Geometry-Aware Approaches for Balancing Performance and Theoretical Guarantees in Linear Bandits

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Abstract

This paper is motivated by recent research in the d-dimensional stochastic linear bandit literature, which has revealed an unsettling discrepancy: algorithms like Thompson sampling and Greedy demonstrate promising empirical performance, yet this contrasts with their pessimistic theoretical regret bounds. The challenge arises from the fact that while these algorithms may perform poorly in certain problem instances, they generally excel in typical instances. To address this, we propose a new data-driven technique that tracks the geometric properties of the uncertainty ellipsoid around the main problem parameter. This methodology enables us to formulate a data-driven frequentist regret bound, which incorporates the geometric information, for a broad class of base algorithms, including Greedy, OFUL, and Thompson sampling. This result allows us to identify and "course-correct" problem instances in which the base algorithms perform poorly. The course-corrected algorithms achieve the minimax optimal regret of order $\widetilde{\mathcal{O}}(d\sqrt{T})$ for a T-period decision-making scenario, effectively maintaining the desirable attributes of the base algorithms, including their empirical efficacy. We present simulation results to validate our findings using synthetic and real data.

1 Introduction

Multi-armed bandits (MABs) have garnered significant attention as they provide well-defined framework and techniques for investigating the trade off between experimentation (learning) and rewards (earning) and in sequential decision-making problems. In MAB problems, a decision-maker sequentially selects actions from a given set and observes corresponding uncertain rewards. The MAB setting also extends to scenarios where the decision rewards can be personalized by the presence of features or covariates, leading to contextual bandits, as showcased in a large number of recent applications (Langford & Zhang, 2008; Li et al., 2010; Tewari & Murphy, 2017; Zhou et al., 2020; Villar et al., 2015; Bastani & Bayati, 2020; Cohen et al., 2020). This paper focuses on a well-studied class of models that captures both MABs and contextual bandits as special cases while being amenable to theoretical analysis: the stochastic linear bandit (LB) problem. In this model, the problem parameter $\theta^\star$ represents an unknown vector in $\mathbb{R}^d$, while the actions, also vectors in $\mathbb{R}^d$, yield noisy rewards with a mean equal to the inner product of $\theta^\star$ and the chosen action. The objective of a policy is to maximize the cumulative reward based on the observed data up to the decision time. The policy's performance is measured by the cumulative regret, which quantifies the difference between the total expected rewards achieved by the policy and the maximum achievable expected reward.

Achieving this objective necessitates striking a balance between exploration and exploitation. In the context of LB, this entails selecting actions that aid in estimating the true parameter $\theta^\star$ accurately while obtaining optimal rewards. Various algorithms based on the *optimism principle* have been developed to address this challenge, wherein the optimal action is chosen based on the upper confidence bound (UCB) (Lai & Robbins, 1985; Auer,

2002; Dani et al., 2008; Rusmevichientong & Tsitsiklis, 2010). Another popular strategy is Thompson sampling (TS), a Bayesian heuristic introduced by Thompson (1933) that employs randomization to select actions according to the posterior distribution of reward functions. Additionally, the Greedy policy that selects the myopically best action is shown to be effective in contextual bandits (Kannan et al., 2018; Raghavan et al., 2018; Hao et al., 2020; Bastani et al., 2021).

In the linear bandit setting, two types of regret are considered. The Bayesian regret is applicable when the parameter $\theta^\star$ is treated as a random variable with a prior distribution. In this case, the regret is averaged over three sources of randomness: the observation noise, the randomized algorithm, and the random parameter $\theta^\star$. Intuitively, the Bayesian regret measures the expected performance of the algorithm over different realizations of the parameter $\theta^\star$. Russo & Van Roy (2014) and Dong & Van Roy (2018) establish an $\widetilde{\mathcal{O}}(d\sqrt{T})$ upper bound for the Bayesian regret of the Thompson Sampling (TS) heuristic, referred to as LinTS, which matches the minimax optimal bound shown by Dani et al. (2008). Here, $\widetilde{\mathcal{O}}$ refers to the asymptotic order, up to polylogarithmic factors.

On the other hand, the frequentist regret assumes a fixed, unknown parameter $\theta^\star$, and the expectation is taken only with respect to the randomness of the noise and the algorithm. In this frequentist setting, the optimism-based algorithm proposed by Abbasi-Yadkori et al. (2011), known as Optimism in the Face of Uncertainty Linear Bandit Algorithm (OFUL), achieves a $\widetilde{\mathcal{O}}(d\sqrt{T})$ frequentist regret bound, which matches the minimax optimal Bayesian bound. However, for a frequentist variant of LinTS, referred to as TS-Freq, which modifies the posterior distribution by increasing its variance, Agrawal & Goyal (2013) and Abeille et al. (2017) provide a $\widetilde{\mathcal{O}}(d\sqrt{dT})$ upper bound for the frequentist regret. This regret bound falls short of the optimal rate by a factor of $\sqrt{d}$. Recent work by Hamidi & Bayati (2020a) confirms that this modification is necessary, and thus, the frequentist regret of LinTS cannot be improved. For the Greedy algorithm in linear bandit problems, no general theoretical guarantee exists (Lattimore & Szepesvari, 2017), and hence both LinTS and Greedy might perform suboptimally.

Despite the theoretical gaps in performance, LinTS has shown strong empirical performance (Russo et al., 2018), indicating that the inflation of the posterior distribution may be unnecessary in most problem instances, and unfavorable instances are unlikely to occur frequently. Similarly, the Greedy algorithm works well in typical instances (Bietti et al., 2021). Additionally, while optimism-based algorithms are computationally expensive (generally NP-hard as discussed by Dani et al. (2008); Russo & Van Roy (2014); Agrawal (2019)), LinTS and Greedy are known for their computational efficiency. This unsettling disparity between theoretical, computational, and empirical performance has motivated our investigation into the following two questions: Is it possible to identify, in a data-driven fashion, problematic instances where LinTS and Greedy could potentially fail and apply a "course-correction" to ensure competitive frequentist regret bounds? And can this be achieved without compromising their impressive empirical performance and computational efficiency? In this paper, we provide positive answers to both questions. Specifically, we make the following *contributions*.

1. We develop a real-time geometric analysis technique for the d-dimensional confidence ellipsoid surrounding $\theta^\star$. This method is crucial for maximizing the use of historical data, advancing beyond methods that capture only limited information from the confidence ellipsoid, such as a single numerical value. Consequently, this facilitates a more precise "course-correction".

2. We introduce a comprehensive family of algorithms, termed *POFUL* (encompassing OFUL, LinTS, TS-Freq, and Greedy as specific instances), and derive a general, data-driven frequentist regret bound for them. This bound is efficiently computable using data observed from previous decision epochs.

3. We introduce course-corrected variants of LinTS and Greedy that achieve minimax optimal frequentist regret. These adaptations maintain most of the desirable characteristics of the original algorithms.

The distinguishing feature of our study from the existing literature is the geometric analysis of the d-dimensional confidence ellipsoid. Specifically, we conduct an analysis considering the size, shape, position, and orientation of the confidence ellipsoid during the execution of bandit algorithms. This enables real-time characterization of the set of potentially optimal actions, leading to the establishment of a data-driven regret bound.

1.1 Other Related Literature

Our work is closely related to three main research streams: methodological foundations of linear bandits, bandit algorithms utilizing spectral properties, and data-driven exploration techniques. While these works share some similarities with our approach, we highlight the key differences and the unique aspects of our methodology.

From a methodological perspective, our regret analysis builds upon the foundations laid by Abbasi-Yadkori et al. (2011), Agrawal & Goyal (2013), and Abeille et al. (2017). However, a key distinguishing factor is that our approach does not rely on optimistic samples, which is a departure from previous methods. This means that the algorithms we study do not always choose actions that are expected to perform better than the true optimal action. By allowing non-optimistic samples, we avoid the need to inflate the posterior distribution, a requirement in the works of Agrawal & Goyal (2013) and Abeille et al. (2017).

Our use of spectral information in bandit algorithms bears some resemblance to the study of *Spectral Bandits* (Valko et al., 2014; Kocák et al., 2014; Kocák et al., 2020; Kocák & Garivier, 2020). These works represent arm rewards as smooth functions on a graph, leveraging low-rank structures to improve algorithmic performance and obtain regret guarantees independent of the number of actions. In contrast, our approach exploits the spectral properties of the action covariance matrix, which is distinct from graph spectral analysis. Moreover, our research tackles the broader context of stochastic linear bandits without assuming any low-rank structure.

Our work also shares conceptual similarities with research on exploration strategies (Russo & Van Roy, 2016; Kirschner & Krause, 2018) and data-driven exploration reduction (Bastani et al., 2021; Pacchiano et al., 2020; Hamidi & Bayati, 2020a;b). However, our methodology and data utilization differ significantly. For instance, Bastani et al. (2021) focuses on the minimum eigenvalue of the covariance matrix, a single-parameter summary of the observed data, while Hamidi & Bayati (2020b) uses information from one-dimensional reward confidence intervals. The work of Hamidi & Bayati (2020a) is more closely related to ours, as it employs spectral information to improve the performance of Thompson Sampling in linear bandits. They use a single summary statistic called the *thinness coefficient* to decide whether to inflate the posterior. In contrast, our approach leverages the full geometric details of the d-dimensional confidence ellipsoid, harnessing richer geometric information.

2 Setup and Preliminaries

Notations. We use $\|\cdot\|$ to denote the Euclidean 2-norm. For a symmetric positive definite matrix A and a vector x of proper dimension, we let $\|x\|_A := \sqrt{x^\top A x}$ be the weighted 2-norm (or the A-norm). We let $\langle \cdot, \cdot \rangle$ denote the inner product in Euclidean space such that $\langle x, y \rangle = x^\top y$. For a d-dimensional matrix V, we let $\lambda_1(V) \geq \lambda_2(V) \geq \cdots \geq \lambda_d(V)$ be the eigenvalues of V arranged in decreasing order. We let $\mathcal{B}_d$ denote the unit ball in $\mathbb{R}^d$, and $\mathcal{S}_{d-1} = \{x \in \mathbb{R}^d : \|x\| = 1\}$ denote the unit hypersphere in $\mathbb{R}^d$. For an interger $N \geq 1$, we let $[N]$ denote the set $\{1, 2, \ldots, N\}$. We use the $\mathcal{O}(\cdot)$ notation to suppress problem-dependent constants, and the $\widetilde{\mathcal{O}}(\cdot)$ notation further suppresses polylog factors.

Problem formulation and assumptions. We consider the stochastic linear bandit problem. Let $\theta^\star \in \mathbb{R}^d$ be a fixed but unknown parameter. At each time $t \in [T]$, a policy π selects action x_t from a set of action $\mathcal{X}_t \subset \mathbb{R}^d$ according to the past observations and receives a reward $r_t = \langle x_t, \theta^\star \rangle + \varepsilon_t$, where ε_t is mean-zero noise with a distribution specified in Assumption 3 below. We measure the performance of π with the cumulative expected regret $\mathcal{R}(T) = \sum_{t=1}^{T} \langle x_t^\star, \theta^\star \rangle - \langle x_t, \theta^\star \rangle$, where $x_t^\star$ is the best action at time t, i.e.,

$x_t^\star = \arg\max_{x \in \mathcal{X}_t} \langle x, \theta^\star \rangle$. Let $\mathcal{F}_t$ be a σ-algebra generated by the history $(x_1, r_1, \ldots, x_t, r_t)$ and the prior knowledge, $\mathcal{F}_0$. Therefore, $\{\mathcal{F}_t\}_{t \geq 0}$ forms a filteration such that each $\mathcal{F}_t$ encodes all the information up to the end of period t.

We make the following assumptions that are standard in the relevant literature.

Assumption 1 (Bounded parameter)**.** *The unknown parameter $\theta^\star$ is bounded as $\|\theta^\star\| \leq S$, where $S > 0$ is known.*

Assumption 2 (Bounded action sets)**.** *The action sets $\{\mathcal{X}_t\}$ are uniformly bounded and closed subsets of $\mathbb{R}^d$, such that $\|x\| \leq X_t$ for all $x \in \mathcal{X}_t$ and all $t \in [T]$, where X_t's are known and $\sup_{t \geq 1} \{X_t\} < \infty$.*

Assumption 3 (Subgaussian reward noise)**.** *The noise sequence $\{\varepsilon_t\}_{t \geq 1}$ is conditionally mean-zero and R-subgaussian, where R is known. Formally, for all real valued λ, $\mathbb{E}\left[e^{\lambda \varepsilon_t} | \mathcal{F}_t\right] \leq \exp\left(\lambda^2 R^2 / 2\right)$. This condition implies that $\mathbb{E}\left[\varepsilon_t | \mathcal{F}_t\right] = 0$ for all $t \geq 1$.*

2.1 Regularized Least Square and Confidence Ellipsoid

In this subsection, we review the useful frequentist tools developed by Abbasi-Yadkori et al. (2011) for estimating the unknown parameter θ^* in linear bandit (LB) problems.

Consider an arbitrary sequence of actions $(x_1, \ldots, x_t)$ and their corresponding rewards $(r_1, \ldots, r_t)$. In LB problems, the parameter θ^* is typically estimated using the regularized least squares (RLS) estimator. Let λ be a fixed regularization parameter. The sample covariance matrix V_t and the RLS estimate $\widehat{\theta}_t$ are defined as follows:

$$V_t = \lambda_{\text{reg}} I_d + \sum_{s=1}^{t} x_s x_s^\top, \quad \widehat{\theta}_t = V_t^{-1} \sum_{s=1}^{t} x_s r_s. \tag{1}$$

The following proposition from Abbasi-Yadkori et al. (2011) establishes that the RLS estimate $\widehat{\theta}_t$ concentrates around the true parameter θ^* with high probability.

Proposition 1 (Theorem 2 in Abbasi-Yadkori et al. (2011))**.** *Let $\delta \in (0, 1)$ be a fixed confidence level. Then, with probability at least $1 - \delta$, it holds for all $x \in \mathbb{R}^d$ that*

$$\left\| \widehat{\theta}_t - \theta^\star \right\|_{V_t} \leq \beta_{t,\delta,\lambda_{reg}}^{RLS}, \quad \left| \langle x, \widehat{\theta}_t - \theta^\star \rangle \right| \leq \|x\|_{V_t^{-1}} \beta_{t,\delta,\lambda_{reg}}^{RLS}$$

where the confidence bound $\beta_{t,\delta,\lambda_{reg}}^{RLS}$ is defined as

$$\beta_{t,\delta,\lambda_{reg}}^{RLS} = R \sqrt{2 \log \frac{(\lambda_{reg} + t)^{d/2} \lambda_{reg}^{-d/2}}{\delta}} + \sqrt{\lambda_{reg}} S. \tag{2}$$

Hereafter, we might omit the dependence of β_t on δ if there is no ambiguity. Propostion 1 enables us to construct the following sequence of confidence ellipsoids.

Definition 1. *Fix $\delta \in (0, 1)$. We define the RLS confidence ellipsoid as*

$$\mathcal{E}_t^{RLS}(\delta) = \{\theta \in \mathbb{R}^d : \|\theta - \widehat{\theta}_t\|_{V_t} \leq \beta_{t,\delta,\lambda_{reg}}^{RLS}\}.$$

The next proposition, known as the *elliptical potential lemma*, plays a central role in bounding the regret. This proposition provides the key element in the work of Abbasi-Yadkori et al. (2011), showing that the cumulative prediction error incurred by the action sequence used to estimate θ^* is small.

Proposition 2 (Lemma 11 in Abbasi-Yadkori et al. (2011))**.** *If $\lambda_{reg} > 1$, for an arbitrary sequence $(x_1, \ldots, x_t)$, it holds that $\sum_{s=1}^{t} \|x_s\|_{V_s^{-1}}^2 \leq 2 \log \frac{\det(V_{t+1})}{\det(\lambda_{reg} I)} \leq 2d \log\left(1 + \frac{t}{\lambda_{reg}}\right)$.*

3 POFUL Algorithms

In this section, we introduce POFUL (Pivot OFUL), a generalized framework of OFUL. This framework enables a unified analysis of frequentist regret for common algorithms.

At a high level, POFUL is designed to encompass the exploration mechanism of OFUL and LinTS. POFUL takes as input a sequence of *inflation* parameters $\{\iota_t\}_{t\in[T]}$, feasible (randomized) *pivots* $\{\widetilde{\theta}_t\}_{t\in[T]}$ and *optimism* parameters $\{\tau_t\}_{t\in[T]}$. The inflation parameters are used to construct confidence ellipsoids that contain $\{\widetilde{\theta}_t\}_{t\in[T]}$ with high probability. This is formalized in the next definition.

Definition 2. *Fix $\delta \in (0,1)$ and $\delta' = \delta/2T$. Given the inflation parameters $\{\iota_t\}_{t\in[T]}$, we call random variables $\{\widetilde{\theta}_t\}_{t\in[T]}$ feasible pivots if for all $t \in [T]$, $\mathbb{P}\left[\widetilde{\theta}_t \in \mathcal{E}_t^{PVT}(\delta')|\mathcal{F}_t\right] \geq 1-\delta'$, where we define the "pivot ellipsoid" as $\mathcal{E}_t^{PVT}(\delta) := \left\{\theta \in \mathbb{R}^d : \|\theta - \widehat{\theta}_t\|_{V_t} \leq \iota_t \beta^{RLS}_{t,\delta,\lambda_{reg}}\right\}$.*

At each time t, POFUL chooses the action that maximizes the optimistic reward

$$\widetilde{x}_t = \arg\max_{x\in\mathcal{X}_t} \left(\langle x, \widetilde{\theta}_t\rangle + \tau_t \|x\|_{V_t^{-1}} \beta^{RLS}_{t,\delta',\lambda_{\text{reg}}} \right), \tag{3}$$

as shown in a pseudocode representation in Algorithm 1 and illustrated in Figure 1a.

Recall OFUL encourages exploration by introducing the uncertainty term $\tau_t \|x\|_{V_t^{-1}} \beta^{RLS}_{t,\delta',\lambda_{\text{reg}}}$ in the reward, while LinTS explores through random sampling within the confidence ellipsoid. We let POFUL select an arbitrary pivot (which can be random) from $\mathcal{E}_t^{PVT}$ and maximize the optimistic reward to encompass arbitrary exploration mechanisms within $\mathcal{E}_t^{PVT}$.

Algorithm 1 POFUL

Require: T, δ, λ_{reg}, $\{\iota_t\}_{t\in[T]}$, $\{\tau_t\}_{t\in[T]}$
  Initialize $V_0 \leftarrow \lambda\mathbb{I}$, $\widehat{\theta}_1 \leftarrow 0$, $\delta' \leftarrow \delta/2T$
  for t = 0, 1, . . . , T **do**
    Sample a feasible pivot $\widetilde{\theta}_t$ with respect to ι_t according to Definition 2
    $\widetilde{x}_t \leftarrow \arg\max_{x\in\mathcal{X}_t} \left(\langle x, \widetilde{\theta}_t\rangle + \tau_t \|x\|_{V_t^{-1}} \beta^{RLS}_{t,\delta',\lambda_{\text{reg}}} \right)$
    Observe reward r_t
    $V_{t+1} \leftarrow V_t + \widetilde{x}_t \widetilde{x}_t^\top$
    $\widehat{\theta}_{t+1} \leftarrow V_{t+1}^{-1} \sum_{s=1}^{t} \widetilde{x}_s r_s$.
  end for

We demonstrate that POFUL encompasses OFUL, LinTS, TS-Freq, and Greedy as special cases, as illustrated in Figure 1b.

Example 1 (OFUL)**.** *For stochastic linear bandit problems, OFUL chooses actions by solving the optimization problem $\max_{x\in\mathcal{X}_t} \langle x, \widehat{\theta}_t\rangle + \|x\|_{V_t^{-1}} \beta^{RLS}_{t,\delta',\lambda_{reg}}$. Therefore, OFUL is a specially case of POFUL where $\iota_t = 0$, $\tau_t = 1$ and $\widetilde{\theta}_t = \widehat{\theta}_t$, the center of the confidence ellipsoid, for all $t \in [T]$.*

Before describing how TS can be derived as an instance of POFUL, we introduce a definition.

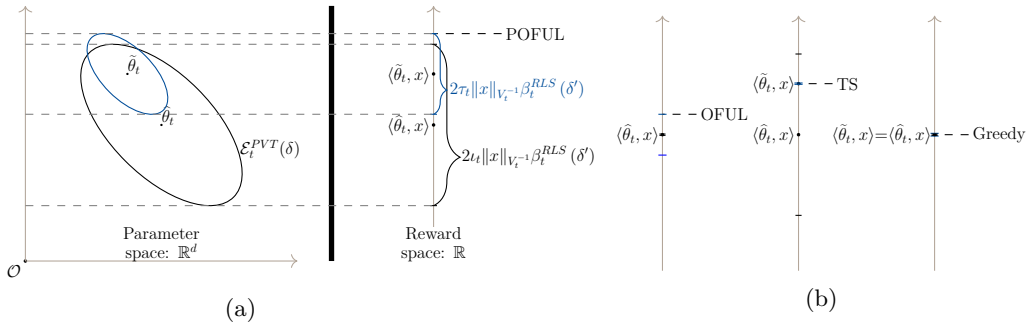


Figure 1: a) POFUL algorithms illustration. (b) Special cases: Greedy, TS, and OFUL.

Definition 3. *Let $\delta \in (0,1)$. We define $\mathcal{D}^{SA}(\delta)$ as a distribution satisfying $\mathbb{P}_{\eta\sim\mathcal{D}^{SA}(\delta)}\left[\|\eta\| \le 1\right] \ge 1-\delta$.*

Example 2 (TS)**.** *Linear Thompson Sampling (LinTS) algorithm is a generic randomized algorithm that samples from a distribution constructed from the RLS estimate at each step. At time t, LinTS samples as $\widetilde{\theta}_t = \widehat{\theta}_t + \iota_t^{TS}\beta_t^{RLS}(\delta')V_t^{-\frac{1}{2}}\eta_t$, where $\delta' = \delta/2T$, and ι_t^{TS} is an inflation parameter controlling the scale of the sampling range, and η_t is a random sample from a normalized sampling distribution $\mathcal{D}^{SA}(\delta')$ that concentrates with high probability. LinTS is a special case of POFUL where $\iota_t = \iota_t^{TS}$, $\tau_t = 0$ and $\widetilde{\theta}_t = \widehat{\theta}_t + \iota_t^{TS}\beta_t^{RLS}(\delta')V_t^{-\frac{1}{2}}\eta_t$. Setting the inflation parameter $\iota_t = \widetilde{\mathcal{O}}(1)$ corresponds to the original LinTS algorithm. On the other hand, setting $\iota_t = \widetilde{\mathcal{O}}(\sqrt{d})$ corresponds to the frequentist variant of LinTS studied in Agrawal & Goyal (2013); Abeille et al. (2017), namely TS-Freq. This means TS-Freq inflates the posterior by a factor of order $\sqrt{d}$.*

Example 3 (Greedy)**.** *Greedy is a special case of POFUL with $\iota_t = \tau_t = 0$, $\widetilde{\theta}_t = \widehat{\theta}_t$, $\forall t$.*

4 Frequentist Regret Analysis of POFUL

In this section, we present the frequentist regret analysis of POFUL algorithms. We defer all proofs to Appendix C. We first introduce useful concentration events that hold with high-probability.

Definition 4. *Fix $\delta \in (0,1)$ and $\delta' = \delta/2T$. We define $\beta_{t,\delta',\lambda_{reg}}^{PVT} := \iota_t(\delta)\beta_{t,\delta',\lambda_{reg}}^{RLS}$ and*

$$\widehat{\mathcal{A}}_t := \left\{\forall s \le t : \left\|\widehat{\theta}_t - \theta^\star\right\|_{V_t} \le \beta_{t,\delta',\lambda_{reg}}^{RLS}\right\}, \quad \widetilde{\mathcal{A}}_t := \left\{\forall s \le t : \left\|\widetilde{\theta}_t - \widehat{\theta}_t\right\|_{V_t} \le \beta_{t,\delta',\lambda_{reg}}^{PVT}\right\}.$$

We also define $\mathcal{A}_t := \widehat{\mathcal{A}}_t \cap \widetilde{\mathcal{A}}_t$.

Proposition 3. *Under Assumptions 1, 2 and 3 , we have $\mathbb{P}\left[\mathcal{A}_T\right] \ge 1-\delta$.*

4.1 An Data-Driven Regret Bound for POFUL

In the following, we condition on the event $\mathcal{A}_T$ which holds with probability $1-\delta$. The following proposition bounds the instantaneous regret of POFUL.

Proposition 4. *Suppose $\theta^\star \in \mathcal{E}_t^{RLS}(\delta')$ and $\widetilde{\theta}_t \in \mathcal{E}_t^{PVT}(\delta')$, it holds that*

$$\langle x_t^\star, \theta^\star\rangle - \langle \widetilde{x}_t, \theta^\star\rangle \le (1+\iota_t-\tau_t)\|x_t^\star\|_{V_t^{-1}}\beta_{t,\delta',\lambda_{reg}}^{RLS} + (1+\iota_t+\tau_t)\|\widetilde{x}_t\|_{V_t^{-1}}\beta_{t,\delta',\lambda_{reg}}^{RLS}. \quad (4)$$

Note that this upper bound is different from what's used in the optimism-based methods (Abbasi-Yadkori et al., 2011; Agrawal & Goyal, 2013; Abeille et al., 2017), we reproduce their upper bound and discuss the relationship of our method and theirs in Appendix D.

On the right-hand side of equation 4, since the oracle optimal action sequence $\{x_t^\star\}_{t\in[T]}$ is unknown to the algorithm and is different from the action sequence $\{\widetilde{x}_t\}_{t\in[T]}$ played by POFUL, one cannot apply Proposition 2 to bound the summation $\sum_{t=1}^T \|\widetilde{x}_t\|_{V_t^{-1}}^2$ and get an upperbound of the regret. To fix the problem due to this discrepancy, the key point is connecting $\{\widetilde{x}_t\}_{t\in[T]}$ and $\{x_t^\star\}_{t\in[T]}$ in terms of the V_t^{-1}-norm. This motivates the following definition.

Definition 5. *For each $t \ge 1$, let $\widetilde{x}_t$ and $x_t^\star$ respectively denote the action chosen by POFUL and the optimal action. We define the* uncertainty ratio *at time t as $\alpha_t := \|x_t^\star\|_{V_t^{-1}}/\|\widetilde{x}_t\|_{V_t^{-1}}$. We also define the* (instantaneous) regret proxy *at time t as $\mu_t := \alpha_t(1+\iota_t-\tau_t)+1+\iota_t+\tau_t$.*

Note that $\langle x, \widehat{\theta}_t - \theta^\star\rangle \le \|x\|_{V_t^{-1}}\beta_t^{RLS}$ holds with high probability, we have that $\|x\|_{V_t^{-1}}$ essentially determines the length of the confidence interval of the reward $\langle x, \theta^\star\rangle$. Hence, α_t serves as the ratio of uncertainty degrees of the reward obtained by the optimal action $x_t^\star$ and the chosen action $\widetilde{x}_t$.

The intuition behind the definition for μ_t is constructing a regret upper bound similar to that of OFUL. Specifically, Proposition 4 indicates $\langle x_t^\star, \theta^\star \rangle - \langle \widetilde{x}_t, \theta^\star \rangle \leq \mu_t \|\widetilde{x}_t\|_{V_t^{-1}} \beta_t^{RLS}$, and we can check that the instantaneous regret of OFUL satisfies $\langle x_t^\star, \theta^\star \rangle - \langle \widetilde{x}_t, \theta^\star \rangle \leq 2\|\widetilde{x}_t\|_{V_t^{-1}} \beta_t^{RLS}$. In this sense, μ_t is a proxy of the instantaneous regret incurred by POFUL at time t. Moreover, OFUL can be regarded as a POFUL algorithm whose μ_t is fixed at 2, and we could extend the definition of α_t to OFUL by solving $\mu_t = \alpha_t(1 + \iota_t - \tau_t) + 1 + \iota_t + \tau_t$ and set $\alpha_t = 1$ for all $t \in [T]$ for OFUL (recall that in OFUL, $\iota_t = 0$ and $\tau_t = 1$ for all $t \in [T]$).

The following Theorem connects $\{\mu_t\}_{t\in[T]}$ and $\mathcal{R}(T)$. It provides an oracle but general frequentist regret upper bound for all POFUL algorithms.

Theorem 1 (Oracle frequentist regret bound for POFUL)**.** *Fix $\delta \in (0, 1)$ and let $\delta' = \delta/2T$. Under Assumptions 1, 2 and 3, with probability $1 - \delta$, POFUL achieves a regret of*

$$\mathcal{R}(T) \leq \sqrt{2d \left(\sum_{t=1}^{T} \mu_t^2 \right) \log \left(1 + \frac{T}{\lambda_{reg}} \right)} \beta_{T,\delta',\lambda_{reg}}^{RLS}. \tag{5}$$

Remark 1. *We call Theorem 1 an* oracle *regret bound as $\{\mu_t\}_{t\in[T]}$ for general POFUL depends on the unknown system parameter $\theta^\star$. In general, they cannot be calculated by the decision-maker. Nevertheless, when we have upper bounds for ι_t and τ_t, as well as computable upper bounds $\{\widehat{\alpha}_t\}_{t\in[T]}$ for $\{\alpha_t\}_{t\in[T]}$ respectively, using $\mu_t^2 \leq 2\alpha_t^2(1 + \iota_t - \tau_t)^2 + 2(1+\iota_t+\tau_t)^2$, we could calculate upper bounds for $\{\mu_t\}_{t\in[T]}$ as well. Consequently, Theorem 1 instantly turns into a data-driven regret bound for POFUL and could be utilized later for course correction, which will be the aim of the next section. When we additionally know that $1 + \iota_t - \tau_t$ is non-negative, we would use the equality $\mu_t = \alpha_t(1 + \iota_t - \tau_t) + 1 + \iota_t + \tau_t$ directly for the bound.*

Remark 2. *In the Discussion section of Abeille et al. (2017), the authors introduce a concept similar to the reciprocal of our α_t. They suggest that the necessity of proving LinTS samples are optimistic could be bypassed if for some $\alpha > 0$ LinTS samples $\widetilde{\theta}_t$ such that $\|x^\star(\widetilde{\theta}_t)\|_{V_t^{-1}} \geq \alpha \|x^\star(\theta_t^\star)\|_{V_t^{-1}}$ with constant probability ,where $x^\star(\widetilde{\theta}_t)$ and $x^\star(\theta_t^\star)$ represent the optimal actions corresponding to $\widetilde{\theta}_t$ and $\theta_t^\star$, respectively. They pose this as an open question regarding the possibility of relaxing the requirement of inflating the posterior. In the following section, we provide a positive answer to this question by studying the reciprocal of their α using geometric arguments. This investigation offers an explanation for the empirical success of LinTS without the need for posterior inflation.*

5 A Data-Driven Approach

In this section, we present the main contribution of this work which provides a data-driven approach to calibrating POFUL. Note that ι_t and τ_t are parameters of POFUL that can be controlled by a decision-maker, the essential point is to find a computable, non-trivial upper bound $\widehat{\alpha}_t$ for the uncertainty ratio α_t, which turns into an upper bound $\widehat{\mu}_t$ for the regret proxy μ_t that's deeply related to the frequentist regret of POFUL.

Typically, we can check that $\widehat{\alpha}_t$ is no less than one because when $\widetilde{x}_t = x_t^\star$, we have $\alpha_t = \|x_t^\star\|_{V_t^{-1}} / \|\widetilde{x}_t\|_{V_t^{-1}} = 1$ and $\widehat{\alpha}_t$ is an upper bound for α_t. As a result, it holds that $\widehat{\mu}_t = (1 + \widehat{\alpha}_t)(1 + \iota_t) + (1 - \widehat{\alpha}_t)\tau_t \leq (1 + \widehat{\alpha}_t)(1 + \iota_t)$, i.e., setting $\tau_t = 0$ yields a valid upper bound for $\widehat{\mu}_t$. Given this observation, we will focus on scenarios where $\tau_t = 0$ for all $t \in [T]$. Such scenarios include LinTS and its variants like TS-Freq as well as Greedy - all of which are standard algorithms that still lack theoretical regret guarantee results.

In the subsequent analysis, we construct upper bounds $\{\widehat{\alpha}_t\}_{t\in[T]}$ for the continuous-action scenario. Bounds for the discrete-action scenario are in Appendix E.

5.1 Continuous action space.

Our strategy capitalizes on geometric insights related to the properties of the confidence ellipsoids, providing upper bounds that can be computed efficiently.

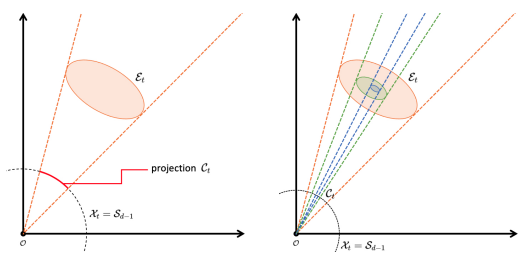
For the sake of a better illustration, we consider $\mathcal{X}_t = \mathcal{S}_{d-1}$ for all $t \in [T]$ for this scenario, where $\mathcal{S}_{d-1} = \{x \in \mathbb{R}^d : \|x\| = 1\}$ is the unit hypersphere in $\mathbb{R}^d$.This is a standard example of continuous action space, and is the same as the setting considered in Abeille et al. (2017). We remark that for this specific setting, the problem is still hard. This is because we don't have a closed-form solution for the set of potentially optimal actions.

In this setting, the optimal action $x_t^\star(\theta) := \arg\max_{x \in \mathcal{X}_t} \langle x, \theta \rangle$ takes the form $x_t^\star(\theta) = \theta / \|\theta\|$. To upper bound α_t, we consider respectively the smallest and largest value of $\|x_t^\star(\theta)\|_{V_t^{-1}}$ for θ in the confidence ellipsoids of θ, namely, $\mathcal{E}_t^{RLS}$ and $\mathcal{E}_t^{PVT}$. Specifically, we have

$$\alpha_t \leq \frac{\sup_{\theta \in \mathcal{E}_t^{RLS}} \|x_t^\star(\theta)\|_{V_t^{-1}}}{\inf_{\theta \in \mathcal{E}_t^{PVT}} \|x_t^\star(\theta)\|_{V_t^{-1}}}. \tag{6}$$

As is illustrated in Figure 2, the set of potentially optimal actions $\mathcal{C}_t$ is the projection of the confidence ellipsoid $\mathcal{E}_t$ onto $\mathcal{S}_{d-1}$. It's hard to get a closed-form expression for $\mathcal{C}_t$, so we cannot directly calculate the range of V_t^{-1}-norm of actions in $\mathcal{C}_t$. Nevertheless, we can approximate the range by investigating the geometric properties of the ellipsoids.

The intuition here is that, when POFUL has implemented sufficient exploration so that $\mathcal{E}_t$ is small enough, $\mathcal{C}_t$ concentrates accordingly to a small cap on $\mathcal{S}_{d-1}$. All actions within $\mathcal{C}_t$ point to similar directions and thus have similar V_t-norm. (Note that for a unit vector x, we have that $\|x\|_{V_t}$ can be written as a weighted summation of the eigenvalues of V_t, where the weights are determined by the direction of x.) Therefore, it is possible to estimate the range of the V_t-norm by employing geometric reasoning. Subsequently, this estimated range will be utilized to ascertain the range of the V_t^{-1}-norm.



(a) (b)

Figure 2: Illustration of potentially optimal actions set $\mathcal{C}_t$ in $\mathbb{R}^2$. (a): $\mathcal{C}_t$ is $\mathcal{E}_t$'s projection onto $\mathcal{S}_{d-1}$. (b): As more data is collected, $\mathcal{E}_t$ shrinks (colors show exploration levels). Potentially optimal actions point in similar directions, determining their V_t-norm. This suggests their V_t-norm range could be estimated geometrically.

The main theorem (proved in Section A) derives an upper bound for α_t based on this idea.

Theorem 2. *Suppose $\mathcal{X}_t = \mathcal{S}_{d-1}$ for all $t \in [T]$. Define $m_t = (\|\widehat{\theta}_t\|_{V_t}^2 - (\beta_t^{RLS})^2)/(\|\widehat{\theta}_t\| + \beta_t^{RLS}/\lambda_d(V_t))^2$, $M_t = \|\widehat{\theta}_t\|_{V_t^2}^2/(\|\widehat{\theta}_t\|_{V_t}^2 - (\beta_t^{PVT})^2)$. Let $k \in [d]$ be the integer that satisfies $\lambda_k(V) \leq M_t \leq \lambda_{k+1}(V)$. Define $\beta_t^{PVT} := \iota_t \beta_t^{RLS}$ and*

$$\Phi_t = \begin{cases} (\lambda_1^{-1}(V_t) + \lambda_d^{-1}(V_t) - m_t \lambda_1^{-1}(V_t)\lambda_d^{-1}(V_t))^{\frac{1}{2}}, & \text{if } \|\widehat{\theta}_t\|_{V_t} \geq \beta_t^{RLS} \\ \lambda_d^{-\frac{1}{2}}(V_t), & \text{if } \|\widehat{\theta}_t\|_{V_t} < \beta_t^{RLS} \end{cases},$$

$$\Psi_t = \begin{cases} (\lambda_k^{-1}(V_t) + \lambda_{k+1}^{-1}(V_t) - M_t \lambda_k^{-1}(V_t)\lambda_{k+1}^{-1}(V_t))^{\frac{1}{2}}, & \text{if } \|\widehat{\theta}_t\|_{V_t} \geq \beta_t^{PVT} \\ \lambda_1^{-\frac{1}{2}}(V_t), & \text{if } \|\widehat{\theta}_t\|_{V_t} < \beta_t^{PVT} \end{cases}.$$

Then for all $t \in [T]$, conditioned on $\widehat{\mathcal{A}}_t \cap \widetilde{\mathcal{A}}_t$, it holds for all $s \leq t$ that $\alpha_s \leq \widehat{\alpha}_s := \Phi_s / \Psi_s$.

To better understand what Theorem 2 implies, we discuss some special cases in Appendix G and provide empirical validations for them.

6 A Meta-Algorithm for Course-Correction

This section demonstrates how the data-driven regret bound can enhance standard bandit algorithms. We propose a meta-algorithm that creates course-corrected variants of base algorithms, achieving minimax-optimal frequentist regret guarantees while preserving most original characteristics, including computational efficiency and typically low regret.

We take LinTS as an example of the base algorithm, and propose the algorithm Linear Thompson Sampling with Maximum Regret (Proxy) (TS-MR). The idea is to measure the performance of LinTS using $\widehat{\mu}_t$ and avoid bad LinTS actions by switching to OFUL actions. Specifically, at each time t, TS-MR calculates the upper bound $\widehat{\mu}_t$ and compares it with a preset threshold μ. If $\widehat{\mu}_t > \mu$, LinTS might be problematic and TS-MR takes an OFUL action to ensure a low instantaneous regret; if $\widehat{\mu}_t \leq \mu$, TS-MR takes the LinTS action. We remark that setting $\iota_t = 0$ for all $t \in [T]$ yields the corresponding Greedy-MR algorithm. The pseudocode is presented in Algorithm 2 in Appendix H.

By design, course-corrected algorithms maintain $\mu_t \leq \max\{\mu, 2\}$ for all $t \in [T]$. Theorem 1 yields their optimal frequentist regret, up to a constant factor.

Corollary 1. *TS-MR and Greedy-MR achieve a frequentist regret of* $\widetilde{\mathcal{O}}(\max\{\mu, 2\}d\sqrt{T})$.

Proof. Note that $\mu_t \leq \max\{\mu, 2\}$, by Theorem 1, we have

$$\mathcal{R}(T) \leq \sqrt{2dT(\max\{\mu,2\})^2 \log\left(1 + \frac{T}{\lambda_{\text{reg}}}\right)\beta^{RLS}_{T,\delta',\lambda_{\text{reg}}}} = \widetilde{\mathcal{O}}(\max\{\mu, 2\}d\sqrt{T}).$$

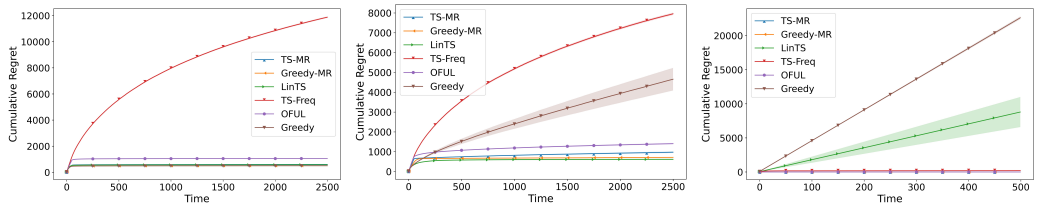
□

Remark 3. *In practice, the choice of the threshold μ depends on the problem settings. In a high-risk setting where LinTS and Greedy fail with high probability, one can set a small μ so that TS-MR and Greedy-MR select more OFUL actions to guarantee the necessary amount of exploration. In a low-risk setting where original LinTS and Greedy algorithms work well, one can set a large μ and hence TS-MR and Greedy-MR select TS and greedy actions respectively to avoid unnecessary exploration and save the computational cost.*

7 Simulations

We aim to compare TS-MR, Greedy-MR, and key baseline algorithms, via simulation.

7.1 Synthetic datasets



(a) example 1 (b) example 2 (c) example 3

Figure 3: Comparison of the cumulative regret incurred by TS-MR and Greedy-MR, versus the baseline algorithms in Examples 1-3.

We conduct simulations on three representative synthetic examples. The detailed experimental setups for these examples are presented in Appendix F.

Example 1. Stochastic linear bandit with uniformly and independently distributed actions. This is a basic example of standard stochastic linear bandit problems without any extra structure. TS-Freq shows pessimistic regret due to the inflation of the posterior, while other algorithms in general perform well.

Example 2. Contextual bandits embedded in the linear bandit problem (Abbasi-Yadkori, 2013). In this setting, Greedy performs suboptimally due to a lack of exploration for some arms. Nevertheless, Greedy-MR outperforms both Greedy and OFUL by adaptively choosing OFUL actions only when it detects large regret proxy $\widehat{\mu}_t$.

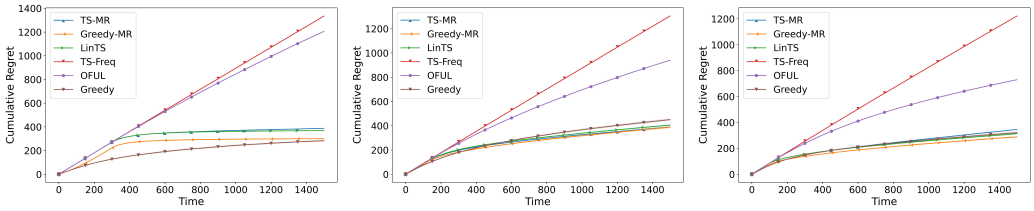
Example 3. Prior mean mismatch (Hamidi & Bayati, 2020a). This is an example in which LinTS is proven to incur linear Bayesian regret. We see both LinTS and Greedy incur linear regrets as expected, while TS-MR and Greedy-MR, switch to OFUL adaptively to tackle this hard problem and achieve sublinear regret.

7.2 Real-world datasets

We explore the performance of standard POFUL algorithms and the proposed TS-MR and Greedy-MR algorithms on real-world datasets. We consider three datasets for classification tasks on the OpenML platform, Cardiotocography, JapaneseVowels and Segment. They focus on healthcare, pattern recognition, and computer vision problems respectively.

Setup. We follow the approach in the literature (Bietti et al., 2021; Bastani et al., 2021) that converts classification tasks to contextual bandit problems, and then embeds it into linear bandit problems in the same way as Example 2 in Section 7.1. Specifically, we regard each class as an action so that at each time, the decision-maker assigns a class to the feature observed and receives a binary reward, namely 1 for assigning the correct class and 0 otherwise, plus a Gaussian noise.

We plot the cumulative regret (averaged over 100 runs) for all algorithms. Figure 4 shows that for all real-world datasets: OFUL and TS-Freq perform poorly due to their conservative exploration; LinTS and Greedy are achieving empirical success even though they don't have theoretical guarantees; TS-MR and Greedy-MR retain the desirable empirical performance of LinTS and Greedy, while enjoying the minimax optimal frequentist regret bound.



(a) Cardiotocography dataset. (b) JapaneseVowels dataset. (c) Segment dataset.

Figure 4: Cumulative regret of all algorithms on real-world datasets.

8 Conclusion

In this work, we propose a data-driven framework to analyze the frequentist regret of POFUL, a family of algorithms that includes OFUL, LinTS, TS-Freq, and Greedy as special cases. Our approach allows for the computation of a data-driven frequentist regret bound for POFUL during implementation, which subsequently informs the course-correction of the algorithm. Our technique conducts a novel real-time geometric analysis of the d-dimensional confidence ellipsoid to fully leverage the historical information and might be of independent interest. As applications, we propose TS-MR and Greedy-MR algorithms that enjoy provable minimax optimal frequentist regret and demonstrate their ability to adaptively switch to OFUL when necessary in hard problems where LinTS and Greedy fail. We hope this work provides a steady step towards bridging the gap between theoretical guarantees and empirical performance of bandit algorithms such as LinTS and Greedy.

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