
Preference-based Pure Exploration

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Abstract

We study the preference-based pure exploration problem for bandits with vector-valued rewards. The rewards are ordered using a (given) preference cone $\mathcal{C}$ and our goal is to identify the set of Pareto optimal arms. First, to quantify the impact of preferences, we derive a novel lower bound on sample complexity for identifying the most preferred policy with a confidence level $1 - \delta$. Our lower bound elicits the role played by the geometry of the preference cone and punctuates the difference in hardness compared to existing best-arm identification variants of the problem. We further explicate this geometry when the rewards follow Gaussian distributions. We then provide a convex relaxation of the lower bound and leverage it to design the Preference-based Track and Stop (PreTS) algorithm that identifies the most preferred policy. Finally, we show that the sample complexity of PreTS is asymptotically tight by deriving a new concentration inequality for vector-valued rewards.

1 Introduction

Following COVID-19, the importance of reliable clinical trials and corresponding data acquisition to design effective drugs has gained wider recognition. However, conducting large-scale clinical trials is cost and time intensive as it requires working with large number of patients and following up their medical conditions over time. In the past two decades, this has led to doubling in the cost to bring a drug to the market, i.e., to \$2.6 billion with a 12-year drug development horizon and 90% failure rate during the clinical trial (Mullard, 2014; Sun et al., 2022). However, due to the rise of systematic data acquisition about biological systems, pharmaceutical firms are interested in harvesting the collected data for drug discovery (Gaulton et al., 2012; Reker and Schneider, 2015). Thus, machine learning-based methods are increasingly studied and deployed as a promising avenue for identifying potentially successful drugs with less patient involvement, increasing the “hit rate”, and speeding up the development process (Jayatunga et al., 2022; Smer-Barreto et al., 2023; Sadybekov and Katritch, 2023; Hasselgren and Oprea, 2024). But deciding whether a drug is successful depends on multiple and often conflicting objectives regarding safety, efficacy, and pharmacokinetic constraints (Lizotte and Laber, 2016). For example, COV-BOOST (Munro et al., 2021) demonstrates a phase II vaccine clinical trial conducted on 2883 participants to measure the immunogenicity indicators (e.g. cellular response, anti-spike IgG and NT₅₀) of different Covid-19 vaccines as a booster (third dose). Experts decide how different indicators are preferred over one another, and above different thresholds (Jayatunga et al., 2022). This motivates us to study a sequential decision-making problem, where we aim to conduct minimum number of experiments to acquire informative data, and to reliably validate a hypothesis with multiple objectives by imposing preferences over them.

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Problems of such nature can be modeled as a multi-armed bandit (in brief, bandits), which is an established framework for sequential decision-making under uncertainty (Lattimore and Szepesvári, 2020). In bandits, a learner has access to an instance of K decisions (or arms). Each arm $k \in \{1, \dots, K\}$ corresponds to a probability distribution P_k of feedback (rewards) with unknown mean μ_k . At each step $t \in \mathbb{N}$, the learner interacts with the instance by taking a decision k_t (analogously pulling an arm), and observes a noisy reward R_t from the corresponding distribution of rewards P_{k_t} . The goal of the learner is to identify the arm with the highest expected reward over a certain confidence level through minimum number of interactions with the instance. This is popularly known as a fixed-confidence Best Arm Identification (BAI) in bandit literature (Jamieson and Nowak, 2014; Garivier and Kaufmann, 2016; Soare et al., 2014), which is a special case of pure exploration problems (Even-Dar et al., 2006; Bubeck et al., 2009; Auer et al., 2016).

The bandit literature spanning over a century mostly focuses on a scalar reward, i.e., a single objective. In our problem, each reward R_t is a real-valued vector of $L \in \mathbb{N}$ objectives, and thus, the unknown mean vector of each arm $M_k \in \mathbb{R}^L$. Since the objectives can be often conflicting, there might not exist a single best arm. Rather, there exists a Pareto Optimal Set of arms (Drugan and Nowe, 2013; Auer et al., 2016). Given a set of preferences over the objectives, the Pareto Optimal Set consists of arms whose mean vectors dominate the mean vectors of any other arm outside the set. Keeping generality, we assume that preferences are defined by a cone of vectors $\mathcal{C} \subseteq \mathbb{R}^L$. Every $\mathcal{C}$ induces a set of partial or incomplete orders over the L objectives (Jahn et al., 2009; Löhne, 2011). Given the preference cone $\mathcal{C}$, we aim to *exactly* identify the complete Pareto Optimal Set with a confidence level $(1 - \delta) \in [0, 1]$ using as few interactions as possible. We refer to this problem Preference-based Pure Exploration (**PrePEX**). Recently, Auer et al. (2016); Kone et al. (2023a,b); crepon et al. (2024) consider a special case of PrePEX, where the preference is known. To the best of our knowledge, Ararat and Tekin (2023) and Korkmaz et al. (2023) are the only studies of PrePEX from frequentist and Bayesian angles, respectively. Here, we consider a frequentist approach as in (Ararat and Tekin, 2023). However, their goal is to identify points that are in the Pareto Optimal Set or very close to it. In contrast, we focus on exactly identifying the Pareto Optimal Set. Additionally, Ararat and Tekin (2023) propose a gap-based elimination algorithm to solve the problem that generalises the algorithm of Even-Dar et al. (2006). But in BAI, there is another paradigm of designing efficient algorithms that solves and tracks the exact lower bound on the expected time to identify the best arm $(1 - \delta)$ correctly (Garivier and Kaufmann, 2016; Degenne and Koolen, 2019). We explore this paradigm for PrePEX and ask two questions:

What is the exact lower bound of PrePEX for identifying the Pareto Optimal Set, and how to design a computationally tractable algorithm matching this bound?

We address them affirmatively in our contributions:

1. Lower Bound for PrePEX. In Theorem 3.1, we study hardness of PrePEX problems by deriving the novel lower bound on the expected sample complexity of any algorithm to yield the exact Pareto Optimal Set with confidence $(1 - \delta)$. The challenge here is to extend the classical BAI lower bound (Garivier and Kaufmann, 2016) to a set of confusing instances given $\mathcal{C}$. We observe that unlike BAI, distinguishability of two arms in PrePEX depends on their projections on the cone polar to $\mathcal{C}$. We also show that our lower bound generalises the lower bound for pure exploration under known constraints (Carlsson et al., 2024). Additionally, we provide an exact characterization the lower bound further for Gaussian reward distributions in Theorem 3.2. It shows that the hardness depends on the bilinear projection of the mean matrix of arms onto the boundary of a normal cone of policies and the preferences. This is novel w.r.t. the existing gap-dependent lower bounds that hold either for a narrow range of μ_a 's (Ararat and Tekin, 2023), or fixed preference (Kone et al., 2023a).

2. Algorithm Design. First, we observe that the optimisation problem in our lower bound involves minimisation over a non-convex set. We provide a convex relaxation of the problem based on ideas from disjunctive programming (Theorem 4.1 and 4.2). We then leverage this lower bound to propose a novel Track-and-Stop (Garivier and Kaufmann, 2016) style algorithm, called PreTS (Preference-based Track-and-Stop). In Theorem 4.3, we devise a new stopping rule that can handle the preference-aligned suboptimality gaps between the arms.

3. Sample Complexity Analysis. Finally, we provide an upper bound on sample complexity of PreTS. This requires us to define a distance metric between two pareto sets of arms, and proving a concentration bound with respect to this metric (Theorem 5.1). In Theorem 5.2, we prove that sample complexity of PreTS matches the convexified lower bound up to constants.

1.1 Related Works

In the past decade, works on multi-armed bandits also focus on pure-exploration in addition to regret minimization. Regret minimization and pure-exploration differ in the sense when arms in pure-exploration are immediately discarded upon being deemed as sub-optimal, whereas, in the regret minimization setting, sub-optimal arms may still be played since they provide additional information about other arms. Pure-exploration problems have been considered in two settings: fixed-budget and fixed-confidence. The fixed-budget setting aims at bounding the probability of underestimating the best arm given a budget of samples. Audibert and Bubeck (2010) propose the first algorithm for the fixed budget setting. Here, the budget is divided into $K - 1$ rounds and at the end of every round, the arms with the lowest empirical mean are discarded. On the other hand, best-arm identification is a version of the pure-exploration problem with scalar rewards (Even-Dar et al., 2006). In this setting, we are given a $\delta \in (0, 1)$ and the goal is to identify the best-arm with probability at least $1 - \delta$. Several strategies such as those based on elimination, adaptivity, racing, upper-confidence bounds have been proposed to minimize the number of expected pulls of an arm in the fixed confidence setting by (Kalyanakrishnan et al., 2012; Gabillon et al., 2012; Jamieson et al., 2014; Garivier and Kaufmann, 2016; Jedra and Proutiere, 2020). Arm rewards can be modeled as a vector with Gaussian Process (Zuluaga et al., 2016), linear rewards (Drugan and Nowe, 2013; Lu et al., 2019), and non-parametric rewards (Turgay et al., 2018), which can include contextual bandit formulations (Tekin and Turgay, 2017; Shukla, 2022). In recent past, the pure exploration techniques have been successfully applied in hyperparameter tuning (Li et al., 2018) and black-box optimization problems (Contal et al., 2013; Wang et al., 2021, 2022) demonstrating considerable performance gains.

In a marked deviation, given an instance of the bandit problem, the goal of this paper is to identify the entire Pareto front. A key observation in this regard is that there might be arms, which are sub-optimal for almost every objective but still lie on the Pareto front. Further, since sampling an arm returns a vector of rewards determining an arm-strategy that reduces the uncertainty in the estimate of every reward function is challenging. An immediate consequence of these differences is the fact that the complexity of identifying the Pareto front is different from that of best arm identification. Auer et al. (2016) consider the Pareto front identification problem in the multi-armed bandit model and establish sample complexity bounds for the problem in terms of relevant problem parameters in the fixed-confidence setting. The multi-armed bandit problem is further studied under cone-based preferences by Ararat and Tekin (2023). The main contribution of (Ararat and Tekin, 2023) are bounds on the sample complexity of the problem in terms of gap-based notions that depend on the cone. Karagözlü et al. (2024) builds upon this work to introduce adaptive elimination based algorithms for learning the Pareto front under incomplete preferences. When the reward vectors are Gaussian processes Korkmaz et al. (2023) propose an elimination based algorithm based for identifying the Pareto front. The goal in these works is to identify the set of arms that are ϵ close to the Pareto front as the sample complexity to identify the exact Pareto set can be very large. Kone et al. (2023a) consider the problem of identifying a relevant subset of the Pareto set using a single sampling strategy Adaptive Pareto Exploration, along with different stopping rules to consider variations of the Pareto Set Identification problem. crepon et al. (2024) consider the exact Pareto front identification problem in the multi-armed bandit setting but with fixed and known preference cone. They propose a lower bound and a computationally efficient gradient-based algorithm to implement a track-and-stop based strategy. To the best of our knowledge, ours is the first work to consider *the exact Pareto front identification problem from a pure-exploration perspective*. Therefore, our proposed framework can be used for identifying the Pareto front given a preference cone for several variants of the bandit problem including the standard multi-armed bandit problem, linear bandits, etc.

2 Preference-based Pure Exploration Problem

In this section, we formalise the fixed-confidence setting of preference-based pure exploration and introduce the notations.

Notations. For $n \in \mathbb{N}$, let $[n]$ denote the set $\{1, 2, \dots, n\}$. We use $\|\cdot\|_1, \|\cdot\|_2, \|\cdot\|_\infty$ to denote the ℓ_1 -norm, ℓ_2 -norm and ℓ_∞ -norm, respectively. For a vector z , $z^{(\ell)}$ denotes its ℓ^{th} component. Let e_ℓ denote the vector with 1 in the ℓ^{th} position and zero otherwise. Δ_K denotes the simplex on $[K]$. $d_{KL}(P, Q)$ measures the KL-divergence between distributions P and Q . $\text{vect}(A)$ is the vectorized version of matrix A . $\mathbf{1}$ is the vector of all 1's. Further details of notations are deferred to Appendix A.

PrePEX: Problem Formulation. In PrePEX, a learner can access a bandit instance with K arms. Each arm $k \in [K]$ corresponds to a reward distribution P_k over $\mathbb{R}^L$ with unknown mean $M_k \in \mathbb{R}^L$ and known covariance $\Sigma = \text{Diag}(\sigma_1^2, \dots, \sigma_L^2)$. Here, L denotes the number of objectives corresponding to each arm. Thus, a bandit instance can be specified with the vector of mean rewards $\{M_k\}_{k=1}^K$. For brevity, we represent them with a matrix $M \in \mathbb{R}^{L \times K}$ such that its k^{th} column is M_k . At each time $t \in \mathbb{N}$, the learner pulls an arm $k_t \in [K]$ and observes the corresponding reward vector R_t sampled from ν_{k_t} . In pure exploration, the learner typically focuses on finding the best arm, i.e. the arm with highest mean (Garivier and Kaufmann, 2016). In pure exploration, a more general setting of BAI, the learner aims to find a policy $\pi \in \Delta_K$ that dictates the arm-proportion to choose to maximize the expected reward from the instance.

Following the vector optimization literature (Jahn et al., 2009; Ararat and Tekin, 2023), we assume that the learner has additionally access to an ordering cone $\mathcal{C}$.

Definition 2.1 (Ordering Cone). A set $\mathcal{C} \subseteq \mathbb{R}^L$ is called a cone if $v \in \mathcal{C}$ implies that $\alpha v \in \mathcal{C}$ for all $\alpha \geq 0$. A solid cone has a non-empty interior, i.e., $\text{int}(\mathcal{C}) \neq \emptyset$. A pointed cone contains the origin. A closed convex, pointed and solid cone is called an ordering cone.

An ordering cone can be both polyhedral and non-polyhedral. Following the literature (Ararat and Tekin, 2023; Karagözlü et al., 2024), we consider access to a polyhedral ordering cone.

Definition 2.2 (Polyhedral Ordering Cone). An ordering cone $\mathcal{C}$ is a polyhedral cone if $\mathcal{C} \triangleq \{x \in \mathbb{R}^L \mid Ax \geq 0\}$, where $A \in \mathbb{R}^{K \times L}$ with rows $a_i^\top$. A is called the half-space representation of $\mathcal{C}$.

Each polyhedral ordering cone induces a set of partial order on the reward vectors in $\mathbb{R}^L$. To ignore the redundancies and to focus on the bandit problem, we further assume that A is full row-rank and $\|A_i\|_2 = 1$ (Ararat and Tekin, 2023). Hereafter, we call them *preference cones*, and the vectors in the cone as the *preferences*. We refer to (Jahn et al., 2009; Löhne, 2011) for further details on cones.

Example 2.1 (Preference cones). The positive orthant $\mathbb{R}_+^L$ is a polyhedral ordering cone. This is the one used in the pareto-set identification literature (Auer et al., 2016; Kone et al., 2023b; crepon et al., 2024). The cones with all non-negative entries are called solvency cones and used in finance (Kabanov, 2009). Another simple example is $\mathcal{C}_{\pi/3} \triangleq \{(r \cos \theta, r \sin \theta) \in \mathbb{R}^2 \mid r \geq 0 \wedge \theta \in [0, \pi/3]\}$, i.e., all the 2-dimensional vectors that make an angle less than $\pi/3$ with the x -axis.

Definition 2.3 (Partial Order). For every $\mu, \mu' \in \mathbb{R}^L$, $\mu \preceq_{\mathcal{C}} \mu'$ if $\mu \in \mu' + \mathcal{C}$ and $\mu \prec_{\mathcal{C}} \mu'$ if $\mu \in \mu' + \text{int}(\mathcal{C})$. Alternatively, $\mu \preceq_{\mathcal{C}} \mu'$ is equivalent to $z^\top (\mu - \mu') \leq 0, \forall z \in \mathcal{C}$.

The partial order induced by $\mathcal{C}$ induces further order over the set of arms $[K]$.

Definition 2.4 (Order over arms). Consider two arms $i, j \in [K]$. (i) Arm i is weakly dominated by arm j iff $M_i \preceq_{\mathcal{C}} M_j$. (ii) Arm i dominates arm j iff $M_j \prec_{\mathcal{C} \setminus \{0\}} M_i$. (iii) Arm i strongly dominates arm j iff $M_j \prec_{\mathcal{C}} M_i$.

Definition 2.5 (Pareto Optimal Set). An arm $i \in [K]$ is Pareto Optimal if it is not dominated by any other arm w.r.t. the cone $\mathcal{C}$. The Pareto Optimal Set $\mathcal{P}^*$ is defined as the set of all Pareto Optimal arms.

Given a preference cone, a learner aims to identify exactly the Pareto Optimal Set from a finite set of arms $[K]$ whose mean rewards belong to the Pareto Optimal Set w.r.t. $\mathcal{C}$. Alternatively, this vector optimization problem can be represented in the policy space as finding a policy $\pi \in \Delta_K$ supported on the Pareto Optimal Set of arms. The following vector optimization problem yields this:

$$V(M) \triangleq \max_{\pi \in \Delta_K} M\pi \text{ over } \mathcal{C}. \quad (1)$$

In this context, we denote the set of Pareto optimal policies as $\Pi^*(M) \triangleq \arg \max_{\pi \in \Delta_K} M\pi \text{ over } \mathcal{C}$. We assume that $\Pi^*(M)$ is non-empty.

Example 2.2 (Pareto Optimal Sets for different cones). Figure 1 illustrates the Pareto Optimal Sets among 2-dimensional mean vectors of 200 randomly selected arms under preference cones $\mathcal{C}_{\pi/2}$

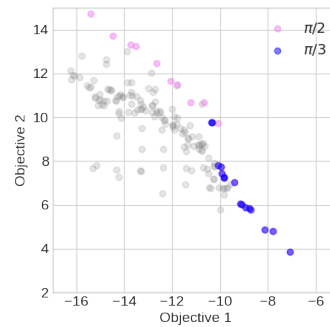


Figure 1: Effect of cone selection on size of Pareto optimal set

and $\mathcal{C}_{\pi/3}$. We observe that the Pareto Optimal Sets for them (in pink and blue respectively), are completely different for the same set of arms. Thus, we have to adapt to the available preferences to solve the aforementioned problem. As noted later, the geometry of this cone plays a crucial role in determining the Pareto front.

In PrePEX, we consider the problem of Equation (1), when the mean matrix M is unknown a priori but bounded, i.e., the entries of M , $M_{ij} \in [M_{\min}, M_{\max}]$. We denote all such mean matrices by $\mathcal{M}$. Identifying the policy will lead us to identify the true Pareto front $\mathcal{P}^*$. In the noisy feedback setting, the reward at time t is $R_t = M_{k_t} + \eta_t$, where $\eta_t \in \mathbb{R}^L$ is the noise vector. We assume that the noise vectors η_t are independent of M_{k_t} and also across time. Further, they are sub-Gaussian with parameter σ and adapted to the filtration $\mathcal{F}_t$, which is a standard assumption in the literature. A policy $\pi \in \Pi \subset \Delta^K$ is a randomized mapping from the history $\mathcal{H}_t$ to the probability simplex over the set of arms $[K]$. In Preference-based Pure EXploration (PrePEX) problem, the goal of the learner is to identify a Pareto optimal policy in Π^* (Equation (1)) given an instance M and a preference cone $\mathcal{C}$ while observing only noisy rewards from the arms, and also using as few observations as possible.

Definition 2.6 ($(1 - \delta)$ -correct PrePEX). *An algorithm for Preference-based Pure Exploration (PrePEX) is said to be $(1 - \delta)$ correct if with probability $1 - \delta$, it recommends a Pareto optimal policy $\pi \in \Pi^*$.*

For example, a pareto optimal policy for $\mathcal{C}_{\pi/2}$ would be a distribution in Δ_K with support on the arms corresponding to the pink reward vectors (Figure 1). For $\mathcal{C}_{\pi/3}$, it would be one with support on blue points. Finally, we make the standard assumption on the mean rewards.

Assumption 2.1 (Single Parameter Exponential Family). *Let $X = (X_1, \dots, X_d)$ be a d -dimensional random vector with a distribution $P_\theta, \theta \in \Theta$. Suppose $X_1, \dots, X_d$ are jointly continuous. The family of distributions $\{P_\theta, \theta \in \Theta\}$ is said to belong to the one parameter Exponential family if the density of X may be represented in the form $f(x|\theta) \triangleq h(x) \exp(\eta(\theta)T(x) - \psi(\theta))$. We assume that the mean reward for each vector belongs to a single-parameter exponential family with variance bounded by 1.*

3 Lower Bound on Sample Complexity

We begin by deriving a KL-divergence based lower bound for PrePEX using techniques from (Garivier and Kaufmann, 2016). Our lower bound is based on establishing a change-of-measure argument in the spirit of (Graves and Lai, 1997; Kaufmann et al., 2016). The lower bounds are derived first by defining a set of alternating instances Λ for a given bandit instance and then by trying to compute an optimal allocation policy $w \in \Delta_K$ that maximises the sum of minimum KL-divergence between any instance in Λ and the bandit instance under interaction. *The key insight of our work is to formulate the identification of Pareto Set problem in the policy space rather than in the arm space as done in antecedent literature.* This formulation helps us to derive the KL-based lower bound, which is more general than the existing suboptimality gap-based lower bounds (Auer et al., 2016; Ararat and Tekin, 2023; crepon et al., 2024).

The Alternating Instances with respect to Pareto Fronts. The learner needs to distinguish between all instance $\tilde{M} \in \mathcal{M} \setminus \{M\}$ for which the Pareto front associated with $\tilde{M}$ is different from the one associated with M . At first, given an optimal policy of M , say π^* , it would appear that the set of confusing instances is $\Lambda_{\pi^*}(M)^{\text{naive}} \triangleq \{\tilde{M} \in \mathcal{M} : \tilde{M}\pi^* \preceq_{\mathcal{C}} \max_{\pi \in \Pi} \tilde{M}\pi\}$. However, this is fallacious since the instances whose rewards dominate M can also confuse a policy π . Given a π^* , the correct alternating set is the set of instances in $\mathcal{M}$ whose Pareto optimal set is not dominated by π^* corresponding to M .

$$\begin{aligned} \Lambda_{\pi^*}(M) &\triangleq \left\{ \tilde{M} \in \mathcal{M} \setminus \{M\} : \max_{\pi \in \Pi} \tilde{M}\pi \not\preceq_{\mathcal{C}} \tilde{M}\pi^* \right\} \\ &= \left\{ \tilde{M} \in \mathcal{M} \setminus \{M\} : \exists z \in \mathcal{C} \text{ s.t. } \max_{\pi \in \Pi} z^\top \tilde{M}\pi > z^\top \tilde{M}\pi^* \right\}. \end{aligned}$$

With this new alternate set defined, we now establish lower bounds on the performance of any PrePEX algorithm.

Theorem 3.1 (Lower Bound). *Given a bandit model $M \in \mathcal{M}$, a preference cone $\mathcal{C}$, and a confidence level $\delta \in [0, 1)$, the expected stopping time of any $(1 - \delta)$ -correct PrePEX algorithm, to identify the*

Pareto Optimal Set is

$$\mathbb{E}[\tau] \geq \mathcal{T}_{M,\mathcal{C}} \log \left(\frac{1}{2.4\delta} \right), \quad (2)$$

where, the expectation is taken over the stochasticity of both the algorithm and the bandit instance. Here, $\mathcal{T}_{M,\mathcal{C}}$ is called the characteristic time of the PrePEX instance $(M, \mathcal{C})$ and is expressed as

$$(\mathcal{T}_{M,\mathcal{C}})^{-1} \triangleq \sup_{w \in \Delta^K} \inf_{\substack{\pi \in \Pi \setminus \{\pi^*\} \\ \pi^* \in \Pi^*(M)}} \inf_{\tilde{M} \in \partial \Lambda_{\pi^*}(M)} \inf_{z \in \mathcal{C}} \sum_{k=1}^K w_k d_{KL} \left(z^\top M_k, z^\top \tilde{M}_k \right), \quad (3)$$

such that $\partial \Lambda_{\pi^*}(M) \triangleq \cup_{\Pi \setminus \{\pi^*\}} \left\{ \tilde{M} \in \mathcal{M} : \exists z \in \mathcal{C}, \langle \text{vect}(z(\pi - \pi^*)^\top), \text{vect}(\tilde{M}) \rangle = 0 \right\}$.

Proof Intuition. First, we observe that an instance $\tilde{M}$ is in alternating set if there exists a $\pi \in \Pi \setminus \{\pi^*\}$ and $z \in \mathcal{C}$, such that $z^\top \tilde{M}(\pi - \pi^*) > 0$. If π and π^* were pure strategies, it would have been exactly $\inf_{z \in \mathcal{C} \setminus \{0\}} z^\top (\tilde{M}_a - \tilde{M}_{a^*}) > 0$. Let us denote the z achieving the inf as z_{inf} , i.e., the preference for which $\tilde{M}_a$ and $\tilde{M}_{a^*}$ are least distinguishable. Thus, we observe that $z_{\text{inf}}^\top \tilde{M}_a$ exactly functions as the mean of the arm a in an instance $\tilde{M}$, whereas $z_{\text{inf}}^\top (\tilde{M}_{a^*} - \tilde{M}_a)$ acts as the suboptimality gap. Now, we extend this idea in the classical lower bound scheme to get a nested optimization problem with inf over $z \in \mathcal{C}$ and $\tilde{M}$ in the alternating set, and a sup over allocations $w \in \Delta_K$. We further show that the inf for $\tilde{M}$ appears at the boundary of the alternating set defined as $\partial \Lambda(M)$.

Discussions. (i) Novelty: In the best of our knowledge, this is the first lower bound for PrePEX with fixed confidence with an explicit KL-based dependence. All the existing lower bounds are gap dependent, and valid for a narrow range on mean vectors or known preference cone, i.e. the right orthant. Our proof does not need such assumptions. The gap-dependent bounds are special case of ours (cf. Theorem 3.2 for the case of Gaussian rewards).

(ii) Geometric Insights. Theorem 3.1 provides multiple geometric insights into the affect of the ordering cone $\mathcal{C}$ on the characteristic time. *First*, the alternating set $\Lambda_{\pi^*}(M)$ is piece-wise polyhedral and non-convex. We address consequent issues in Section 4.1. *Second*, there is an additional minimization over the vectors lying in the cone $\mathcal{C}$. We interpret the minimization over vectors in the cone as a *instance- and preference-dependent scalarization of the distance between the given instance M and the corresponding most-confusing instance in $\Lambda_{\pi^*}(M)$* . *Third*, in the proof, we show that the reward gap using the best policy π^* and a given policy π for the most confusing instance belongs to the polar cone $\mathcal{C}^\circ$ of the preference cone $\mathcal{C}$. The most confusing lies on the boundary of this polar cone and its projection the policy gaps $(\pi^* - \pi)$. Further insights can be obtained by imagining the polar cone to be orthogonal to the cone $\mathcal{C}$. Then, the vector of reward-gaps for the most confusing instance for every objective is orthogonal to the generating rays of $\mathcal{C}$. These novel geometric insights are complementary to the existing algebraic and statistical insights available in the lower bound literature (Kone et al., 2023a; Ararat and Tekin, 2023).

3.1 Characterization of Lower Bounds for Gaussians

To understand our lower bound better and to compare it with the literature, we present a reduction for Gaussian bandits. In Gaussian bandits, we assume that the reward vectors of arm $a \in [K]$ are generated from a multivariate Gaussian distribution $\mathcal{N}(\mu_a, \Sigma)$, where the covariance is a diagonal matrix: $\Sigma \triangleq \text{Diag}(\sigma_1^2, \dots, \sigma_L^2)$.

Theorem 3.2 (Lower Bound for Gaussian Bandits). *1. Given any $\pi^* \in \Pi^*(M)$ and $N(\pi^*)$ being the set of neighbouring policies of π^* , the most confusing instance of M belongs to the set*

$$\left\{ \tilde{M} \in \mathcal{M} \setminus \{M\} : \tilde{M}_{k,\ell} = M_{k,\ell} - \beta \frac{\sigma_\ell^2 (\pi^* - \pi)_k}{z_\ell w_k}, \quad \forall \pi \in N(\pi^*), z \in \mathcal{C} \setminus \{0\}, k \in [K], \ell \in [L] \right\},$$

$$\text{where } \beta \triangleq \frac{z^\top M(\pi^* - \pi)}{\text{Tr}(\Sigma) \|\pi^* - \pi\|_{\text{Diag}(1/w)}^2}.$$

2. The inverse of characteristic time, i.e. $(\mathcal{T}_{M,\mathcal{C}}^{\text{Gauss}})^{-1}$, for an instance $(M, \mathcal{C})$ is

$$\inf_{\substack{\pi \in N(\pi^*) \\ \pi^* \in \Pi^*(M)}} \min_{z \in \mathcal{C} \setminus \{0\}} \frac{(z^\top M(\pi^* - \pi))^2}{2 \text{Tr}(\Sigma) \|\pi^* - \pi\|_2^2}.$$

Consequences. *First*, we observe an interesting phenomenon that a bilinear projection of mean matrix M on the preferences and policy gaps operates as an extension of suboptimality gap in classical BAI. This is reminiscent of the lower bound for pure exploration under known linear constraints as in Carlsson et al. (2024) who show that the hardness of the problem depends only on the projection of the mean vector on the policy gap. In addition to similar projection structure, preferences introduce a novel bilinearity here. *Second*, we show how the lower bound inflates with the covariance matrix for each objective. This shows the richness of our KL-divergence based lower bound as opposed to gap-based bounds which have difficulty accommodating variance related terms directly.

Connection to existing results. Our result generalizes several existing lower bounds for BAI.

1. *BAI lower bound.* Our lower bound is able to recover that of Kaufmann et al. (2016) for the standard BAI problem with fixed confidence. In the case of the standard BAI problem, the ordering cone is given by $\mathcal{C} \triangleq \mathbb{R}_+$ and therefore the minimization over $\mathcal{C}$ in (3) becomes redundant. The definition of the alternating set is then given by the set of instances which have a different optimal arm than μ which is exactly the set considered in (Kaufmann et al., 2016).

2. *Pure exploration under known constraints.* Our lower bound is able to recover the lower bound of Carlsson et al. (2023) for the BAI problem with fixed confidence and linear constraints. This is the case with $L = 1$ and the ordering cone being $\mathcal{C} \triangleq \mathbb{R}_+$ making the minimization over $z \in \mathcal{C}$ in (3) redundant. $\Lambda_{\pi^*}(M)$ becomes $\Lambda_{\pi^*}(M) = \{\tilde{\mu} : \max_{\pi \in \Pi} \tilde{\mu}^\top \pi \geq \mu^\top \pi^*\}$ and we retrieve exactly their Corollary 1.

4 Algorithm Design: PreTS

In this section, we propose an algorithm that tracks the lower bound. However, this is not straightforward since the alternating set is non-convex. We first propose a convex relaxation for this set and then, design a Track and Stop style algorithm, called PreTS.

4.1 Convex Relaxation of the Lower Bound

One of the major differences regarding the structure of lower bounds compared to a standard BAI problem is that $\Lambda_{\pi^*}(M)$ is a piece-wise polyhedron, i.e., a union of hyperplanes. Each hyperplane corresponds to a policy $\pi \in \Pi \setminus \{\pi^*\}$. To make the optimization problem tractable and obtain a convex program, we relax $\Lambda_{\pi^*}(M)$ using its convex closure, denoted by $\text{ch}(\Lambda_{\pi^*}(M))$. We note that the construction of such a convex relaxation for track-and-stop (when the lower bound problem is non-convex) has been done in the MDP setting Al Marjani and Proutiere (2021). We define $\text{ch}(\Lambda_{\pi^*}(M))$ in Theorem 4.1 by formulating it as a disjunctive program, which we can reformulate further as a linear program (Balas, 1985).

Theorem 4.1. Let $\mathcal{F} \triangleq \cup_{\Pi \setminus \pi^*} \{\tilde{M} \in \mathcal{M} : \exists z \in \mathcal{C}, \langle \text{vect}(z^\top(\pi - \pi^*)), \text{vect}(\tilde{M}) \rangle = 0\}$. Fix $z \in \mathcal{C}$ such that $z = \sum_i \alpha_i v_i$. Then, we have $\text{ch}(\mathcal{F}) = \mathcal{I}$, where $\mathcal{I}$ is defined as

$$\mathcal{I} \triangleq \{\tilde{M} \in \mathcal{M} : \gamma^\top \text{vect}(\tilde{M}) \geq \gamma_0, \gamma = \sum_i u_i \alpha_i \text{vect}(v_i^\top(\pi - \pi^*)), \gamma_0 \leq u_i \sum_i \alpha_i v_i^\top \pi^*\}. \quad (4)$$

Using the convex hull (Eq. (4)), we quantify the optimal value for a given allocation w as

$$\bar{\mathcal{V}}_{\mathcal{C}}(w, M) \triangleq \min_{\tilde{M} \in \text{ch}(\Lambda_{\pi^*}(M))} \inf_{z \in \mathcal{C}} \sum_{k=1}^K w_k d_{\text{KL}}(z^\top M, z^\top \tilde{M}).$$

The corresponding optimal allocation is

$$\bar{w}^*(M) = \arg \max_{w \in \Delta^K} \inf_{\substack{\pi \in \Pi \setminus \pi^* \\ \pi^* \in \Pi^*(M)}} \min_{\tilde{M} \in \text{ch}(\Lambda_{\pi^*}(M))} \inf_{z \in \mathcal{C}} \sum_{k=1}^K w_k d_{\text{KL}}(z^\top M, z^\top \tilde{M}). \quad (5)$$

Hereafter, we consider Equation (5) as the optimization problem to be tracked. To compute $\bar{\mathcal{V}}_{\mathcal{C}}(w, M)$, we need access to the true instance M which is not available to us. Our Track-and-Stop strategy is based on repeatedly sampling an arm to construct an estimate of M , i.e. M_t , and exploiting continuity properties of $\bar{\mathcal{V}}_{\mathcal{C}}(w, M)$ to show that $\bar{\mathcal{V}}_{\mathcal{C}}(w, M_t) \rightarrow \bar{\mathcal{V}}_{\mathcal{C}}(w, M)$ and the cumulative number of arm plays $N_{t,k} \rightarrow w_k$, $w_k \in \bar{w}^*(M)$. These properties ensure that it makes sense to design a Track and Stop style algorithm for this problem.

Algorithm 1 Preference-based Track-and-Stop (PreTS)

- 1: **Input:** Confidence parameter δ , preference cone $\mathcal{C}$
 - 2: **if** $\sup_{\pi_t^*} \min_{\tilde{M} \in \text{ch}(\partial \Lambda_{\pi_t^*}(\hat{M}_t))} \min_{z \in \mathcal{C}} \sum_k N_{k,t} d_{\text{KL}}(z^\top \hat{M}_t^{(k)}, z^\top \tilde{M}^{(k)}) \geq \beta(t, \delta)$ **then**
 - 3: Compute $w_t \leftarrow \arg \max_{w \in \Delta^K} \bar{V}_{\mathcal{C}}(w, \hat{M}_t)$
 - 4: Play $k_t \leftarrow \arg \min_{k \in [K]} |N_{k,t} - \sum_{s=1}^t w_s|$
 - 5: Observe reward r_t
 - 6: Construct an empirical estimator $\hat{M}_t$
 - 7: **end if**
 - 8: Construct a Pareto Front $\hat{\mathcal{P}}_\tau$ from empirical means $\hat{M}_\tau$
 - 9: Return: $\hat{\mathcal{P}}_\tau$
-

Theorem 4.2 (Analytical Properties). *For all $M \in \mathbb{R}^{L \times K}$ and all preference cones $\mathcal{C}$, we get 1. The mapping $(w, M) \rightarrow \bar{V}_{\mathcal{C}}(w, M)$ is continuous. 2. The characteristic time mapping $M \rightarrow \bar{\mathcal{T}}_{M, \mathcal{C}}$ is continuous. 3. The set valued function $M \rightarrow \bar{w}^*(M)$ is upper-hemicontinuous. 4. The set $\bar{w}^*(M)$ is convex.*

Discussion: Cost of Convexification. For Gaussian bandits, as we can get the analytical form of the most confusing instance $\tilde{M}$ (Theorem 3.2), we do not pay any extra cost of convexification. In the non-Gaussian settings, where we cannot find such analytical forms for the most confusing instances, the minimum value of the inner minimisation problem under the convex hull (Equation (5)) can go lower than the minimum value found in the original non-convex set of instances (Equation (3)). Thus, the characteristic time attained by solving the convex relaxation might be higher than that of the original lower bound. Hence, an algorithm solving the convex relaxation has a higher stopping time. However, convexification is essential for the computational feasibility of a lower bound-tracking algorithm for PrePEX. This computational-statistical trade-off will be interesting to study in the future.

4.2 Algorithm: Preference-based Track-and-Stop (PreTS)

We now construct a general recipe to design a PrePEX algorithm when we do not have access to the true instance M . The fundamental element of any such recipe is constructing an estimate of M . For a given set of observed rewards $\{R_t\}_{t=1}^T$, we obtain a column-wise empirical average of the observed rewards and use it as our estimator of M . Now, we elaborate the three key components of our PrePEX algorithm Preference-based Track and Stop (PreTS, Algorithm 1).

1. **Sampling Rule:** For the sampling rule, we consider a Track-and-Stop strategy (Garivier and Kaufmann, 2016). It tracks the optimal proportion of arm sampling by plugging in the empirical estimates of means and empirical count $N_{k,t}$ in the convexified lower bound. This leads to an allocation policy with improved information acquisition.

2. **Stopping Rule:** Our ultimate stopping goal is to identify arms that are on the Pareto front. Based on this, we define the confidence set as:

$$c(t, \delta) \triangleq \left\{ \tilde{M} \in \mathcal{M} : \min_{z \in \mathcal{C}} \sum_k N_{k,t} d_{\text{KL}}(z^\top \hat{M}_t^{(k)}, z^\top \tilde{M}^{(k)}) \leq \beta(t, \delta) \right\}, \quad (6)$$

where $\beta(t, \delta) \triangleq \sum_{a \in \mathcal{S}} 3 \ln(1 + \ln(N_{k,t})) + K\mathcal{T}\left(\frac{\ln(\frac{1}{\delta})}{K}\right)$ and $\mathcal{T}$ is defined in Equation (17). Our first claim is to show that the true instance belongs to the confidence ellipsoid with high probability.

Lemma 4.1 (Confidence Ball). *For any $t \in \mathbb{N}$ and $c(t, \delta)$ is defined in Equation (6), we have $\mathbb{P}(M \notin c(t, \delta)) \leq \delta$.*

Thus, we can now formalise the corresponding Chernoff-stopping rule as

$$\min_{\tilde{M} \in \text{ch}(\partial \Lambda_{\pi_t^*}(\hat{M}_t))} \min_{z \in \mathcal{C}} \sum_k N_{k,t} d_{\text{KL}}(z^\top \hat{M}_t^{(k)}, z^\top \tilde{M}^{(k)}) \geq \beta(t, \delta) \quad (7)$$

Given the estimates $\hat{M}_t$, the problem in Equation (7) can be solved efficiently. Next, we show that upon stopping with Equation (7), PreTS returns the true Pareto Front $\mathcal{P}^*$ with probability $1 - \delta$. Let

$\hat{\mathcal{P}}_t$ denote the estimated Pareto Front at time t , which is constructed using estimates $\hat{M}_t$. Then at stopping time τ , we have

$$\begin{aligned} \mathbb{P}(\mathcal{P}^* \neq \hat{\mathcal{P}}_t) &\leq \mathbb{P}\left(\exists t \in \mathbb{N} : \sum_{k,\ell} N_{k,t} d_{\text{KL}}\left(z^\top \hat{M}_t^{(k)}, z^\top M^{(k)}\right) \geq \beta(t, \delta)\right) \\ &\leq \sum_{t=1}^{\infty} \mathbb{P}\left(\sum_{k,\ell} N_{k,t} d_{\text{KL}}\left(z^\top \hat{M}_t^{(k)}, z^\top M^{(k)}\right) \geq \beta(t, \delta)\right) \leq \delta \end{aligned}$$

where, the last inequality is true due to Theorem 4.3, a concentration result on the KL-divergence with preference projected mean rewards.

Theorem 4.3. For all $\rho \geq (K+1)$, $z \in \mathcal{C}$ and $t \in \mathbb{N}$, we have that:

$$\mathbb{P}\left[\sum_{k \in [K]} N_{k,t} d_{\text{KL}}\left(z^\top \hat{M}_t^{(k)}, z^\top M^{(k)}\right) \geq \rho\right] \leq \exp(-\rho) \left(\frac{\lceil \rho \log(t) \rceil}{K}\right)^K \exp(K+1)$$

3. Recommendation Rule: At the end of stopping time τ , the algorithm returns an estimate of the Pareto Front $\hat{\mathcal{P}}_\tau$.

5 Upper Bound on Sample Complexity

Now, we prove upper bound on the expected sample complexity of PreTS. This requires us to the Track-an-Stop proof technique. But the challenge is to show concentration of the pareto fronts under a suitable metric.

Concentrating to the Pareto Front. To show that upon stopping the algorithm returns the true Pareto Frontier, we need to establish a valid metric to show such convergence. Usually, the distance between sets is measured using the Hausdorff metric (Costantini and Vitolo, 1995), i.e. $d_H(\hat{\mathcal{P}}_\tau, \mathcal{P}) \triangleq \max\left\{\sup_{k \in \hat{\mathcal{P}}_\tau} \inf_{k' \in \mathcal{P}} \|M_k - M_{k'}\|_\infty, \sup_{k \in \mathcal{P}} \inf_{k' \in \hat{\mathcal{P}}_\tau} \|M_k - M_{k'}\|_\infty\right\}$. But the Hausdorff distance only defines a pseudo-distance between sets and $\mathcal{Z}$ may not be closed under this metric. To circumvent this issue, we build upon the notion of a gap-based metric considered in the antecedent literature (Auer et al., 2016) to measure the distance between the mean reward of an arm and a given Pareto Front. We extend it to a distance metric between elements in the space of Pareto Fronts $\mathcal{Z}$.

Definition 5.1 (Distance from Pareto Front). The distance of the mean of arm k from the Pareto Front $\mathcal{P}^*$ is $d(k, \mathcal{P}^*) \triangleq \inf_{\varepsilon \geq 0} \varepsilon$, such that $M_k + \varepsilon \mathbf{1} \not\prec_{\mathcal{C}} M_{k'}, k' \in \mathcal{P}^*$. Equivalently,

$$d(k, \mathcal{P}^*) \triangleq \inf_{k' \in \mathcal{P}^*} \max\left\{0, \sup_{z \in \mathcal{C} \cap \mathbb{B}(1)} z^\top (M_{k'} - M_k)\right\}. \quad (8)$$

Definition 5.2 (Distance between Pareto Fronts). We define the metric between Pareto Fronts $d_P((\cdot, \cdot), \cdot) : \mathcal{Z} \times \mathcal{Z} \rightarrow \mathbb{R}_{\geq 0}$ as $d_P(\hat{\mathcal{P}}, \mathcal{P}^*) \triangleq \max\left\{\sup_{k \in \hat{\mathcal{P}}} d(k, \mathcal{P}^*), \sup_{k \in \mathcal{P}^*} d(k, \hat{\mathcal{P}})\right\}$.

In the appendix, we establish that (i) $d(\cdot, \cdot)$ is a valid metric on $\mathcal{Z}$, and (ii) $\mathcal{Z}$ is compact and complete under $d(\cdot, \cdot)$. Now, we leverage this metric to show that the Pareto Front defined by the arm-wise constructed estimator $\hat{M}_t$ concentrates towards the true Pareto Front.

Theorem 5.1 (Concentration of mean estimates). For any pair $(i, j) \in [K] \times [K]$ and $z \in \mathcal{C}$, we have

$$\left|z^\top (M_i - M_j) - z^\top (\hat{M}_{i,t} - \hat{M}_{j,t})\right| \leq \beta_{ij}(t),$$

where $\beta_{ij}^2(t) \triangleq 4\|z\|_1^2 \left(h\left(\frac{\log(\frac{K_1}{\delta})}{2}\right) + \sum_{a \in \{i,j\}} \log(4 + \log(N_a(t)))\right) \left(\sum_{a \in \{i,j\}} \frac{1}{N_a(t)}\right)$, $K_1 \triangleq \frac{K(K-1)}{2}$, and $h(x) \approx x + \log(x)$.

Proof Sketch. This is a consequence of jointly applying a vectorial concentration result for multiple-objectives of each arm (Kaufmann and Koolen, 2021), and pairwise time-uniform concentration bounds (Kone et al., 2023a). A key observation here is that the confidence radii depends on the magnitude of the preference vector z and scales with different objectives accordingly.

Sample Complexity of PreTS. Using this new concentration result for the Pareto Front and the stopping rule in Equation 7, we derive an upper bound on the expected stopping time of PreTS.

Theorem 5.2 (Upper Bound on Sample Complexity). *For any $\alpha > 0$ and $c(t, \delta)$ defined in (7), we have that the stopping time satisfies*

$$\lim_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau]}{\log\left(\frac{1}{\delta}\right)} \leq \overline{\mathcal{T}_{M,c}} \quad \forall M \in \mathbb{R}^{L \times K}$$

The basic outline of the proof follows a general strategy to prove Track-and-Stop result. However, the new arguments lie in establishing that the Pareto fronts converge under a suitable metric sufficiently fast. Our proof implies that PreTS matches the convex relaxation of the lower bound asymptotically at the corresponding risk level δ . Strictly, speaking this is not *asymptotically optimal* since, we do not track the exact lower-bound.

6 Conclusion and Future Works

We study the fixed-confidence version of preference-based pure exploration problem under linear stochastic bandit feedback, where each arm corresponds to a reward vector ordered according to a preference cone. We derive a novel lower bound for this problem. We leverage the lower bound further to derive a track-and-stop based algorithm for PrePEX problem. As future work, it would be interesting to verify our results on a real-world datasets.

Additionally, it would be interesting and challenging to study how other asymptotically optimal pure exploration strategies, e.g. gamified explorers (Degenne and Koolen, 2019), top-two algorithms (Jourd'han et al., 2022), can be adapted to this setting. In general, improving the computational efficiency and studying the optimality gap with respect to the non-convex lower-bound problem would be of fundamental interest.

References

- Al Marjani, A. and Proutiere, A. (2021). Adaptive sampling for best policy identification in markov decision processes. In *International Conference on Machine Learning*, pages 7459–7468. PMLR.
- Ararat, C. and Tekin, C. (2023). Vector optimization with stochastic bandit feedback. In *International Conference on Artificial Intelligence and Statistics*, pages 2165–2190. PMLR.
- Audibert, J.-Y. and Bubeck, S. (2010). Best arm identification in multi-armed bandits.
- Auer, P., Chiang, C.-K., Ortner, R., and Drugan, M. (2016). Pareto front identification from stochastic bandit feedback. In *Artificial intelligence and statistics*, pages 939–947. PMLR.
- Balas, E. (1985). Disjunctive programming and a hierarchy of relaxations for discrete optimization problems. *SIAM Journal on Algebraic Discrete Methods*, 6(3):466–486.
- Berge, C. (1877). *Topological spaces: Including a treatment of multi-valued functions, vector spaces and convexity*. Oliver & Boyd.
- Bubeck, S., Munos, R., and Stoltz, G. (2009). Pure exploration in multi-armed bandits problems. In *Algorithmic Learning Theory: 20th International Conference, ALT 2009, Porto, Portugal, October 3-5, 2009. Proceedings 20*, pages 23–37. Springer.
- Carlsson, E., Basu, D., Johansson, F., and Dubhashi, D. (2024). Pure exploration in bandits with linear constraints. In *International Conference on Artificial Intelligence and Statistics*, pages 334–342. PMLR.
- Carlsson, E., Basu, D., Johansson, F. D., and Dubhashi, D. (2023). Pure exploration in bandits with linear constraints. *arXiv preprint arXiv:2306.12774*.

- Contal, E., Buffoni, D., Robicquet, A., and Vayatis, N. (2013). Parallel gaussian process optimization with upper confidence bound and pure exploration. In *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*, pages 225–240. Springer.
- Costantini, C. and Vitolo, P. (1995). On the infimum of the hausdorff metric topologies. *Proceedings of the London Mathematical Society*, 3(2):441–480.
- crepon, e., Garivier, A., and M Koolen, W. (2024). Sequential learning of the Pareto front for multi-objective bandits. In Dasgupta, S., Mandt, S., and Li, Y., editors, *Proceedings of The 27th International Conference on Artificial Intelligence and Statistics*, volume 238 of *Proceedings of Machine Learning Research*, pages 3583–3591. PMLR.
- Degenne, R. and Koolen, W. M. (2019). Pure exploration with multiple correct answers. In *Neural Information Processing Systems*.
- Donsker, M. D. and Varadhan, S. S. (1975). Asymptotic evaluation of certain markov process expectations for large time, i. *Communications on pure and applied mathematics*, 28(1):1–47.
- Drugan, M. M. and Nowe, A. (2013). Designing multi-objective multi-armed bandits algorithms: A study. In *The 2013 international joint conference on neural networks (IJCNN)*, pages 1–8. IEEE.
- Even-Dar, E., Mannor, S., and Mansour, Y. (2006). Action elimination and stopping conditions for the multi-armed bandit and reinforcement learning problems. *Journal of machine learning research*, 7(Jun):1079–1105.
- Gabillon, V., Ghavamzadeh, M., and Lazaric, A. (2012). Best arm identification: A unified approach to fixed budget and fixed confidence. In *Advances in Neural Information Processing Systems*, pages 3212–3220.
- Garivier, A. and Kaufmann, E. (2016). Optimal best arm identification with fixed confidence. In *Conference on Learning Theory*, pages 998–1027.
- Gaulton, A., Bellis, L. J., Bento, A. P., Chambers, J., Davies, M., Hersey, A., Light, Y., McGlinchey, S., Michalovich, D., Al-Lazikani, B., et al. (2012). ChEMBL: a large-scale bioactivity database for drug discovery. *Nucleic acids research*, 40(D1):D1100–D1107.
- Graves, T. L. and Lai, T. L. (1997). Asymptotically efficient adaptive choice of control laws in uncontrolled markov chains. *SIAM journal on control and optimization*, 35(3):715–743.
- Hasselgren, C. and Oprea, T. I. (2024). Artificial intelligence for drug discovery: Are we there yet? *Annual Review of Pharmacology and Toxicology*, 64:527–550.
- Jahn, J. et al. (2009). *Vector optimization*. Springer.
- Jamieson, K., Malloy, M., Nowak, R., and Bubeck, S. (2014). lil’ucb: An optimal exploration algorithm for multi-armed bandits. In *Conference on Learning Theory*, pages 423–439.
- Jamieson, K. and Nowak, R. (2014). Best-arm identification algorithms for multi-armed bandits in the fixed confidence setting. In *2014 48th Annual Conference on Information Sciences and Systems (CISS)*, pages 1–6. IEEE.
- Jayatunga, M. K., Xie, W., Ruder, L., Schulze, U., and Meier, C. (2022). Ai in small-molecule drug discovery: a coming wave. *Nat. Rev. Drug Discov*, 21(3):175–176.
- Jedra, Y. and Proutiere, A. (2020). Optimal best-arm identification in linear bandits. *Advances in Neural Information Processing Systems*, 33:10007–10017.
- Jourdan, M., Degenne, R., Baudry, D., de Heide, R., and Kaufmann, E. (2022). Top two algorithms revisited. *Advances in Neural Information Processing Systems*, 35:26791–26803.
- Kabanov, Y. (2009). *Markets with Transaction Costs Mathematical Theory*. Springer.
- Kalyanakrishnan, S., Tewari, A., Auer, P., and Stone, P. (2012). Pac subset selection in stochastic multi-armed bandits. In *ICML*, volume 12, pages 655–662.

- Karagözlü, E. M., Yıldırım, Y. C., Ararat, C., and Tekin, C. (2024). Learning the pareto set under incomplete preferences: Pure exploration in vector bandits. In *International Conference on Artificial Intelligence and Statistics*, pages 3070–3078. PMLR.
- Kaufmann, E., Cappé, O., and Garivier, A. (2016). On the complexity of best arm identification in multi-armed bandit models. *Journal of Machine Learning Research*, 17:1–42.
- Kaufmann, E. and Koolen, W. M. (2021). Mixture martingales revisited with applications to sequential tests and confidence intervals. *Journal of Machine Learning Research*, 22(246):1–44.
- Kone, C., Kaufmann, E., and Richert, L. (2023a). Adaptive algorithms for relaxed pareto set identification. *Advances in Neural Information Processing Systems*, 36:35190–35201.
- Kone, C., Kaufmann, E., and Richert, L. (2023b). Bandit pareto set identification: the fixed budget setting. *arXiv preprint arXiv:2311.03992*.
- Korkmaz, İ. O., Ararat, C., and Tekin, C. (2023). Bayesian vector optimization with gaussian processes.
- Lattimore, T. and Szepesvári, C. (2020). *Bandit Algorithms*. Cambridge University Press.
- Li, L., Jamieson, K., DeSalvo, G., Rostamizadeh, A., and Talwalkar, A. (2018). Hyperband: A novel bandit-based approach to hyperparameter optimization. *Journal of Machine Learning Research*, 18(185):1–52.
- Lizotte, D. J. and Laber, E. B. (2016). Multi-objective markov decision processes for data-driven decision support. *Journal of Machine Learning Research*, 17(210):1–28.
- Löhne, A. (2011). *Vector optimization with infimum and supremum*. Springer Science & Business Media.
- Lu, S., Wang, G., Hu, Y., and Zhang, L. (2019). Multi-objective generalized linear bandits. *arXiv preprint arXiv:1905.12879*.
- Magureanu, S., Combes, R., and Proutiere, A. (2014). Lipschitz bandits: Regret lower bound and optimal algorithms. In *Conference on Learning Theory*, pages 975–999. PMLR.
- Mullard, A. (2014). New drugs cost us \$2.6 billion to develop. *Nature reviews drug discovery*, 13(12).
- Munro, A. P., Janani, L., Cornelius, V., Aley, P. K., Babbage, G., Baxter, D., Bula, M., Cathie, K., Chatterjee, K., Dodd, K., et al. (2021). Safety and immunogenicity of seven covid-19 vaccines as a third dose (booster) following two doses of chadox1 ncov-19 or bnt162b2 in the uk (cov-boost): a blinded, multicentre, randomised, controlled, phase 2 trial. *The Lancet*, 398(10318):2258–2276.
- Peskun, P. H. (1973). Optimum monte-carlo sampling using markov chains. *Biometrika*, 60(3):607–612.
- Reker, D. and Schneider, G. (2015). Active-learning strategies in computer-assisted drug discovery. *Drug discovery today*, 20(4):458–465.
- Sadybekov, A. V. and Katritch, V. (2023). Computational approaches streamlining drug discovery. *Nature*, 616(7958):673–685.
- Shukla, A. (2022). *Optimization and Learning in Dynamic Environments: Models and Algorithms*. Columbia University.
- Smer-Barreto, V., Quintanilla, A., Elliott, R. J., Dawson, J. C., Sun, J., Campa, V. M., Lorente-Macías, Á., Unciti-Broceta, A., Carragher, N. O., Acosta, J. C., et al. (2023). Discovery of senolytics using machine learning. *Nature communications*, 14(1):3445.
- Soare, M., Lazaric, A., and Munos, R. (2014). Best-arm identification in linear bandits. In *Advances in Neural Information Processing Systems*, pages 828–836.

- Sun, D., Gao, W., Hu, H., and Zhou, S. (2022). Why 90 *Acta Pharmaceutica Sinica B*, 12(7):3049–3062.
- Tekin, C. and Turgay, E. (2017). Multi-objective contextual bandits with a dominant objective. In *2017 IEEE 27th International Workshop on Machine Learning for Signal Processing (MLSP)*, pages 1–6. IEEE.
- Turgay, E., Oner, D., and Tekin, C. (2018). Multi-objective contextual bandit problem with similarity information. In *International Conference on Artificial Intelligence and Statistics*, pages 1673–1681. PMLR.
- Wang, J., Basu, D., and Trummer, I. (2022). Procrastinated tree search: Black-box optimization with delayed, noisy, and multi-fidelity feedback. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 36, pages 10381–10390.
- Wang, J., Trummer, I., and Basu, D. (2021). Demonstrating udo: A unified approach for optimizing transaction code, physical design, and system parameters via reinforcement learning. In *Proceedings of the 2021 International Conference on Management of Data*, pages 2794–2797.
- Zuluaga, M., Krause, A., et al. (2016). e-pal: An active learning approach to the multi-objective optimization problem. *Journal of Machine Learning Research*, 17(104):1–32.

Appendix

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A Notations

Notation	Description
$\mathcal{C}, \prec_{\mathcal{C} \setminus \{0\}}$	Given convex cone and induced partial order
K, L	number of arms and objectives
$\mathcal{P}^*, \hat{\mathcal{P}}_t$	Ground truth Pareto set and estimated Pareto set
$\mathcal{Z}$	Space of all Pareto Frontiers on $[0, 1]^K$
$M \in \mathbb{R}^{K \times L}$	matrix with mean reward of K arms
r_{k_t}, M_{k_t}, η_t	observed reward, mean reward and noise
$c(t, \delta)$	Confidence ball at time t with confidence δ
$d_H(X, Y)$	Hausdroff distance between sets X and Y
$d_P(P, \hat{P})$	Distance metric between Pareto Fronts P and $\hat{P}$
w	Allocation vector
Π	Family of policies
$\hat{M}_{\ell, k} t, M_{\ell} k$	Estimated and true of mean rewards
$\text{ch}(S)$	Convex hull of set S
$\Lambda_{\pi^*}(M)$	Set of alternating instances associated with M

Table 1: Table of Notations

B Proofs of Lower Bounds

B.1 Generic Lower Bound: Proof of Theorem 3.1

Proof. The proof follows the basic structure of constructing a lower bound as in Kaufmann et al. (2016). Recall that their inverse of characteristic time is given by

$$\mathcal{T} = \sup_{w \in \Pi} \inf_{\tilde{M} \in \Lambda_{\pi^*}(M)} \sum_k w_k d_{\text{KL}}(M_k, \tilde{M}_k) \quad (9)$$

The main challenge for our setting is describing the alternating set $\Lambda_{\pi^*}(M)$ and scalarization of the given instance $M \in \mathcal{M}$. Given a matrix of arm-objective mean-rewards M , ordering cone $\mathcal{C}$ and a family of policies Π , the Pareto front is the set of optimal values (ordered wrt $\mathcal{C}$) of

$$\max_{\pi \in \Pi} M\pi. \quad (10)$$

- **Step 1: Constructing set of alternative instances** Let $\pi^* \in \arg \max_{\pi \in \Pi} M\pi$.

The set of confusing instances given Π and $\mathcal{C}$ is the set of all matrices $\tilde{M}$ which have a different Pareto front than M when using the policy π^* . Therefore, the optimal values of (10) with instance M are not-dominated by those of instance $\tilde{M}$. Hence, the set of alternative instances, $\Lambda_{\pi^*}(M)$ is given by:

$$\Lambda_{\pi^*}(M) := \left\{ \tilde{M} \in \mathcal{M} : \max_{\pi \in \Pi} \tilde{M}\pi \not\leq_{\mathcal{C}} \tilde{M}\pi^* \right\}$$

Let $\pi' \in \arg \max_{\pi \in \Pi} \tilde{M}\pi$ over $\mathcal{C}$ which implies $\tilde{M}\pi' \not\leq_{\mathcal{C}} \tilde{M}\pi^*$ or equivalently:

$$\exists z \in \mathcal{C}, \pi \in \Pi \setminus \{\pi^*\} \text{ s.t. } z^\top \tilde{M}\pi > z^\top \tilde{M}\pi^*$$

Therefore, the alternative set can be written as:

$$\begin{aligned} \Lambda_{\pi^*}(M) &\triangleq \cup_{\pi \in \Pi \setminus \{\pi^*\}} \left\{ \tilde{M} \in \mathcal{M} : \exists z \in \mathcal{C}, z^\top \tilde{M}\pi > z^\top \tilde{M}\pi^* \right\} \\ &= \cup_{\pi \in \Pi \setminus \{\pi^*\}} \left\{ \tilde{M} \in \mathcal{M} : \exists z \in \mathcal{C} : z^\top \tilde{M} \cdot (\pi - \pi^*) > 0 \right\} \end{aligned}$$

where, $\cdot$ represents a bilinear product and, its complement is given by:

$$\begin{aligned} \overline{\Lambda_{\pi^*}(M)} &\triangleq \cap_{\pi \in \Pi \setminus \{\pi^*\}} \left\{ \tilde{M} \in \mathcal{M} : \forall z \in \mathcal{C} : z^\top \tilde{M} \cdot (\pi - \pi^*) \leq 0 \right\} \\ &= \cap_{\pi \in \Pi \setminus \{\pi^*\}} \left\{ \tilde{M} \in \mathcal{M} : \tilde{M} \cdot (\pi - \pi^*) \in \mathcal{C}^\circ \right\} \end{aligned}$$

where, $\text{ri}(\mathcal{C}^\circ)$ denotes the relative interior of the polar cone to $\mathcal{C}$. Since $\mathcal{C}$ is a polyhedral cone, it is closed and convex and therefore, its polar cone is non-empty, closed and convex. Therefore, $\overline{\Lambda_{\pi^*}(M)}$ is non-empty.

- **Step 2: Hardest instance lies on the boundary** We now show that given π^* , and π , the hardest instances $\tilde{M} \in \mathcal{M}$ are such that:

$$\tilde{M} \cdot (\pi - \pi^*) \in \text{bd}(\mathcal{C}^\circ).$$

Fix $\pi' \in \Pi \setminus \{\pi^*\}$ and let $M' \in \left\{ \tilde{M} \in \mathcal{M} : \tilde{M} \cdot (\pi' - \pi^*) \in \text{ri}(\mathcal{C}^\circ) \right\}$. Then, by convexity of $\left\{ \tilde{M} \in \mathcal{M} : \exists z \in \mathcal{C} : z^\top \tilde{M} \cdot (\pi - \pi^*) > 0 \right\}$ there exists $M'' \in \left\{ \tilde{M} \in \mathcal{M} : \tilde{M} \cdot (\pi' - \pi^*) \in \text{bd}(\mathcal{C}^\circ) \right\}$ such that $|z^\top M_k - z^\top M'_k| \geq |z^\top M_k - z^\top M''_k|, \forall z \in \mathcal{C}$. Since $d_{\text{KL}}(z^\top M, \cdot)$ is decreasing, we have: $d_{\text{KL}}(z^\top M_k, z^\top M'_k) \geq d_{\text{KL}}(z^\top M_k, z^\top M''_k)$.

Using the above arguments we see that the minimum argument of $\sum_k w_k d_{\text{KL}}(z^\top M', z^\top M'')$ is such that $M'' \in \left\{ \tilde{M} \in \mathcal{M} : \tilde{M} \cdot (\pi - \pi^*) \in \text{bd}(\mathcal{C}^\circ) \right\}$.

The optimization problem now becomes:

$$\begin{aligned} & \sup_{w \in \Pi} \inf_{\tilde{M} \in \Lambda_{\pi^*}(M)} \inf_{z \in \mathcal{C}} \sum_k w_k d_{\text{KL}}(z^\top M_k, z^\top \tilde{M}_k) \\ &= \sup_{w \in \Delta^K} \inf_{\pi \in \Pi \setminus \pi^*} \min_{\tilde{M} \in \partial \Lambda_{\pi^*}(M)} \inf_{z \in \mathcal{C}} \sum_{k=1}^K w_k d_{\text{KL}}(z^\top M_k, z^\top \tilde{M}_k), \end{aligned}$$

where

$$\begin{aligned} \partial \Lambda_{\pi^*}(M) &\triangleq \cup_{\Pi \setminus \pi^*} \left\{ \tilde{M} \in \mathcal{M} : \exists z \in \mathcal{C}, z^\top \tilde{M}(\pi - \pi^*) = 0 \right\} \\ &= \cup_{\Pi \setminus \pi^*} \left\{ \tilde{M} \in \mathcal{M} : \exists z \in \mathcal{C}, \langle \text{vect}(z^\top(\pi - \pi^*)), \text{vect}(\tilde{M}) \rangle = 0 \right\}. \end{aligned} \quad (11)$$

Finally, to accommodate for multiple optimal policies π^* , the inner minimisation problem becomes

$$\sup_{w \in \Delta^K} \inf_{\substack{\pi \in \Pi \setminus \pi^* \\ \pi^* \in \Pi^*(M)}} \min_{\tilde{M} \in \partial \Lambda_{\pi^*}(M)} \inf_{z \in \mathcal{C}} \sum_{k=1}^K w_k d_{\text{KL}}(z^\top M_k, z^\top \tilde{M}_k)$$

This concludes the proof. □

B.2 Lower Bound for Gaussians: Proof of Theorem 3.2

Proof.

Step 1. Simplifying the KL-divergence for a Gaussian bandit instance with identical variance across all objectives yields

$$\mathcal{V}_{\mathcal{C}}(w, M) = \min_{\tilde{M} \in \partial \Lambda_{\pi^*}(M)} \min_{z \in \mathcal{C}} \sum_{k=1}^K w_k \sum_{\ell=1}^L (z^{(\ell)})^2 \frac{(\mu_k^{(\ell)} - \tilde{M}_k^{(\ell)})^2}{2\sigma_\ell^2}. \quad (12)$$

Recalling that due to the projection lemma, the $\tilde{M}$ achieving the minimum satisfies

$$z^\top \sum_{k=1}^K \tilde{M}_k^\top (\pi_k^* - \pi_k) = 0, \quad \forall z \in \mathcal{C} \quad (13)$$

Now, we formulate the Lagrangian of (12) with dual variables β for (13) as

$$\begin{aligned} & \mathcal{L}(w, M, \tilde{M}, \gamma, \beta) \\ &= \sum_{k=1}^K w_k \sum_{\ell=1}^L (z^{(\ell)})^2 \left(\frac{\mu_k^{(\ell)} - \tilde{M}_k^{(\ell)}}{\sqrt{2}\sigma_\ell} \right)^2 + \beta z^\top \tilde{M} (\pi^* - \pi) \\ &= \sum_{k=1}^K w_k \sum_{\ell=1}^L (z^{(\ell)})^2 \left(\frac{\mu_k^{(\ell)} - \tilde{M}_k^{(\ell)}}{\sqrt{2}\sigma_\ell} \right)^2 + \beta z^\top \tilde{M} (\pi^* - \pi) \end{aligned} \quad (14)$$

Step 2. Taking the derivative w.r.t. $\tilde{M}$, we have

$$\frac{\partial \mathcal{L}}{\partial \tilde{M}_k^{(\ell)}} = w_k (z^{(\ell)})^2 \left(\frac{-2}{2\sigma_\ell^2} \right) (\mu_k^{(\ell)} - \tilde{M}_k^{(\ell)}) + \beta z^{(\ell)} (\pi^* - \pi)_k,$$

and setting it to zero, we get

$$\begin{aligned} & w_k (z^{(\ell)})^2 \left(\frac{2}{2\sigma_\ell^2} \right) (\mu_k^{(\ell)} - \tilde{M}_k^{(\ell)}) = \beta z^{(\ell)} (\pi^* - \pi)_k \\ \implies \tilde{M}_k^{(\ell)} &= \mu_k^{(\ell)} - \frac{2\sigma_\ell^2 \beta (z^{(\ell)} (\pi^* - \pi)_k)}{2w_k (z^{(\ell)})^2} = \mu_k^{(\ell)} - \frac{\sigma_\ell^2 \beta (\pi^* - \pi)_k}{w_k z^{(\ell)}}. \end{aligned} \quad (15)$$

The last equality holds for any $z^{(\ell)} \neq 0$. Therefore, the Lagrangian now becomes

$$\begin{aligned} \mathcal{L}(w, M, \beta) &= \sum_{k=1}^K w_k \sum_{\ell=1}^L (z^{(\ell)})^2 \left(\frac{\mu_k^{(\ell)} - \tilde{M}_k^{(\ell)}}{\sqrt{2}\sigma_\ell} \right)^2 + \beta \sum_{i=1}^N \lambda_i \sum_{\ell=1}^L v_i^{(\ell)} \sum_{k=1}^K \tilde{M}_k^{(\ell)} (\pi^* - \pi)_k \\ &= \sum_{k=1}^K w_k \sum_{\ell=1}^L (z^{(\ell)})^2 \frac{(\pi^* - \pi)_k^2}{(z^{(\ell)})^2 w_k^2} \frac{\beta^2 \sigma_\ell^2}{2} + \beta \sum_{\ell=1}^L z^{(\ell)} \sum_{k=1}^K (\pi^* - \pi)_k \left(\mu_k^{(\ell)} - \beta \sigma_\ell^2 \frac{(\pi^* - \pi)_k}{z^{(\ell)} w_k} \right) \\ &= -\frac{\beta^2}{2} \sum_{k=1}^K \sum_{\ell=1}^L \sigma_\ell^2 \frac{(\pi^* - \pi)_k^2}{w_k} + \beta \sum_{\ell=1}^L \sum_{k=1}^K z^{(\ell)} (\pi^* - \pi)_k \mu_k^{(\ell)} \end{aligned}$$

Step 3. By taking the derivative with respect to β , we have

$$\frac{\partial \mathcal{L}}{\partial \beta} = -\beta \sum_{k=1}^K \sum_{\ell=1}^L \sigma_\ell^2 \frac{(\pi^* - \pi)_k^2}{w_k} + \sum_{\ell=1}^L \sum_{k=1}^K z^{(\ell)} (\pi^* - \pi)_k \mu_k^{(\ell)},$$

and setting it to zero, leads to:

$$\beta = \frac{\sum_{\ell=1}^L \sum_{k=1}^K z^{(\ell)} (\pi^* - \pi)_k \mu_k^{(\ell)}}{\sum_{k=1}^K \sum_{\ell=1}^L \sigma_\ell^2 \frac{(\pi^* - \pi)_k^2}{w_k}} = \frac{z^\top M \Delta}{\sigma_o^2 \|\Delta\|_{\text{Diag}(1/w)}^2}, \quad (16)$$

where $\sigma_o^2 \triangleq \sum_{\ell=1}^L \sigma_\ell^2$, and $\Delta \triangleq \pi^* - \pi$.

From (15), excluding for the origin lying within the cone, we get:

$$\begin{aligned} \tilde{M}_k^{(\ell)} &= \mu_k^{(\ell)} - \beta \sigma_\ell^2 \frac{(\pi^* - \pi)_k}{z^\ell w_k} \\ &= \mu_k^{(\ell)} - \frac{\sigma_\ell^2}{z^\ell} \frac{\Delta_k}{w_k} \frac{z^\top M \Delta}{\sigma_o^2 \|\Delta\|_{\text{Diag}(1/w)}^2} \end{aligned}$$

Finally, the Lagrangian from (14) leads to

$$\begin{aligned} \mathcal{L}(w, M) &= -\frac{1}{2} \left(\frac{z^\top M \Delta}{\sigma_o^2 \|\Delta\|_{\text{Diag}(1/w)}^2} \right)^2 \sigma_o^2 \|\Delta\|_{\text{Diag}(1/w)}^2 + \frac{(z^\top M \Delta)^2}{\sigma_o^2 \|\Delta\|_{\text{Diag}(1/w)}^2} \\ &= \frac{(z^\top M \Delta)^2}{2\sigma_o^2 \|\Delta\|_{\text{Diag}(1/w)}^2}. \end{aligned}$$

Thus, the characteristic time inverse is given by,

$$\max_{w \in \Delta^K} \inf_{\substack{\pi \in N(\pi^*) \\ \pi^* \in \Pi^*(M)}} \min_{z \in \mathcal{C} \setminus \{0\}} \frac{(z^\top M \Delta)^2}{2\sigma_o^2 \|\Delta\|_{\text{Diag}(1/w)}^2} = \inf_{\substack{\pi \in N(\pi^*) \\ \pi^* \in \Pi^*(M)}} \min_{z \in \mathcal{C} \setminus \{0\}} \frac{(z^\top M \Delta)^2}{2\sigma_o^2 \|\Delta\|_2^2}.$$

□

B.3 Proof of Theorem 4.1

This proof follows directly from Theorem 3.1 in Balas (1985). Recall that the set $\mathcal{F}$ is given by:

$$\mathcal{F} \triangleq \cup_{\Pi \setminus \{\pi^*\}} \left\{ \tilde{M} \in \mathcal{M} : \langle \text{vect}(z^\top (\pi - \pi^*)), \text{vect}(\tilde{M}) \rangle = 0 \right\}$$

Any $z \in \mathcal{C}$, we have $z = \sum_i \alpha_i v_i$. Rewriting, every hyperplane in $\mathcal{F}$ as $P_\pi = \left\{ \tilde{M} \in \mathcal{M} \mid \langle \text{vect}(\sum_i \alpha_i v_i^\top \pi), \text{vect}(\tilde{M}) \rangle = \sum_i \alpha_i v_i^\top \pi^* \right\}$. Then, by Theorem 3.1 in Balas (1985), $\mathcal{C}(\mathcal{F})$ is given by:

$$\mathcal{C}(\mathcal{F}) = \left\{ \gamma^\top \text{vect}(\tilde{M}) \geq \gamma_0, \gamma = \sum_i u_i \alpha_i \text{vect}(v_i^\top (\pi - \pi^*)) \right. \\ \left. \gamma_0 \leq u_i \sum_i \alpha_i v_i^\top \pi^*, \tilde{M} \in \mathcal{M} \right\}$$

B.4 Proof of Theorem 4.2

Recall that:

$$\bar{\mathcal{V}}_{\mathcal{C}}(w, M) \triangleq \min_{\tilde{M} \in \text{ch}(\partial \Lambda_{\pi^*}(M))} \inf_{z \in \mathcal{C}} \sum_{k=1}^K w_k d_{\text{KL}}(z^{\top} M, z^{\top} \tilde{M})$$

$$\bar{w}^*(M) \triangleq \arg \max_{w \in \Delta^K} \inf_{\substack{\pi \in \Pi \setminus \pi^* \\ \pi^* \in \Pi^*(M)}} \min_{\tilde{M} \in \text{ch}(\partial \Lambda_{\pi^*}(M))} \min_{z \in \mathcal{C}} \sum_{k=1}^K w_k d_{\text{KL}}(z^{\top} M, z^{\top} \tilde{M})$$

- For (1) and (2) observe that $(z, M) \rightarrow z^{\top} M$ and $(z, M, \tilde{M}) \rightarrow d_{\text{KL}}(z^{\top} M, z^{\top} \tilde{M})$ are continuous maps for all $(z, M) \in \mathcal{C} \times \mathcal{M}$ and $(z, M, \tilde{M}) \in \mathcal{C} \times \mathcal{M} \times \text{ch}(\partial \Lambda_{\pi^*}(M))$. Further, $\sum_k w_k d_{\text{KL}}(z^{\top} M, z^{\top} \tilde{M})$ is continuous in all its elements. Fix a sequence $(w_t, z_t, M_t) \in \Pi \times \mathcal{C} \times \mathcal{M}$ such that $(w_t, z_t, M_t) \rightarrow (w, z, M)$. For any ϵ , $\exists t' \geq 1$ such that $\|(w_t, z_t, M_t) - (w, z, M)\| \leq \epsilon \forall t \geq t'$. Further, $\text{ch}(\Lambda_{\pi^*}(M_t)) \rightarrow \text{ch}(\Lambda_{\pi^*}(M))$. Therefore, for every ϵ' , $\exists t'' \geq 1$ such that $\forall t \geq t''$ we

$$\left| \sum_k w_{k,t} d_{\text{KL}}(z_t^{\top} M_t, z_t^{\top} \tilde{M}_t) - \sum_k w_k d_{\text{KL}}(z^{\top} M, z_t^{\top} \tilde{M}_t) \right| \leq \epsilon' \forall \tilde{M}_t \in \mathbb{R}^{K \times L}$$

Taking $t \geq \max\{t', t''\}$, we have:

$$\begin{aligned} & \left| \inf_{\tilde{M} \in \partial \Lambda_{\pi^*}(M)} \inf_{z \in \mathcal{C}} \sum_k w_{k,t} d_{\text{KL}}(z_t^{\top} M_t, z_t^{\top} \tilde{M}_t) - \inf_{\tilde{M} \in \partial \Lambda_{\pi^*}(M)} \inf_{z \in \mathcal{C}} \sum_k w_k d_{\text{KL}}(z^{\top} M, z_t^{\top} \tilde{M}_t) \right| \\ & \leq \left| \inf_{\tilde{M} \in \partial \Lambda_{\pi^*}(M)} \inf_{z \in \mathcal{C}} \sum_k w_{k,t} d_{\text{KL}}(z_t^{\top} M_t, z_t^{\top} \tilde{M}_t) - \sum_k w_k d_{\text{KL}}(z^{\top} M, z_t^{\top} \tilde{M}_t) \right| \\ & \leq \epsilon' \end{aligned}$$

- For (3), we define $f(w, M) = \inf_{\tilde{M} \in \text{ch}(\partial \Lambda_{\pi^*}(M))} \inf_{z \in \mathcal{C}} \sum_k w_k d_{\text{KL}}(z^{\top} M, z^{\top} \tilde{M})$ and $C(w) = \Pi$. Then, from Berge's Theorem (Theorem F.1 in Appendix), we get $w^*(M)$ is upper-hemicontinuous.
- For (4), the convexity of $w^*(M)$ follows since the optimal solution

$$\max_{w \in \Pi} \inf_{\tilde{M} \in \text{ch}(\partial \Lambda_{\pi^*}(M))} \inf_{z \in \mathcal{C}} \sum_k w_k d_{\text{KL}}(z^{\top} M, z^{\top} \tilde{M})$$

is concave for any given π and π^* .

C Proof of the Stopping Time

C.1 Proof of Lemma 4.1

The proof follows by showing that $\inf_{z \in \mathcal{C}} \sum_k N_{k,t} d_{\text{KL}}(z^\top \hat{M}_{k,t}, z^\top M_k)$ is an appropriate stochastic process and can be bounded using the mixture of martingales technique of Kaufmann and Koolen (2021).

To this end, given a $z \in \mathcal{C}$, we define the random variable as

$$X_k(t) \triangleq \sum_k \max\{0, N_{k,t} d_{\text{KL}}(z_{\text{inf}}^\top \hat{M}_{k,t}, z_{\text{inf}}^\top M_k) - 3 \ln(1 + \ln N_{k,t})\},$$

where $z_{\text{inf}} \triangleq \arg \inf_{z \in \mathcal{C}} \sum_k N_{k,t} d_{\text{KL}}(z^\top \hat{M}_{k,t}, z^\top M_k)$

Since we assume $M_{k,\ell}$ belongs to exponential family of distributions, for any given $z_{\text{inf}} \neq \mathbf{0}$, $z_{\text{inf}}^\top M_k$ being a non-degenerate linear transform also belongs to the exponential family.

Now, plugging in $X_k(t)$ in Theorem 7 of (Kaufmann and Koolen, 2021) yields

$$\mathbb{P} \left[\exists t \in \mathbb{N} : \sum_{k \in [K]} N_{k,t} d_{\text{KL}}(z_{\text{inf}}^\top \hat{M}_{k,t}, z_{\text{inf}}^\top M_k) \geq \sum_{k \in [K]} 3 \ln(1 + \ln(N_{k,t})) + K \mathcal{T} \left(\frac{\ln(\frac{1}{\delta})}{K} \right) \right] \leq \delta.$$

Here, $\mathcal{T} : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ is such that

$$\mathcal{T}(x) \triangleq 2\tilde{h}_{3/2} \left(\frac{h^{-1}(1+x) + \ln(2\zeta(2))}{2} \right) \quad (17)$$

with

$$\forall u \geq 1, \quad h(u) = u - \ln(u) \quad (18)$$

$$\forall z \in [1, e], \forall x \geq 0, \quad \tilde{h}_z(x) = \begin{cases} \exp\left(\frac{1}{h^{-1}(x)}\right) h^{-1}(x) & \text{if } x \geq h^{-1}\left(\frac{1}{\ln(z)}\right) \\ z(x - \ln(\ln(z))) & \text{else} \end{cases}, \quad (19)$$

and $\zeta(2) = \sum_{n=1}^{\infty} n^{-2}$.

C.2 Proof of Theorem 4.3

First, we prove the following lemma required to proceed with Theorem 4.3.

Lemma C.1. For any $k = 1, 2, \dots, K$, let $1 \leq t_k \leq t$. Let $\eta > 0$ and define the event:

$$C \triangleq \cap_{k \in [K]} C_k \triangleq \cap_{k \in [K]} \{t_k \leq N_{k,t} \leq (1 + \eta)t_k\}$$

and let $\mathbb{1}_C$ indicate whether the event holds. For $\rho \geq (1 + \eta)K$, for all $z \in \mathcal{C}$ we have:

$$\mathbb{P} \left[\mathbb{1}_C \sum_{k \in [K]} N_{k,t} d_{\text{KL}}(z^\top \hat{M}_{k,t}, z^\top M_k) \geq \rho \right] \leq \left(\frac{\rho e}{K} \right)^K \exp \left(\frac{-\rho}{1 + \eta} \right).$$

Proof. Fix $\zeta \in \mathbb{R}_+^K$ and $t \geq 0$. Define $m_{k,t}$ such that:

$$m_{k,t} = \begin{cases} m, & \text{if } \exists 0 \leq m \leq z^\top M_k, \text{ s.t. } t d_{\text{KL}}(m, z^\top M_k) = \zeta_k \\ 0, & \text{otherwise} \end{cases}$$

By monotonicity of $t d_{\text{KL}}(\cdot, z^\top M_k)$, $t \rightarrow m_{k,t}$ is increasing. With $t = N_{k,t}$, we have that

$$N_{k,t} d_{\text{KL}}(m_{k,N_{k,t}}, z^\top M_k) = \zeta_k \leq N_{k,t} d_{\text{KL}}(z^\top \hat{M}_{k,t}, z^\top M_k), \implies z^\top \hat{M}_{k,t} \stackrel{(a)}{\leq} m_{k,N_{k,t}} \stackrel{(b)}{\leq} m_{k,(1+\eta)t_k},$$

where (a) follows from monotonicity of $d_{\text{KL}}(\cdot, \cdot)$ and (b) follows from monotonicity of $m_{k,t}^{(\ell)}$.

With $t_k d_{\text{KL}}(z^\top \hat{M}_{k,t_k(1+\eta)}, z^\top M_k) = \frac{\zeta_k}{1+\eta}$ and non-negativity of $d_{\text{KL}}(\cdot, \cdot)$ we have:

$$\begin{aligned} & \mathbb{P}\left(\bigcap_{k \in [K]} \left\{ \mathbb{1}_{C_k} N_{k,t} d_{\text{KL}}(z^\top \hat{M}_{k,t}, z^\top M_k) \geq \zeta_k \right\}\right) \\ & \leq \mathbb{P}\left(\bigcap_{k \in [K]} \left\{ z^\top \hat{M}_{k,t} \leq m_{k,N_{k,t}, C_k} \right\}\right) \\ & \leq \mathbb{P}\left(\bigcap_{k \in [K]} \left\{ z^\top \hat{M}_{k,t} \leq m_{k,(1+\eta)t_k, C_k} \right\}\right) \\ & \leq \mathbb{P}\left(\bigcap_{k \in [K]} \left\{ z^\top \hat{M}_{k,t} \leq m_{k,(1+\eta)t_k, C_k} \right\}\right) \\ & \stackrel{(a)}{\leq} \exp\left(-\sum_{k \in [K]} t_k d_{\text{KL}}(m_{k,(1+\eta)t_k}, z^\top M_k)\right) \\ & = \exp\left(-\sum_{k \in [K]} \frac{\zeta_k}{1+\eta}\right), \end{aligned}$$

where (a) follows from Lemma F.2.

Using Lemma F.3, with $Z_k = N_{k,t} d_{\text{KL}}(z^\top \hat{M}_{k,t}, z^\top M_k)$ and $a = \frac{1}{(1+\eta)}$, we have that:

$$\mathbb{P}\left[\mathbb{1}_C \sum_{k \in [K]} N_{k,t} d_{\text{KL}}(z^\top \hat{M}_{k,t}, z^\top M_k) \geq \rho\right] \leq \left(\frac{\rho e}{K}\right)^K \exp\left(\frac{-\rho}{1+\eta}\right)$$

This concludes the proof. $\square$

Now, we provide the proof of Theorem 4.3.

Proof. Let us define $D = \lceil \frac{\log(t)}{\log(1+\eta)} \rceil$ and set $\mathcal{D} = \{1, 2, \dots, D\}^K$. Let us define

$$\begin{aligned} A &= \left\{ \sum_{k \in [K]} N_{k,t} d_{\text{KL}}(z^\top \hat{M}_{k,t}, z^\top M_k) \geq \rho \right\} \\ B_d &= \bigcap_{k=1}^K \left\{ (1+\xi)^{d_k-1} \leq N_{k,t} \leq (1+\xi)^{d_k} \right\} \end{aligned}$$

We have $A = \bigcup_{d \in \mathcal{D}} (A \cap B_d)$, hence $\mathbb{P}(A) \leq \sum_{d \in \mathcal{D}} \mathbb{P}(A \cap B_d)$.

For $\eta = \frac{1}{\rho-1}$ and $\rho \geq (1+\eta)K$, we get $\rho \geq K+1$.

Now, we use Lemma C.1 with $\eta = \frac{1}{\rho-1}$ and $\bar{t}_k = (1+\eta)^{d_k-1}$ to obtain for all $d \in \mathcal{D}$:

$$\mathbb{P}(A \cap B_d) \leq \left(\frac{\rho e}{K}\right)^K \exp\left(\frac{-\rho}{(1+\eta)}\right)$$

By a union bound on $\mathcal{D}$, we have:

$$\mathbb{P}(A) \leq \left(\frac{D\rho e}{K}\right)^K \exp\left(\frac{-\rho}{1+\eta}\right)$$

Noting that $D = \lceil \frac{\log(t)}{\log(1+\eta)} \rceil$ and $\eta = \frac{1}{\rho-1}$, we get:

$$\mathbb{P}(A) \leq \exp(-\rho) \left(\frac{\rho \lceil \rho \log(t) \rceil}{K}\right)^K e^{K+1}.$$

$\square$

D Proofs for Sample Complexity Upper Bound

D.1 Pairwise Concentration Bounds

Lemma D.1 (Pairwise concentration (Proof of Theorem 5.1)). *Consider the event:*

$$\mathcal{E}_t \triangleq \cap_{i \in [K]} \cap_{j \neq i} \{L_{i,j}(t) \leq z^\top \mu_i - z^\top \mu_j \leq U_{i,j}(t)\} \quad (20)$$

where $L_{ij}(t) = z^\top (\hat{\mu}_{i,t} - \hat{\mu}_{j,t}) - \beta_{ij}(t)$ and $U_{ij}(t) = z^\top (\hat{\mu}_{i,t} - \hat{\mu}_{j,t}) + \beta_{ij}(t)$, and $\beta_{ij}(t)$ is defined as

$$\beta_{ij}^2(t) \triangleq 4\|z\|_1^2 \left(h\left(\frac{\log(\frac{K_1}{\delta})}{2}\right) + \sum_{a \in \{i,j\}} \log(4 + \log(N_a(t))) \right) \left(\sum_{a \in \{i,j\}} \frac{1}{N_a(t)} \right).$$

Here, $K_1 \triangleq \frac{K(K-1)}{2}$, $h(\cdot) \approx x + \log(1+x)$. Then, we get

$$\mathbb{P}(\cap_{t=1}^{\infty} \mathcal{E}_t) \geq 1 - \delta.$$

Proof. We have the following:

$$\begin{aligned} \mathcal{E}_t &= \cap_{(i,j)} \{L_{i,j} \leq z^\top \mu_i - z^\top \mu_j \leq U_{i,j}\} \\ &= \cap_{(i,j)} \{|z^\top (\hat{\mu}_{i,t} - \hat{\mu}_{j,t}) - z^\top (\mu_i - \mu_j)| \leq \beta_{ij}(t)\} \end{aligned}$$

where, $(i, j) \in [K] \times [K]$ is the set of arm pairs. By a union bound, we have the following:

$$\begin{aligned} \mathbb{P}(\bar{\mathcal{E}}_t) &= \mathbb{P}(\exists t \geq 1 : \bar{\mathcal{E}}_t \text{ holds}) \\ &= \mathbb{P}(\exists t \geq 1 : |z^\top (\hat{\mu}_{i,t} - \hat{\mu}_{j,t}) - z^\top (\mu_i - \mu_j)| \geq \beta_{ij}(t)) \\ &\leq \mathbb{P}(\exists t \geq 1 : |z^\top (\hat{\mu}_{i,t} - \mu_i) - z^\top (\hat{\mu}_{j,t} - \mu_j)| \geq \beta_{ij}(t)) \\ &\stackrel{(a)}{\leq} \sum_{(i,j)} \frac{\delta}{K(K-1)} \\ &= \delta \end{aligned}$$

(a) follows from

1. $z^\top (\hat{\mu}_{i,t} - \mu_i)$ is a $\|z\|_1$ sub-Gaussian as $\hat{\mu}_{i,t} - \mu_i$ is 1-sub-Gaussian, and
2. Lemma 7 of (Kone et al., 2023a) that states that for two 1-sub-Gaussian and centred random variables X and Y , the following holds true with probability $1 - \delta$.

$$\left| \frac{1}{p} \sum_i X_i - \frac{1}{q} \sum_i Y_i \right| \leq 2 \sqrt{\left(h\left(\frac{\log(\frac{1}{\delta})}{2}\right) + \log \log(e^4 p) + \log \log(e^4 q) \right) \left(\frac{1}{p} + \frac{1}{q} \right)},$$

given $h(x) \approx x + \ln x$.

□

We now show that the Pareto fronts under the metric d_p .

Lemma D.2. $(\mathcal{Z}, d_p)$ is a complete metric space.

Proof. From Definition 5.2, for two Pareto fronts $\mathcal{P}_1, \mathcal{P}_2 \in \mathcal{Z}$, we have that:

$$d_p(\mathcal{P}_1, \mathcal{P}_2) \triangleq \max \left\{ \sup_{k \in \mathcal{P}_1} d(k, \mathcal{P}_2), \sup_{k \in \mathcal{P}_2} d(k, \mathcal{P}_1) \right\}$$

where,

$$d(k, \mathcal{P}) = \inf_{k' \in \mathcal{P}} \max \left\{ 0, \sup_{z \in \mathcal{C} \cap \mathbb{B}(1)} z^\top (\mu_{k'} - \mu_k) \right\}$$

1. We first show that $d_p(\mathcal{P}_1, \mathcal{P}_2)$ is a metric. Let $\mathcal{P}_1, \mathcal{P}_2 \in \mathcal{Z}$. To show that d_p is a metric, we show that:

(a) Symmetry: $d_p(\mathcal{P}_1, \mathcal{P}_2)$ is symmetric by definition

(b) Triangle Inequality: We show that $d_p(\mathcal{P}_1, \mathcal{P}_3) \leq d_p(\mathcal{P}_1, \mathcal{P}_2) + d_p(\mathcal{P}_2, \mathcal{P}_3)$.

$$d_p(\mathcal{P}_1, \mathcal{P}_3) = \max \left\{ \max_{k \in \mathcal{P}_1} \min_{k' \in \mathcal{P}_3} \mu_{k'}(X_3) - \mu_k(X_1), \max_{k \in \mathcal{P}_3} \min_{k' \in \mathcal{P}_1} \mu_{k'}(X_1) - \mu_k(X_3) \right\}$$

We have that:

$$\begin{aligned} & \max_{k \in \mathcal{P}_1} \min_{k' \in \mathcal{P}_3} \mu_{k'}(X_3) - \mu_k(X_1) \\ & \leq \max_{k \in \mathcal{P}_1} \min_{k' \in \mathcal{P}_3} \mu_{k'}(X_3) + \min_{k'' \in \mathcal{P}_2} \mu_{k''}(X_2) - \max_{k'' \in \mathcal{P}_2} \mu_{k''}(X_2) - \mu_k(X_1) \\ & \leq \max_{k'' \in \mathcal{P}(X_2)} \min_{k' \in \mathcal{P}_3} \mu_{k'}(X_3) - \mu_{k''}(X_2) + \max_{k \in \mathcal{P}_1} \min_{k'' \in \mathcal{P}(X_2)} \mu_{k''}(X_2) - \mu_k(X_1) \end{aligned}$$

Using a similar argument:

$$\max_{k \in \mathcal{P}_3} \min_{k' \in \mathcal{P}_1} \mu_{k'}(X_1) - \mu_k(X_2) \leq \max_{k'' \in \mathcal{P}(X_2)} \min_{k' \in \mathcal{P}_1} \mu_{k'}(X_1) - \mu_{k''}(X_2) + \max_{k \in \mathcal{P}_3} \min_{k'' \in \mathcal{P}(X_2)} \mu_{k''}(X_2) - \mu_k(X_3)$$

Noting that for any positive numbers a, b, c, d , $\max\{a + b, c + d\} = \max\{a + c, b + d\}$, we have:

$$\begin{aligned} d_p(\mathcal{P}_1, \mathcal{P}_3) & \leq \max \left\{ \max_{k' \in \mathcal{P}(X_2)} \min_{k' \in \mathcal{P}_3} \mu_{k'}(X_3) - \mu_{k''}(X_2) + \max_{k \in \mathcal{P}_1} \min_{k'' \in \mathcal{P}(X_2)} \mu_{k''}(X_2) - \mu_k(X_1), \right. \\ & \quad \left. \max_{k'' \in \mathcal{P}(X_2)} \min_{k' \in \mathcal{P}_1} \mu_{k'}(X_1) - \mu_{k''}(X_2) + \max_{k \in \mathcal{P}_3} \min_{k'' \in \mathcal{P}(X_2)} \mu_{k''}(X_2) - \mu_k(X_3) \right\} \\ & = \max \left\{ \max_{k' \in \mathcal{P}(X_2)} \min_{k' \in \mathcal{P}_1} \mu_{k'}(X_1) - \mu_{k''}(X_2) + \max_{k \in \mathcal{P}_1} \min_{k'' \in \mathcal{P}(X_2)} \mu_{k''}(X_2) - \mu_k(X_1), \right. \\ & \quad \left. \max_{k'' \in \mathcal{P}(X_2)} \min_{k' \in \mathcal{P}_3} \mu_{k'}(X_3) - \mu_{k''}(X_2) + \max_{k \in \mathcal{P}_3} \min_{k'' \in \mathcal{P}(X_2)} \mu_{k''}(X_2) - \mu_k(X_3) \right\} \\ & = d_p(\mathcal{P}_1, \mathcal{P}_2) + d_p(\mathcal{P}_2, \mathcal{P}_3) \end{aligned}$$

(c) We now show that $d_p(\mathcal{P}_1, \mathcal{P}_2) = 0 \iff \mathcal{P}_1 = \mathcal{P}_2$. The implication $\mathcal{P}_1 = \mathcal{P}_2 \implies d_p(\mathcal{P}_1, \mathcal{P}_2) = 0$ is immediate. For the other side, note that by Definition 5.2, we have:

$$\begin{aligned} & d_p(\mathcal{P}_1, \mathcal{P}_2) = 0 \\ \implies & \sup_{k \in \mathcal{P}_1} \Delta(k, \mathcal{P}_2) = 0 \text{ and } \sup_{k \in \mathcal{P}_2} \Delta(k, \mathcal{P}_1) = 0 \end{aligned}$$

Further, $\sup_{k \in \mathcal{P}_1} \Delta(k, \mathcal{P}_2) = 0$ implies:

$$\forall k \in \mathcal{P}_1, k \not\leq_C k', k' \in \mathcal{P}_2 \iff \forall k \in \mathcal{P}_1, k \in \mathcal{P}_2$$

A similar argument using $\sup_{k \in \mathcal{P}_2} \Delta(k, \mathcal{P}_1) = 0$ implies that $\forall k \in \mathcal{P}_2, k \not\leq_C k', k' \in \mathcal{P}_1$.

2. We now show that $\mathcal{Z}$ is compact under the metric d_p . Consider a sequence of Pareto fronts $\mathcal{P}_1, \mathcal{P}_2, \dots, \mathcal{P}_n \in \mathcal{Z}$ and $\mathcal{P}$ be the candidate for limiting Pareto front.

- Boundedness of $\mathcal{P}$ is immediate.
- $\mathcal{P}_n \rightarrow \mathcal{P}$, therefore, $\forall \epsilon > 0, \exists N(\epsilon)$ s.t. $\forall n > N(\epsilon)$ and $d_p(\mathcal{P}_n, \mathcal{P}) < \epsilon$. Let μ_k be a limit point of $\mathcal{P}$, i.e., $\exists$ a sequence $\mu_{k,n} \in \mathcal{P}$ such that $\mu_{k,n} \rightarrow \mu_k$. Since $d_p(\mathcal{P}_n, \mathcal{P}) \rightarrow 0$ for each $\mu_{k,n} \in \mathcal{P}$ there exists $\mu_{k,n,m} \in \mathcal{P}_n$ s.t. $\mu_{k,n,m} \rightarrow \mu_{k,n}$. Using a diagonalization argument, we can obtain a subsequence $\mu_{k,n,m} \rightarrow \mu_k$.
- Since $\mathcal{P}_n$ is compact, μ_k must lie in $\mathcal{P}$ and therefore, $\mathcal{P}$ is closed.

□

D.2 Concentration to the Pareto Front

Lemma D.3. *There exists constants $C > 0$ such that:*

$$\mathbb{P}(\bar{\mathcal{G}}_T) \leq 2K^2 \frac{1}{1 - \exp(-C)} T \exp(-CT^{1/8}),$$

where $\mathcal{G}_T = \cap_{t=h(T)}^T \left\{ d_P(\hat{\mathcal{P}}_t, \mathcal{P}^*) \leq \epsilon \right\}$.

Proof. We then have that:

$$\begin{aligned}\mathbb{P}\left(d_{\mathcal{P}}\left(\hat{\mathcal{P}}_t, \mathcal{P}^*\right) \geq \epsilon\right) &= \mathbb{P}\left(\max \left\{d_{\mathcal{P}}\left(\hat{\mathcal{P}}_t, \mathcal{P}^*\right), d_{\mathcal{P}}\left(\mathcal{P}^*, \hat{\mathcal{P}}_t\right)\right\} \geq \epsilon\right) \\ &\leq \mathbb{P}\left(d_{\mathcal{P}}\left(\hat{\mathcal{P}}_t, \mathcal{P}^*\right) \geq \epsilon\right) + \mathbb{P}\left(d_{\mathcal{P}}\left(\mathcal{P}^*, \hat{\mathcal{P}}_t\right) \geq \epsilon\right)\end{aligned}$$

Focusing on the first term we have:

$$\begin{aligned}d_{\mathcal{P}}\left(\hat{\mathcal{P}}_t, \mathcal{P}^*\right) &= \inf_{k \in \hat{\mathcal{P}}_t} \sup_{k' \in \mathcal{P}^*} \max \left\{0, \max_{z \in \mathcal{C} \cap \mathbb{B}(1)} z^{\top}\left(M_{k'} - \hat{M}_{k,t}\right)\right\} \\ &\stackrel{(a)}{=} \min_{k \in \hat{\mathcal{P}}_t} \max_{k' \in \mathcal{P}^*} \max \left\{0, \max_{z \in \mathcal{C} \cap \mathbb{B}(1)} z^{\top}\left(M_{k'} - \hat{M}_{k',t} + \hat{M}_{k',t} - \hat{M}_{k,t}\right)\right\} \\ &\stackrel{(b)}{\leq} \max_{k' \in \mathcal{P}^*} \max \left\{0, \max_{z \in \mathcal{C} \cap \mathbb{B}(1)} z^{\top}\left(M_{k'} - \hat{M}_{k',t}\right)\right\} \\ &\quad + \max_{k' \in \mathcal{P}^*} \max \left\{0, \max_{z \in \mathcal{C} \cap \mathbb{B}(1)} z^{\top}\left(\hat{M}_{k',t} - \hat{M}_{k,t}\right)\right\}\end{aligned}$$

Recall that $\bar{\mathcal{G}}_T = \cup_{t=h(T)}^T \left\{d_{\mathcal{P}}\left(\hat{\mathcal{P}}_t, \mathcal{P}^*\right) \geq \epsilon\right\}$, then using a union bound, we have:

$$\begin{aligned}\mathbb{P}\left(\bar{\mathcal{G}}_T\right) &\leq \sum_{t=h(T)}^T \mathbb{P}\left(d_{\mathcal{P}}\left(\hat{\mathcal{P}}_t, \mathcal{P}^*\right) \geq \epsilon\right) \\ &\leq \sum_{t=h(T)}^T \left[\sum_{(k,k')} \mathbb{P}\left(z^{\top}\left(\hat{M}_{k,t} - \hat{M}_{k',t}\right) \leq z^{\top}\left(M_k - M_{k'}\right) - \xi\right) \right. \\ &\quad \left. + \mathbb{P}\left(z^{\top}\left(\hat{M}_{k,t} - \hat{M}_{k',t}\right) \geq z^{\top}\left(M_k - M_{k'}\right) + \xi\right) \right].\end{aligned}$$

Let T be such that $h(T) \geq K^2$. Since $t \geq h(T)$, one has that $N_{k,t} \geq \sqrt{t} - K$.

Then using a union bound on each pair and number of arms, as well as a Chernoff bound, we have that each of the terms in the above inequality are bounded as

$$\begin{aligned}&\mathbb{P}\left(z^{\top}\left(\hat{M}_{k,t} - \hat{M}_{k',t}\right) \leq z^{\top}\left(M_k - M_{k'}\right) - \xi\right) \\ &= \mathbb{P}\left(z^{\top}\left(\hat{M}_{k,t} - \hat{M}_{k',t}\right) \leq z^{\top}\left(M_k - M_{k'}\right) - \xi, N_{k,t} \geq \sqrt{t}\right) \\ &\leq \sum_{s=\sqrt{t}-K}^t \mathbb{P}\left(z^{\top}\left(\hat{M}_{k,s} - \hat{M}_{k',s}\right) \leq z^{\top}\left(M_k - M_{k'}\right) - \xi\right) \\ &\leq \sum_{s=\sqrt{t}-K}^t \mathbb{P}\left(z^{\top}\left(\hat{M}_{k,s} - M_k\right) - z^{\top}\left(\hat{M}_{k',s} - M_{k'}\right) \leq -\xi/2 - \xi/2\right) \\ &\leq \sum_{s=\sqrt{t}-K}^t \left(\mathbb{P}\left(z^{\top}\left(\hat{M}_{k,s} - M_k\right) \leq -\xi/2\right) + \mathbb{P}\left(z^{\top}\left(\hat{M}_{k',s} - M_{k'}\right) \geq \xi/2\right)\right) \\ &\leq \sum_{s=\sqrt{t}-K}^t \left(\exp\left(-sd_{\text{KL}}\left(z^{\top} M_k - \xi/2, z^{\top} M_k\right)\right) + \exp\left(-sd_{\text{KL}}\left(z^{\top} M_{k'} + \xi/2, z^{\top} M_{k'}\right)\right)\right) \\ &\leq \frac{\exp\left(-(\sqrt{t}-K)d_{\text{KL}}\left(z^{\top} M_k - \xi/2, z^{\top} M_k\right)\right)}{1 - \exp\left(-d_{\text{KL}}\left(z^{\top} M_k - \xi/2, z^{\top} M_k\right)\right)} + \frac{\exp\left(-(\sqrt{t}-K)d_{\text{KL}}\left(z^{\top} M_{k'} + \xi/2, z^{\top} M_{k'}\right)\right)}{1 - \exp\left(-d_{\text{KL}}\left(z^{\top} M_{k'} + \xi/2, z^{\top} M_{k'}\right)\right)} \\ &\leq \left(\frac{1}{1 - \exp\left(-d_{\text{KL}}\left(z^{\top} M_k - \xi/2, z^{\top} M_k\right)\right)} + \frac{1}{1 - \exp\left(-d_{\text{KL}}\left(z^{\top} M_{k'} + \xi/2, z^{\top} M_{k'}\right)\right)}\right) \\ &\quad \times \exp\left(-(\sqrt{t}-K) \min_{k,k'}\left\{d_{\text{KL}}\left(z^{\top} M_k - \xi/2, z^{\top} M_k\right), d_{\text{KL}}\left(z^{\top} M_{k'} + \xi/2, z^{\top} M_{k'}\right)\right\}\right)\end{aligned}$$

Similarly, we have:

$$\begin{aligned} & \mathbb{P} \left(z^\top (\hat{M}_{k,t} - \hat{M}_{k',t}) \geq z^\top (M_k - M_{k'}) + \xi \right) \\ & \leq \left(\frac{1}{1 - \exp(-d_{\text{KL}}(z^\top M_k + \xi/2, z^\top M_k))} + \frac{1}{1 - \exp(-d_{\text{KL}}(z^\top M_{k'} - \xi/2, z^\top M_{k'}))} \right) \\ & \quad \times \exp \left(-(\sqrt{t} - K) \min_{k,k'} \{d_{\text{KL}}(z^\top M_k + \xi/2, z^\top M_k), d_{\text{KL}}(z^\top M_{k'} - \xi/2, z^\top M_{k'})\} \right) \end{aligned}$$

Now, we set

$$C \triangleq \min_k \{d_{\text{KL}}(z^\top M_k + \xi/2, z^\top M_k), d_{\text{KL}}(z^\top M_k - \xi/2, z^\top M_k)\}$$

and

$$\begin{aligned} B \triangleq \sum_{(k,k')} & \left(\frac{1}{1 - \exp(-d_{\text{KL}}(z^\top M_k - \xi/2, z^\top M_k))} + \frac{1}{1 - \exp(-d_{\text{KL}}(z^\top M_{k'} + \xi/2, z^\top M_{k'}))} \right. \\ & \left. + \frac{1}{1 - \exp(-d_{\text{KL}}(z^\top M_k + \xi/2, z^\top M_k))} + \frac{1}{1 - \exp(-d_{\text{KL}}(z^\top M_{k'} - \xi/2, z^\top M_{k'}))} \right). \end{aligned}$$

We observe that $B \leq 2K^2 \frac{1}{1 - \exp(-C)}$. Now, we get that

$$\mathbb{P}(\bar{\mathcal{G}}_T) \leq \sum_{t=h(T)}^T B \exp(-C\sqrt{t}) \leq 2K^2 \frac{1}{1 - \exp(-C)} T \exp(-CT^{1/8}).$$

□

D.3 Proof of Theorem 5.2

Theorem D.1 (Restating Theorem 5.2). *For any $\alpha > 0$ and $c(t, \delta)$ defined in (7), we have that the stopping time satisfies :*

$$\lim_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau]}{\log(\frac{1}{\delta})} \leq \alpha \bar{\mathcal{T}}_{\mathcal{F}}(M) \quad \forall M \in \mathbb{R}^{K \times L}$$

Proof. **Step 1: Good Event** Let $T \in \mathbb{N}$, and $h(T) = \sqrt{T}$, define the good event:

$$\mathcal{G}_T = \cap_{t=h(T)}^T \left\{ d_p(\hat{\mathcal{P}}_t, \mathcal{P}^*) \leq f(\epsilon) \right\} \quad (21)$$

where, $f(\epsilon)$ is such that:

$$d_p(\hat{\mathcal{P}}_t, \mathcal{P}^*) \leq f(\epsilon) \implies \sup_{w' \in w^*(\hat{\mathcal{P}}_t)} \sup_{w \in w^*(\mathcal{P}^*)} \|w' - w\| \leq \epsilon$$

Step 2: Concentration of Good Event In Lemma D.3, we show that:

$$\mathbb{P}(\bar{\mathcal{G}}_T) \leq 2K^2 \frac{1}{1 - \exp(-C)} T \exp(-CT^{\frac{1}{8}})$$

Step 3: Tracking Lemma We have:

$$\begin{aligned} |N_{k,t} - w_k^*(M)| & \leq \left| \frac{N_{k,t}}{t} - \frac{1}{t} \sum_{s=1}^{t-1} w_k^*(\hat{M}_s) \right| + \left| \frac{1}{t} \sum_{s=1}^{t-1} w_k^*(\hat{M}_s) - w_k^*(M) \right| \\ & \leq \frac{N_{k,t}}{t} + \frac{h(T)}{t} + \left| \frac{1}{t} \sum_{s=1}^{t-1} w_k^*(\hat{M}_s) - w_k^*(M) \right| \\ & \leq \frac{K(\sqrt{t} + 1)}{t} + \frac{h(T)}{t} + \left| \frac{1}{t} \sum_{s=1}^t w_k^*(\hat{M}_s) - w_k^*(M) \right| \end{aligned}$$

From (Garivier and Kaufmann, 2016), we have that:

$$\max_k \left| N_{k,t} - \sum_t w_{k,t} \right| \leq K \left(1 + \sqrt{t} \right)$$

Step 4: Complexity of the good event

Assume $t \geq T_\epsilon$, and let:

$$C_\epsilon(M) \triangleq \inf_{w', M'} \bar{\mathcal{V}}_C(w, M), \forall (w, M) \text{ s.t. } \|w' - w\| \leq 3\epsilon, d_P(\hat{P}_t, \mathcal{P}^*) \leq f(\epsilon)$$

Then, we have that:

$$\bar{\mathcal{V}}_C(N_t, \hat{M}_t) \geq t C_\epsilon(M)$$

Step 5: Bounding the stopping time for good and bad events

Let τ_δ be the stopping time, then:

$$\min\{\tau_\delta, T\} \leq \sqrt{T} + \sum_{t=T_\epsilon}^T \mathbb{1}_{\tau_\delta \geq t}$$

From the stopping rule (Equation (7)), we get that:

$$\begin{aligned} T_\epsilon + \sum_{t=T_\epsilon}^T \mathbb{1}_{\bar{\mathcal{V}}_C(N_t, \hat{M}_t) \leq \beta(t, \delta)} &\leq \sqrt{T} + \sum_{t=T_\epsilon}^T \mathbb{1}_{t C_\epsilon(M) \leq \beta(t, \delta)} \\ &\leq \sqrt{T} + \frac{\beta(t, \delta)}{C_\epsilon(M)} \end{aligned}$$

where, $\beta(t, \delta)$ is defined in Equation (6).

Define $T_\delta = \inf \left\{ T \in \mathbb{N} : \sqrt{T} + \frac{c(t, \delta)}{C_\epsilon(M)} \leq T \right\}$. Hence, we have:

$$\mathbb{E}[\tau_\delta] \leq T_\epsilon + T_\delta + \sum_{T=1}^{\infty} 2K^2 \frac{1}{1 - \exp(-C)} T \exp(-CT^{-1/8}) \leq T_\epsilon + T_\delta + T'$$

Let $C(\eta) = \inf \{ T : T - \sqrt{T} \geq \frac{T}{(1+\eta)} \}$. Then:

$$T_\delta \leq C(\eta) + \inf \left\{ T \in \mathbb{N} : \frac{TC_\epsilon(M)}{(1+\eta)} \geq \beta(t, \delta) \right\}$$

Step 6: Obtaining the asymptotic bounds Taking limits:

$$\liminf_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau_\delta]}{\log\left(\frac{1}{\delta}\right)} \leq \alpha \mathcal{T}(M) \forall \alpha \geq 1$$

□

E Reduction to Best-arm Identification

We briefly discuss how the metric $d_P(\cdot, \cdot)$ extends existing notions of gap in best-arm and Pareto-front identification literature. Specifically, we proceed with the three following observations.

1. Observe that $d_P(\mathcal{P}^*, \mathcal{P}^*) = 0$.
2. Further, iff $\mathcal{C}$ represents the component-wise ordering as in Pareto-front identification (Auer et al., 2016; Kone et al., 2023a), then $z^{(\ell)} = 1, \forall \ell \in [L]$.

$$\begin{aligned}
 d_P([K] \setminus \mathcal{P}^*, \mathcal{P}^*) &= \max \left\{ \sup_{k \in [K] \setminus \mathcal{P}^*} d(k, \mathcal{P}^*), \sup_{k \in \mathcal{P}^*} d([K] \setminus \mathcal{P}^*, k) \right\} \\
 &= \max \left\{ \sup_{k \in [K] \setminus \mathcal{P}^*} \inf_{k' \in \mathcal{P}^*} \max \left\{ 0, \min_{\ell \in [L]} (M_\ell k - M_\ell k') \right\}, \right. \\
 &\quad \left. \sup_{k \in \mathcal{P}^*} \inf_{k' \in [K] \setminus \mathcal{P}^*} \max \left\{ 0, \min_{\ell \in [L]} (M_\ell k - M_\ell k') \right\} \right\} \\
 &= \max \left\{ \sup_{k \in [K] \setminus \mathcal{P}^*} \inf_{k' \in \mathcal{P}^*} \max \{0, m(k', k)\}, \right. \\
 &\quad \left. \sup_{k \in \mathcal{P}^*} \inf_{k' \in [K] \setminus \mathcal{P}^*} \max \{0, M(k, k')\} \right\} \\
 &= \sup_{k \in \mathcal{P}^*} \inf_{k' \in [K] \setminus \mathcal{P}^*} \max \{0, M(k, k')\}.
 \end{aligned}$$

3. Finally, when there is only a single objective, i.e., $|L| = 1$ and assuming an unique optimal arm (fairly common assumption in BAI literature), we have:

$$\begin{aligned}
 d_P([K] \setminus \mathcal{P}^*, \mathcal{P}^*) &= \max \left\{ \sup_{k \in [K] \setminus \mathcal{P}^*} d(k, \mathcal{P}^*), \sup_{k \in \mathcal{P}^*} d([K] \setminus \mathcal{P}^*, k) \right\} \\
 &= \max \left\{ \sup_{k \in [K] \setminus k^*} \max \{0, (\mu_k - \mu_{k^*})\}, \right. \\
 &\quad \left. \sup_{k' \in [K] \setminus k^*} \max \{0, (\mu_{k^*} - \mu_{k'})\} \right\} \\
 &= \min_{k' \neq k^*} \Delta_{k'},
 \end{aligned}$$

which is exactly the gap for one-dimensional bandit.

F Useful Existing Results

Theorem F.1 (Berge's Maximum Theorem (Berge, 1877)). *Let $\mathcal{U}$ and $\mathcal{V}$ be topological spaces, $f : \mathcal{U} \times \mathcal{V} \rightarrow \mathbb{R}$ and $C : \mathcal{U} \rightarrow \mathcal{V}$ be non-empty compact set for all $u \in \mathcal{U}$. Then, if C is continuous at u , $f^*(u) = \max_{v \in C(u)} f(u, v)$ is continuous and $C^*(u) = \{v \in C(u) : f^*(u) = f(u, v)\}$ is upper-hemicontinuous.*

Theorem F.2 (Donsker-Vardhan Variational Formula (Donsker and Varadhan, 1975)). *For mutual information $d_{KL}(P, Q)$, we have that:*

$$d_{KL}(P, Q) = \sup_f \mathbb{E}_P[f] - \ln \mathbb{E}_Q[\exp(f)]$$

Lemma F.1 (Peskun Ordering (Peskun, 1973)). *For any two random variables X, Y on $\mathbb{R}^K$ the following are equivalent:*

1. $X \leq_s Y$
2. For all $x \in \mathbb{R}^K$, $\mathbb{P}[X \geq x] \leq \mathbb{P}[Y \geq x]$
3. For all non-negative functions $f_1, f_2, \dots, f_K$, we have that: $\mathbb{E}[\Pi_{i=1}^K f_i] \leq \mathbb{E}[\Pi_{i=1}^K f_i]$

Lemma F.2 (Magureanu et al. (2014)). *For any $k = 1, 2, \dots, K$, let us define $1 \leq t_k \leq t$. Then for all $0 \leq C_k \leq M_k$, we have*

$$\mathbb{P}\left(\bigcap_{k \in [K]} \left\{ \hat{M}_{k,t} \leq C_k, t_k \leq N_{k,t} \right\}\right) \leq \exp\left(-\sum_{k \in [K]} t_k d_{KL}(C_k, M_k)\right).$$

Lemma F.3 (Magureanu et al. (2014)). *Let $a > 0$ and $K \geq 2$ and $Z \in \mathbb{R}^K$ such that for all $\xi \in \mathbb{R}_+^K$ we have:*

$$\mathbb{P}(Z \geq \zeta) \leq \exp\left(-a \sum_{k \in [K]} \zeta_k\right).$$

Then, for all $\rho \geq \frac{K}{a} \in \mathbb{R}_+$, we have

$$\mathbb{P}\left(\sum_{k \in [K]} Z_k \geq \rho\right) \leq \left(\frac{ae\rho}{K}\right)^K \exp(-a\rho).$$

Lemma F.4 (Single-arm concentration Kaufmann and Koolen (2021)). *The following is a δ uniformly valid confidence interval on $z^\top \mu$:*

$$z^\top \mu \in \left[z^\top \hat{\mu} + \sqrt{2 \left(LC^g \left(\frac{\ln(\frac{1}{\delta})}{L} \right) \right) + \sum_{k \in [K]} c \ln(d + \ln \ln(N_{k,t})) \frac{\sum_{\ell \in L} (z^\ell)^2}{N_{k,t}}} \right]$$

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