gap $\Delta_1$ theoretically, we follow the setting of Hoffman et al. [12], i.e., $\epsilon = 0$.

- BayesGap-Oracle: We directly give the algorithm exact information of the required hardness quantity $H_1$.
- BayesGap-Adaptive: Following Hoffman et al. [12], we estimate the required hardness quantity by the three-sigma rule at the beginning of each time step.

**D.2 Further observations on synthetic dataset 2**

It is shown in Figure 3 that BayesGap-Oracle does not outperform its adaptive version BayesGap-Adaptive and sometimes even falls behind Sequential Halving. This is partly because BayesGap-Oracle might be too conservative to converge when $T = 2K$. It is noted that in UGapEb [9],
from which BayesGap is adapted, the exploration parameter that controls how much exploration the algorithm does is tuned even if the required hardness quantity is known to the agent. Nevertheless, our algorithm OD-LinBAI is fully parameter-free.

The empirical means of $\Delta_1$, $H_1$, $H_2$, $H_{1,\text{lin}}$ and $H_{2,\text{lin}}$ for different $d$ with $c = 2$ or 3 are reported in Table 2 and Table 3 respectively while the empirical means of the CPU runtimes for different algorithms are listed in Table 4 and Table 5. From these tables, we have the following observations:

(i) With the increase in the dimension of the linear bandit instances, the empirical means of the minimum optimality gap $\Delta_1$ vary a little. However, for OD-LinBAI, the linear bandit instances become easier since the time budgets grow exponentially.

(ii) Different from synthetic dataset 1, the values of the four hardness quantities $H_1$, $H_2$, $H_{1,\text{lin}}$ and $H_{2,\text{lin}}$ in synthetic dataset 2 are close, which is because they are dominated by several smallest optimality gaps.

(iii) OD-LinBAI shows great superiority in terms of CPU runtimes with the increase in $d$. Whereas BayesGap is computationally intractable for synthetic dataset 2 with large $d$, due to the time-consuming matrix inverse updates at each time step.

### D.3 Real-world dataset: Abalone dataset

We conduct an experiment on the Abalone dataset [34], which includes 4177 groups of 8 attributes (such as sex, length, diameter, etc.) of the abalone as well as its target variable which is the abalone’s age. The age of each abalone is usually hard to determine so it is tempting to predict the age using the 8 attributes from physical measurements. To adapt the dataset into a linear bandit problem, we...
first use the whole dataset to calculate the linear regression coefficient vector \( \theta^* \in \mathbb{R}^9 \) and then form a set of arm vectors by the attributes of 400 abalones with the largest true ages. Therefore, in this real-world dataset, it holds that \( d = 9 \) and \( K = 400 \). We assume that the additive random noise follows a Gaussian distribution \( \mathcal{N}(0, 10^2) \). The experimental results of the 4 different algorithms are shown in Figure 4.

![Figure 4: Error probabilities for different time budgets \( T \).](image)

From Figure 4 we see that OD-LinBAI outperforms the other competitors for all time horizons \( T \).