000 001 002 003 REGRET-OPTIMAL LIST REPLICABLE BANDIT LEARN-ING: MATCHING UPPER AND LOWER BOUNDS

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Paper under double-blind review

ABSTRACT

This paper investigates *list replicability* [Dixon et al.](#page-10-0) [\(2023\)](#page-10-0) in the context of multiarmed (also linear) bandits (MAB). We define an algorithm A for MAB to be (ℓ, δ) -list replicable if with probability at least $1 - \delta$, A has at most ℓ traces in independent executions even with different random bits, where a trace means sequence of arms played during an execution. For k -armed bandits, although the total number of traces can be $\Omega(k^T)$ for a time horizon T, we present several surprising upper bounds that either independent of or logarithmic of T: (1) a $(2^k, \delta)$ list replicable algorithm with near-optimal regret, $\ddot{O}(\sqrt{kT})^1$ $\ddot{O}(\sqrt{kT})^1$, (2) a $(O(k/\delta), \delta)$ -list replicable algorithm with regret $\widetilde{O}\left(\frac{k}{\delta}\right)$ \sqrt{kT} , (3) a $((k+1)^{B-1}, \delta)$ -list replicable algorithm with regret $\widetilde{O}(k^{\frac{3}{2}}T^{\frac{1}{2}+2^{-(B+1)}})$ for any integer $B > 1$. On the other hand, for the sublinear regret regime, we establish a matching lowerbound on the list complexity (parameter ℓ). We prove that there is no $(k - 1, \delta)$ -list replicable algorithm with $o(T)$ -regret. This is optimal in list complexity in the sub-linear regret regime as there is a $(k, 0)$ -list replicable algorithm with $O(T^{2/3})$ -regret. We further show that for linear bandits with d -dimensional features, there is a $\widetilde{O}(d^2T^{1/2+2^{-(B+1)}})$ -regret algorithm with $((2d+1)^{B-1}, \delta)$ -list replicability, for $B > 1$, even when the number of possible arms can be infinite.

1 INTRODUCTION

032 033 034 035 036 037 038 039 040 041 042 043 044 The issue of replicability and reproducibility in science has become a significant concern, attracting substantial attention from the broader scientific community Begley $\&$ Ellis [\(2012\)](#page-10-1); [Ioannidis](#page-10-2) [\(2005\)](#page-10-2); [Baker](#page-10-3) [\(2016\)](#page-10-3); [of Sciences et al.](#page-11-0) [\(2019\)](#page-11-0). Recently the machine learning community also started addressing this issue. Inspired by reproducibility workshops at ICML/ICLR, the ML community has created a dedicated online conference, the ML Reproducibility Challenge (MLRC) [Sinha](#page-11-1) [et al.](#page-11-1) [\(2023\)](#page-11-1), to encourage the publishing and sharing of scientific results that are reliable and reproducible. In machine learning, a common approach to ensure replicability and reproducibility is to make datasets and code publicly available. However, it is unclear if such an approach is sufficient, as machine learning algorithms draw samples from data distributions and are usually randomized. This inherent randomness results in non-replicability. Therefore, it is more desirable to design machine learning algorithms that are replicable, i.e., algorithms that return the same result over multiple runs, even when different runs observe different sets of samples from the data distribution. The aforementioned requirement has recently led to theoretical studies and rigorous definitions of replicability [Impagliazzo et al.](#page-10-4) [\(2022\)](#page-10-4); [Dixon et al.](#page-10-0) [\(2023\)](#page-10-0), with various notions of replicability being proposed.

045 046 047 048 049 050 In this work, we study bandit algorithms with replicability guarantees. The Multi-Armed Bandit (MAB) is a learning task in which a learner interacts with an environment consisting of a set of fixed k distributions (called arms) in discrete time steps. In each of the T steps, the learner selects an arm and receives an i.i.d. sample from that arm, called the reward. The goal of the learner is to maximize the cumulative expected reward, equivalently minimizing the "regret" (defined formally later), which characterizes the total sub-optimality of the actions played over the learning course.

051 052 Ideally, an MAB algorithm with *perfect replicability* guarantees should always select exactly the same trace (i.e., sequence of arms) over multiple runs, even if the algorithm receives a different

¹Here $\widetilde{O}(\cdot)$ omits $\log k$, $\log T$, $\log \frac{1}{\delta}$.

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054 055 056 057 058 set of samples from the data distribution for each run. However, as shown later in the paper (and discussed in [Dixon et al.](#page-10-0) [\(2023\)](#page-10-0)), it is impossible for MAB algorithms with perfect replicability guarantees to have a non-trivial regret bound, as algorithms need to adapt to the randomness from the history to learn effectively. Therefore, we ask, *what is the strongest notion of replicability of a bandit algorithm without suffering significant regret loss?*

059 060 061 062 063 064 065 066 067 068 069 Inspired by a recent study [Dixon et al.](#page-10-0) [\(2023\)](#page-10-0) that investigates replicability in the supervised learning setting, we propose a notion of *list replicability* for bandit learning. In this setting, we require that the trace (sequence of actions) produced by the algorithm during the entire learning course be predictable to a certain extent. That is, no matter how many times we repeat the algorithm for the bandit instance, the resulting sequence of actions comes from a small finite list. Note that in general, a T horizon MAB algorithm with k arms can have k^T possible traces. Such a guarantee would be useful for bandit learning in safety-critical applications, as one can be prepared for the action sequence being played. Bandit algorithms and more general reinforcement learning algorithms are increasingly used in clinical trials and social experiments to personalize treatment decisions for individuals [Zhang et al.](#page-11-2) [\(2024\)](#page-11-2). In such domains, it is highly desirable to limit the possible sequence of actions and limit uncertainty.

070 071 072 The formalization of the concept of replicability in various computational settings is a significant and emerging area of research. This work takes an important step toward understanding the foundational principles of replicability in the context of bandit problems.

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2 PRELIMINARIES

076 077 078 079 For $n \in \mathbb{N}$, we use $[n]$ to denote the set $\{1, \ldots, n\}$ and for $a, b \in \mathbb{R}$ we use $[a, b]$, (a, b) , $[a, b)$, and $(a, b]$ to represent the closed, open intervals, and their corresponding half-open intervals respectively. We use $\tilde{O}(\cdot)$ to subsume $\log k$, $\log \log T$, and $\log \frac{1}{\delta}$. In this paper, we consider the following Multi-Armed Bandit (MAB) instance.

080 081 082 083 Assumption 2.1. *An MAB instance is a tuple* (D, T) *where* D *is a collection of distributions* (D_1, \ldots, D_k) and $T \in \mathbb{N}$ is the horizon such that^{[2](#page-1-0)} each D_i is supported on $[0,1]$ and has a mean μ_i . For any $t \in [T]$, if action $a_t \in [k]$ is played, the reward r_t is an i.i.d. sample drawn from D_{a_t} .

084 085 086 087 088 089 Here, we use k to denote the number of arms and T to denote the horizon. For a collection of means μ_1, \ldots, μ_k we use $\mu^* = \max_{a \in [k]} {\mu_a}$ to denote the highest mean and for each $i \in [k]$, $\Delta_i = \mu^* - \mu_i$ to denote its reward gap. An arm i with $\Delta_i = 0$ is called an optimal arm; otherwise, it is called a sub-optimal arm. Let M be an algorithm for MAB. The algorithm M defines probability distribution P_M on traces $[k]^T$ in the following sense: Given a trace $a \in [k]^T$, probability of a, denoted $P_{\mathcal{M}}(a)$, is the probability that $\mathcal M$ takes trace a . For a set S of traces, $P_{\mathcal{M}}(S) = \sum_{a \in S} P_{\mathcal{M}}(a)$.

090 091 Definition 2.2 ((ℓ, δ) -MAB Replicability). *An algorithm M for MAB is* (ℓ, δ) -list replicable if for e very MAB instance (D,T) , there exists a set of traces $S_{D,T} \subseteq [k]^T$ such that $|S_{D,T}| \leq \ell$ and

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P_{\mathcal{M}}(S_{D,T}) \ge 1 - \delta
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094 *When* $\delta = 0$, then we just say that M is ℓ -list replicable. We call ℓ the list complexity of M.

095 096 097 098 Definition 2.3 (Regret). *We measure the performance of an algorithm by the* regret, which is $R_T =$ $\sum_{t=1}^T \max_a \mu_a - \mu_{a^t}$, where a^t is the action played at time t . An MAB algorithm is effective, if the *regret is sublinear in* T : *in this case the average regret per round is approaching* 0 *as* $T \rightarrow \infty$ *.*

099 100 101 102 Trivially, any MAB algorithm is k^T -list replicable because a trace must be an element of $[k]^T$; and an algorithm playing the same action all the time is a $(1, 0)$ -list replicable algorithm, yet with regret T. We aim to create MAB algorithms that have both low regret and are (ℓ, δ) -list replicable with small ℓ and δ .

103 For the linear bandits, we assume that the rewards r_t satisfy a linear structure. Specifically,

104 105 106 Assumption 2.4. *For any* $a \in \mathcal{A}$, *we assume* $||a||_2 \leq 1$ *and hence* \mathcal{A} *is a compact set. For* any time t, if action a_t is played, the reward r_t satisfies $r_t = \langle a_t, \theta^* \rangle + \eta_t$ where $\hat{\theta}^*$ is unknown

¹⁰⁷ ²For presentation simplicity, we restrict to the $[0, 1]$ setting. Our results generalize to sub-Gaussian distributions straightforwardly.

108 109 110 with $\|\theta^*\|_2 \leq \sqrt{2}$ d, and $η_t$ *is an history independent mean-*0 *σ*-sub-Gaussian random variable that *satisfies* $\mathbb{E}[\eta_t] = 0$ and $(\forall x > 0)$. $\Pr[|\eta_t| > x] \leq 2 \exp\left(\frac{-x^2}{\sigma^2}\right)$ $\frac{-x^2}{\sigma^2}$).

112 113 114 We denote $\mu_a = \langle a, \theta^* \rangle \in [0,1]$ as the unknown true mean of an arm a, and let $a^* =$ arg max_{a∈A} $\langle a, \theta^* \rangle$, which is the unknown optimal action. For presentation simplicity, we assume $\sigma = 1$.

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3 OUR CONTRIBUTIONS

118 119 In this work, we introduce a viable notion of replicability which is called *list replicability* in the context of Multi-Armed Bandit algorithms. We summarize our technical results below.

120 121 122 In Section [5.1,](#page-3-0) we present a $(2^k, \delta)$ -list replicable MAB algorithm with near-optimal regret, $\tilde{O}(\sqrt{kT})$. Importantly, the total number of possible traces is completely independent of T.

123 124 125 In Section [5.2,](#page-4-0) we present a $(O(k/\delta), \delta)$ -list replicable MAB algorithm with $\tilde{O}(k/\delta\sqrt{kT})$ regret. When δ is constant, the total number of possible traces is $O(k)$, while the regret bound is $\tilde{O}(\sqrt{\text{poly}(k)T}).$

127 128 129 130 In Section [5.3,](#page-6-0) we present a $((k + 1)^{B-1}, \delta)$ -list replicable algorithm with regret bound $\tilde{O}(k^{\frac{3}{2}}T^{\frac{1}{2}+2^{-(B+1)}})$ for any $B > 1$. By setting B to be a constant, the total number of possible traces is polynomial in k, while the regret bound is sublinear in k. By setting $B = \log \log T$, the total number of possible traces is $k^{O(\log \log T)}$, while the regret bound is $\tilde{O}(k^{3/2}\sqrt{T})$.

131 132 133 134 In Section [6,](#page-7-0) we further show that the guarantees of our third algorithm are nearly tight by establishing a $(k-1)$ lower bound for any list replicable algorithm with failure probability at most $1/(k+1)$ and regret $o(T)$, almost exactly matching the k-list replicable upper bound for $B = 2$. Interstingly, we use a cubical version of Sperner/KKM lemma for establishing the lower bound.

135 136 137 138 Finally, in Section [7,](#page-8-0) we generalize our third algorithm to the linear bandit setting. For a ddimensional linear bandit instance, we present a $((2d + 1)^{B-1}, \delta)$ -list replicable algorithm with regret $\tilde{O}(d^2T^{\frac{1}{2}+2^{-(B+1)}})$ for any $B>1$.

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4 RELATED WORK

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142 143 144 145 146 147 148 Bandit algorithms have been extensively studied in the general setting Lattimore $\&$ Szepesvári [\(2020\)](#page-11-3); [Slivkins et al.](#page-11-4) [\(2019\)](#page-11-4); [Bubeck et al.](#page-10-5) [\(2012\)](#page-10-5); [Auer et al.](#page-10-6) [\(2002\)](#page-10-6); [Cesa-Bianchi & Fischer](#page-10-7) [\(1998\)](#page-10-7); [Kaufmann et al.](#page-10-8) [\(2012\)](#page-10-8). In the MAB setting, Thomson sampling and UCB achieve an optimal regret of $\tilde{O}(\sqrt{kT})$ [Agrawal & Goyal](#page-9-0) [\(2017\)](#page-9-0); [Auer et al.](#page-10-6) [\(2002\)](#page-10-6). In the *d*-dimensional linear bandit setting, Contextual Thomson sampling and LinUCB achieve a regret of $\tilde O(d\sqrt{T})$ [Lattimore](#page-11-3) [& Szepesvari](#page-11-3) [\(2020\)](#page-11-3). There is extensive work in other bandit variants, and interested readers are ´ referred to Lattimore & Szepesvári [\(2020\)](#page-11-3).

¹⁴⁹ 150 151 152 153 154 155 Several works [Impagliazzo et al.](#page-10-4) [\(2022\)](#page-10-4); [Dixon et al.](#page-10-0) [\(2023\)](#page-10-0); [Bun et al.](#page-10-9) [\(2020\)](#page-10-9); [Ghazi et al.](#page-10-10) [\(2021\)](#page-10-10) studied various notions of replicability in the context of learning tasks. In [Bun et al.](#page-10-9) [\(2020\)](#page-10-9), a notion called stability is introduced. The work of [Impagliazzo et al.](#page-10-4) [\(2022\)](#page-10-4), defined the notion of ρ -replicability. In [Dixon et al.](#page-10-0) [\(2023\)](#page-10-0), the authors introduce list replicability and certificate replicability. The work of [Ghazi et al.](#page-10-10) [\(2021\)](#page-10-10) studied list-global stability and pseudo-global stability. The works of [Esfandiari et al.](#page-10-11) [\(2023\)](#page-10-11); [Karbasi et al.](#page-10-12) [\(2024\)](#page-10-12); [Eaton et al.](#page-10-13) [\(2023\)](#page-10-13) studied replicability in the context of reinforcement learning and Bandits.

¹⁵⁶ 157 158 159 160 161 The work that is closely related to our work is the work of [Esfandiari et al.](#page-10-11) [\(2023\)](#page-10-11) in the context of MAB. Their definition of replicability for MAB is inspired by the notion of ρ -replicability of [Impagliazzo et al.](#page-10-4) [\(2022\)](#page-10-4). Informally, their definition requires that an algorithm for MAB is ρ replicable if multiple runs of an algorithm, where all the runs share the internal random seed, will result in the same trace, with probability greater than $1 - \rho$. Their goal was to design ρ -replicable algorithms for MAB with (near) optimal regret. Our definition of replicability is inspired by the list replicability notion of [Dixon et al.](#page-10-0) [\(2023\)](#page-10-0). In our work, the goal is to design list-replicable

162 163 164 165 166 167 algorithms with *small* list size with (near) optimal regret. In this context, the notions of ρ and list replicability are different as they do not imply each other. Thus our results are significantly different from that of [Esfandiari et al.](#page-10-11) [\(2023\)](#page-10-11). Since their algorithm's replicability depends on the random seeds/certificates, which could be exponentially many, their algorithm can have bad (exponential) list replicability when applied in our setting. Hence, different techniques are required to bound the list size.

5 MULTI-ARM BANDITS: UPPER BOUND

In this section we introduce several list-replicable algorithms for the finite-arm setting. We first present an algorithm with no T dependence yet with less ideal dependence on k. We will then attempt to improve the dependence on k by sacrificing the dependence on other parameters.

5.1 A $(2^k, \delta)$ -LIST REPLICABLE ALGORITHM

177 178 179 180 181 182 This algorithm is a standard phase-elimination type algorithm (yet our analysis for list-replicability is novel). For completeness, we present the full algorithm in Algorithm [1.](#page-3-1) The algorithm proceeds in batches (or rounds) and maintains a set of "good" arms. In each batch, the good arms are played uniformly in a lexicographic order to refine the estimation of the their estimated means. At the completion of the batch, the arms whose estimated means are deemed non-optimal (even considering the estimation uncertainty) are removed.

183 184 185 186 The batch length grows geometrically to provide more accurate estimates of the arms compared to the previous batch. The total number of batches is bounded by $O(\log T)$. Furthermore, the arms being played at every batch are guaranteed to satisfy certain optimality guarantees, and therefore, the overall regret per batch can be bounded with high probability.

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5.1.1 ANALYSIS

Our analysis for replicability relies on the novel observation that the total number of traces is determined by the number of possible batches for a sub-optimal arm to be eliminated. If each sub-optimal is eliminated in at most 2 different batches with high probability, then the overall list complexity is at most 2^k . In particular, a sub-optimal arm is always eliminated in two consecutive batches, with high probability. More formally, the guarantee of the algorithm is presented as follows.

210 211 212 213 214 Theorem 5.1. *For every* $\delta \in (0,1]$, *Algorithm [1](#page-3-1)* is $(2^k, \delta)$ -list replicable, and for every input bandit *instance satisfying Assumption [2.1,](#page-1-1) it enjoys a* $O\left(\sqrt{kT \log \frac{k \log T}{\delta}}\right)$ *regret bound with probability at least* $1 - \delta$ *.*

²¹⁵ Below, we provide the proof of the theorem, which is built on a sequence of lemmas and observations.

216 217 218 219 220 221 222 223 224 Before we make our analysis formal, we recall our definition of the parameters. Note that $B =$ $\lfloor \log_{25} T \rfloor$ is the number of batches. For $b \in [B]$, note that $N_b = \left\lceil \frac{5^{2b}}{|A|} \right\rceil$ is the number of pulls of each arm in the batch. Then each batch has a length of $T_b = |\mathcal{A}_b| \cdot N_b \ge 5^{2b}$. For $\epsilon_b = \sqrt{\frac{ck}{5^{2b}} \log \frac{kB}{\delta}}$, and $\hat{\mu}_{i,(b)}$ be the empirical mean of the arm i, we denote the following event E_b : $\{(\forall i \in A_b), \mu_i - \epsilon_b \leq \}$ $\hat{\mu}_{i,(b)} \leq \mu_i + \epsilon_b$. Define the "good" event $E = \bigcap_{b \in [B]} E_b$. Then, by Hoeffding bound and a union bound, we have that $Pr[E] \ge 1 - \delta$. Conditioned on E, we immediately have, $\forall b \in [B]$, $\mu^* - \epsilon_b \leq \max_{a \in \mathcal{A}_b} \hat{\mu}_{a,(b)} \leq \mu^* + \epsilon_b$ and $\Delta_i - 2\epsilon_b \leq \hat{\Delta}_{i,(b)} \leq \Delta_i + 2\epsilon_b$.

225 226 227 We now define a partition $\{I_1, \ldots, I_{B+1}\}$ on [0, 1]. Let $\epsilon_0 = 1$ and $\epsilon_{B+1} = 0$. For each $m \in [B]$ define $I_m = (\epsilon_m, \epsilon_{m-1}]$ and $I_{B+1} = [\epsilon_{B+1}, \epsilon_B]$. Note for each arm $i \in [k]$, there exists a unique $m \in [B+1]$ such that $\Delta_i \in I_m$. We use m_i to denote this unique partition number.

228 229 230 For $i \in [k]$, let X_i be the random variable that denotes which batch arm i is eliminated; we claim that conditioned on E, X_i can take at most one of two values, namely m_i or $m_i + 1$. This follows because of the geometric nature of ϵ_b . The proof of the following can be found at the Appendix [A.1.](#page-11-5)

Lemma 5.2. For all
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i \in [k]
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, $Pr(m_i \le X_i \le m_i + 1|E) = 1$.

233 234 235 236 To conclude that the algorithm is $(2^k, \delta)$ -list replicable, consider the vectors of deletion sequences (X_1, \ldots, X_k) , with high probability see exactly these 2^k such vectors, each vector corresponds to a single unique trace. The proof of the following can be found in Appendix [A.1.](#page-11-5) Thus concludes the proof of Theorem [5.1.](#page-3-2)

Lemma 5.3. On E, the regret of Algorithm [1](#page-3-1) satisfies $R_T \leq O\left(\sqrt{kT \log{\frac{k \log T}{\delta}}} \right)$ *.*

5.2 A $(O(k/\delta), \delta)$ -LIST REPLICABLE ALGORITHM

242 243 244 245 246 247 248 249 In this section, we present a novel modification to Algorithm [1](#page-3-1) to further boost the list replicablility. For the above $(2^k, \delta)$ -list replicablility, we obtained $2\epsilon_b$ -estimates of Δ_i and eliminated those that were $3\epsilon_b$ away. The algorithm guarantees w.h.p. that each arm will be deleted randomly in one of two rounds. We shall now show that if we perturb the deletion criteria by a random shift picked at the start of the algorithm (while simultaneously getting better approximations for Δ_i by drawing more samples in each batch), then the arm will be deleted in exactly 1 round. Crucially, we show that if we pick at most $C = \left[\frac{12k}{\delta}\right]$ such perturbations, it results in at most C many traces. The algorithm is formally presented in Algorithm [2.](#page-4-1)

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Algorithm 2: $(12k/\delta, \delta)$ -List Replicable for MAB

Input: Horizon T, Actions $[k]$, Failure probability δ Number of shifts: $C \leftarrow \left\lceil \frac{12k}{\delta} \right\rceil$, Number of batches: $B \leftarrow \left\lfloor \log_{25} \frac{T}{C^2} \right\rfloor$, Initial good arm set: $\mathcal{A}_1 \leftarrow [k]$, Random shift: $r \sim \text{Unif}([C])$ for *b=1,. . . ,B* do Denote error parameters: $\epsilon_b \leftarrow \sqrt{\frac{ck}{5^{2b}C^2} \log \frac{2kB}{\delta}}$, $\tau_b \leftarrow \frac{4C\epsilon_b}{3(\sqrt{2}-1)}$ Set deletion criteria: $\mathfrak{D}_b \leftarrow \mathfrak{D}_{b,r} = 3\tau_b + (r-1) \cdot \frac{3(\tau_{b-1} - \tau_b)}{C}$ For each arm $i \in A_b$, play i for $\left[\frac{5^{2b}C^2}{|A_b|}\right]$ times, and obtain an empirical mean $\hat{\mu}_{i,(b)}$ (halt the algorithm if T arms have been played) For all $i \in \mathcal{A}_b$: let $\hat{\Delta}_{i,(b)} \leftarrow \max_{a \in \mathcal{A}_b} \hat{\mu}_{a,(b)} - \hat{\mu}_{i,(b)}$ Eliminate bad arms: $A_{b+1} \leftarrow \{i \in A_b : \hat{\Delta}_{i,(b)} \leq \mathfrak{D}_b\}.$ end

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5.2.1 ANALYSIS

²⁶⁹ Similar to the analysis of Algorithm [1,](#page-3-1) our new algorithm shares a similar structure of bounding the regret: the estimates of arms get increasingly improved, and only arms with better error guarantees

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Figure 1: The deletion criteria \mathfrak{D}_b is randomly chosen from $\mathfrak{D}_{b,1}, \ldots, \mathfrak{D}_{b,C}$

will be played per batch. The challenging part is to show that the algorithm can only produce a small number of traces. The following theorem presents the formal guarantee.

280 281 282 283 Theorem 5.4. *For every* $\delta \in (0,1]$, *Algorithm* [2](#page-4-1) *is* $(\frac{12k}{\delta}, \delta)$ -*list replicable, and for every input* bandit instance satisfying Assumption [2.1,](#page-1-1) the algorithm enjoys an $O\left(\frac{k}{\delta}\cdot\sqrt{kT\log{\frac{k\log{T}}{\delta}}} \right)$ *regret bound with probability at least* $1 - \delta$ *.*

285 286 287 288 289 290 291 292 We now present a proof of the theorem. Recall that $C = \lceil 12k/\delta \rceil$ the number of shifts, $B =$ $\lfloor \log_{25} \frac{T}{C^2} \rfloor$. Let $T_b = 5^{2b}C^2$ and $N_b = \lceil \frac{T_b}{k} \rceil$, we draw T_b samples each round, each arm gets $\geq N_b$ samples. Let $\epsilon_b = \sqrt{\frac{ck}{5^{2b}C^2} \log \frac{2kB}{\delta}}$ (for some $c > 0$) and $\tau_b = \frac{4C\epsilon_b}{3(\sqrt{2}-1)}$ and thus the estimate at each round is ϵ_b -accurate with probability at least $1 - \delta$. For $b \in [B]$, and for $r \in [C]$, consider the deletion criterias in the algorithm: $\mathfrak{D}_{b,r} = 3\tau_b + (r-1) \cdot \frac{3(\tau_{b-1}-\tau_b)}{C}$. For a randomly picked $r \in [C]$, the deletion criteria at round b, denoted by the random variable \mathfrak{D}_b is uniformly picked from $\mathfrak{D}_{b,1}, \ldots, \mathfrak{D}_{b,C}$. Note that the same r is shared across all rounds.

293 294 295 296 297 298 Unlike in Algorithm [1,](#page-3-1) the decision boundary, $\mathfrak{D}_b \propto (C\epsilon_b)$ is much larger than the estimation error ϵ_b . Hence, suppose an arm i has a gap $\Delta_i \in [\mathfrak{D}_b, \mathfrak{D}_{b-1}]$ and is more than $O(\epsilon_b)$ from the boundary of the interval, the algorithm will eliminate it with high probability in batch b. Only the "bad" arms whose gaps are within $O(\epsilon_b)$ to the boundary has the possibilities to be not eliminated in batch b. We will show that for the C we choose, with certain probability no bad arms exists and thus there is unique trace from the algorithm. Below, we make this intuition more formal.

299 300 Observation 5.5. *For all* $b \in [B]$ *and* $r \in [C]$ *,* $3\tau_b \leq \mathfrak{D}_{b,r} < 3\tau_{b-1}$ *. In particular, this always holds for the random variable* \mathfrak{D}_b , $3\tau_b \leq \mathfrak{D}_b < 3\tau_{b-1}$.

302 303 304 305 306 307 Analogous to the analysis of Algorithm [1,](#page-3-1) for $b \in [B]$, we define the event as E_b : $(\forall i \in A_b)$. μ_i $\epsilon_b \le \hat{\mu}_{i,(b)} \le \mu_i + \epsilon_b$, and the "good" event $E = \bigcap_{b \in [B]} E_b$. Via Hoeffding and a union bound, we have for all $b \in [B]$. $Pr(E_b) \ge 1 - \frac{\delta}{2B}$ and $Pr(E) \ge 1 - \frac{\delta}{2}$. Define the partition $\{I_1, \ldots, I_{B+1}\}$ on [0, 1]. Let $\tau_0 = 1$ and $\tau_{B+1} = 0$. For each $m \in [B]$ define $I_m = (\tau_m, \tau_{m-1}]$ and $I_{B+1} =$ $[\tau_{B+1}, \tau_B]$. For each arm $i \in [k]$, there exists a unique $m \in [B+1]$ such that $\Delta_i \in I_m$. We use m_i to denote this unique partition number.

308 309 310 311 We now claim that each arm i will be eliminated in one of three batches, namely $m_i, m_i + 1, m_i + 2$, instead of the two in the case of the previous algorithm. Intuitively, an arm that was supposed to be deleted in the second round might be delayed to the third round because of the perturbation in the deletion criteria. The full proof can be found in Appendix [A.2.](#page-11-6)

312 Lemma 5.6. *For all* $i \in [k]$, $Pr(m_i \leq X_i \leq m_i + 2|E) = 1$.

313 314 315 316 317 318 Referring to Figure [1,](#page-5-0) observe that if $r = C - 1$ were picked, it would be a "bad" because even conditioned on E, sometimes the estimate of Δ_i lies on the left of the deletion criteria, \mathfrak{D}_b and other times Δ_i lies on the right of the \mathfrak{D}_b , i.e., the round the arm is deleted is inconsistent even when estimates are good. The other rs are "good" because the arm consistently either gets eliminated this round b or its deletion gets postponed to a future round.

Definition 5.7. *Let* $i \in [k]$ *,* $r \in [C]$ *, and* $b \in [B]$.

1. r is b-bad for i if $\mathfrak{D}_{b,r} \in [\Delta_i - 2\epsilon_b, \Delta_i + 2\epsilon_b]$.

2. *r is bad for i if it is b-bad for i for some* $b = m_i, m_i + 1, m_i + 2$.

3. r is bad if it is bad for <i>i for some $i \in [k]$ *. Otherwise, r is said to be good.*

324 325 326 327 328 $\mathfrak{D}_{b,r}$ s were carefully chosen so that every batch $b \in [B]$ the length of the approximation interval of Δ_i at round b is exactly equal to the distance between consecutive shifts of the same round $\mathfrak{D}_{b,r}$ and $\mathfrak{D}_{b,r+1}$. As a consequence, there can only be at most 2 $\mathfrak{D}_{b,r}$ s contained in the interval $[\Delta_i - 2\epsilon_b, \Delta_i + 2\epsilon_b]$. With some rudimentary counting, the following lemma holds whose full proof can be found in Appendix [A.2.](#page-11-6)

329 330 Lemma 5.8. *There are at most* 6k *bad* r*s.*

331 332 333 334 335 336 337 338 When a good r is chosen, we see exactly one trace (conditioned on E), because the deletion criteria is always outside the estimation interval for all arms. Thus if we uniformly at random pick an $r \sim$ Unif[C], then with probability at most $\frac{6k}{C} = \frac{\delta}{2}$, r is bad. Therefore, the number of traces is at most $C = \frac{12k}{\delta}$ when both these events occur. The probability that both estimates are good and r is good are independent and is bounded by: $Pr(E \cap r \text{ is good}) \ge (1 - \frac{\delta}{2})^2 \ge 1 - \delta$. The proof of the following lemma is similar to the regret analysis of the previous section and can be found in Appendix [A.2.](#page-11-6) Thus concludes the proof of Theorem [5.4.](#page-5-1)

Lemma 5.9. *On* E *and the event that* r *is good, the regret of Algorithm* [2](#page-4-1) *satisfies*, $R_T \leq$ $O\left(\frac{k}{\delta}\sqrt{kT\log \frac{k\log T}{\delta}}\right)$ *.*

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5.3 A $(k^{O(1)}, \delta)$ -List Replicable Algorithm with $k^{3/2} T^{1/2+O(1)}$ -regret

In this section, we refine the tradeoff between list-replicability and the regret bound. We rely on the following critical routine proposed in [Dixon et al.](#page-10-0) [\(2023\)](#page-10-0).

346 347 348 349 350 351 Theorem 5.10 [\(Dixon et al.](#page-10-0) [\(2023\)](#page-10-0), Replicable Mean Estimation). Let $\epsilon, \delta \in (0, 1]$ and $k \in \mathbb{N}$. For any random vector $V \in \mathbb{R}^k$, suppose there exists an algorithm takes samples from V and produces an estimator \widehat{V} such, that $\|\mathbb{E}[V] - \widehat{V}\|_\infty \leq \frac{\epsilon}{2k}$ with probability at least $1-\delta.$ Then there exists an *algorithm,* ReplicableMeans, which takes $\overline{\hat{V}}$ *as an input and output a* $((k + 1), \delta)$ *-list replicable estimator* \overline{V} *, which satisfies* $\|\mathbb{E}[V] - \overline{V}\|_{\infty} \leq \epsilon$ *, with probability at least* $1 - \delta$ *.*

352 353 354 355 356 357 358 359 360 361 We shall argue about replicability based on the subset of arms that are eliminated. Let $B > 1$ be an integer, denoting the number of batches, and $\delta \in (0, 1]$. Let $\nu \approx \frac{1}{2^{B+1}-2}$ with $\alpha = \frac{1}{2} + \nu$. We shall demonstrate how to create a $((k+1)^{B-1}, \delta)$ -list replicable algorithm with $\tilde{O}(kT^{\nu}\sqrt{kT})$ regret. The algorithm is a constant batched algorithm where B is the number of batches. In each batch, bad arms are deleted in a replicable manner with the help of Theorem [5.10;](#page-6-1) thus, in each batch, only $(k+1)$ possible subset of arms are deleted (instead of the naïve 2^k). Via rule of product, over $B - 1$ batches $(k + 1)^{B-1}$ traces are observed. Note that the eliminations in batch B does not affect the replicability. Therefore the replicability is $(k + 1)^{B-1}$. The algorithm is formally presented in Algorithm [3.](#page-6-2)

362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 Algorithm 3: $((k+1)^{B-1}, \delta)$ -List Replicable for MAB **Input:** Horizon T, Actions [k], Number of Batches $B > 1$, Failure probability δ Regret paramter: $\nu \leftarrow \frac{1}{2^{B+1}-2}, \alpha \leftarrow \frac{1}{2} + \nu$, Initial good arm set: $\hat{\mathcal{A}_1} \leftarrow [k]$ for $b=1,\ldots,B$ do For each arm $i \in A_b$, play i for $N_b = \left[T^{\alpha(2-\frac{1}{2^{b-1}})} / |A_b| \right]$ times and obtain an empirical mean $\hat{\mu}_{i,(b)}$ (the algorithm halts if it has played T arms) Use Replicable Means (Theorem [5.10\)](#page-6-1): $\big\langle \hat{\mu}_{i,(b)} \big\rangle_{i\in\mathcal{A}_b}\leftarrow\texttt{ReplicableMeans}\left(\big\langle \hat{\mu}_{i,(b)} \big\rangle_{i\in\mathcal{A}_b}\right)$ For all $i \in \mathcal{A}_b$: let $\hat{\Delta}_{i,(b)} \leftarrow \max_{a \in \mathcal{A}_b} \hat{\mu}_{a,(b)} - \hat{\mu}_{i,(b)}$ Let $T_b = N_b |\mathcal{A}_b|$ be the total steps of batch b Denote error parameters: $\epsilon_b \leftarrow \sqrt{\frac{ck^3}{T_b} \log \frac{k}{\delta}}$ $\mathcal{A}_{b+1} \leftarrow \{i \in \mathcal{A}_b : \hat{\Delta}_{i,(b)} \leq 2\epsilon_b\}.$ end

378 379 5.3.1 ANALYSIS

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380 381 382 383 Theorem 5.11. For every $\delta \in (0,1]$, and integer $B > 1$, Algorithm [3](#page-6-2) is $((k+1)^{B-1}, \delta)$ -list replica-ble, and for any input bandit instance satisfying Assumption [2.1,](#page-1-1) it suffers a $O\left(kT^{\nu}\sqrt{kT\log\frac{kB}{\delta}}\right)$). *regret with probability at least* $1 - \delta$ *, where* $\nu = \frac{1}{2^{B+1}-2}$ *.*

385 386 387 Remark 5.12. We note that when $B = 2$, the algorithm is $(k + 1, \delta)$ -list replicable while en*joys a regret bound of* $O(k^{3/2}T^{2/3})$ *. For* $B = \log \log T$ *, the algorithms enjoys a regret bound of* $\widetilde{O}(k^{3/2}\sqrt{T})$, while with $k^{\log \log T}$ list-complexity [Cesa-Bianchi et al.](#page-10-14) [\(2013\)](#page-10-14).

388 389 390 391 392 393 394 We present the proof of Theorem [5.11.](#page-7-1) For $b \in [B]$, let $T_b = \Theta(T^{\alpha(2-\frac{1}{2^{b-1}})})$ be the batch length. Note that if $\nu = \frac{1}{2^{B+1}-2}$ then $T_B = T$. Therefore $\nu \approx \frac{1}{2^{B+1}-2}$ is sufficient to guarantee $\sum_{b \in [B]} T_b \approx T$. Let $\epsilon_b = \sqrt{\frac{ck^3}{T_b} \log \frac{kB}{\delta}}$ for some c. Therefore, for each $b \in [B]$, with probability at least $1 - \delta/B$, for each $i \in A_b$, $|\hat{\mu}_{i,(b)} - \mu_i| \leq \frac{\epsilon_b}{2k}$. Therefore, by Theorem [5.10,](#page-6-1) RelicableMeans outputs a $(k+1,\delta/B)$ -list means with error at most ϵ_b to each arm.

395 396 397 398 399 We now argue Algorithm [3](#page-6-2) is $((k+1)^{B-1}, \delta)$ -list replicable. Due to the list replicability of the mean estimators, we see at most $(k + 1)$ possible subset deletions at each $b = 1, \ldots, B - 1$ with high probability. Therefore, we see at most $(k+1)^{B-1}$ traces with probability $\geq 1-\delta$. The proof of the following lemma similar to the previous regret analysis, and the proof can be found in Appendix [A.3.](#page-12-0) Thus concludes the proof of Theorem [5.11.](#page-7-1)

Lemma 5.13. *The regret of Algorithm [3](#page-6-2) with probability at least* $1 - \delta$ *is bounded by* $R_T \leq$ $O\left(kT^{\nu}\sqrt{kT\log{\frac{kB}{\delta}}} \right)$ *.*

6 MULTI-ARM BANDITS: LOWER BOUND

406 407 In this section, we prove that any algorithm for k-MAB that has a regret $o(T)$ with high probability can not be $(k - 1)$ list replicable.

408 409 Theorem 6.1. *There is no* $(k - 1, \delta)$ -list replicable algorithm for k-MAB that has $o(T)$ regret with *probability* $1 - \delta$ *, for* $\delta \leq \frac{1}{k+1}$ *.*

410 411 412 413 The proof of this lower bound theorem makes use of a cubical version of Sperner/KKM lemma [De](#page-10-15) [Loera et al.](#page-10-15) [\(2002\)](#page-10-15). Informally, Sperner/KKM lemma says the following: if we "properly color" a d dimensional cube with $d+1$ colors, then there is a point p in the cube so that any arbitrary small neighborhood of p contains $d + 1$ points with different colors.

414 415 416 417 We prove Theorem [6.1](#page-7-2) in two steps. Step (1): we establish that any $(k - 1)$ -list replicable algorithm with $o(T)$ regret yields a $(k-1)$ list replicable algorithm for a problem known as (k, ϵ, δ) -BESTARM. Step (2): we establish that (k, ϵ, δ) -BESTARM does not admit $(k - 1)$ -list replicable algorithm.

418 419 We provide a proof sketch after stating relevant definitions and necessary results. The detailed proofs are given in Appendix [A.4.1.](#page-13-0)

420 We say an arm *a* is an ϵ -best arm if $\mu^* - \mu_a < \epsilon$.

421 422 423 Definition 6.2 ((k, ϵ, δ) -BESTARM). *Let* $k \in \mathbb{N}$ *and* $\epsilon, \delta \in (0, 1)$. *The* (k, ϵ, δ) -BESTARM *is following problem: given k arms with unknown means* μ_1, \ldots, μ_k *. Output an ∈-best arm. with probability* $\geq 1-\delta$. The algorithm can sample from the distribution of the arms.

424 425 426 Definition 6.3 (List replicable algorithms). An algorithm A for (k, ϵ, δ) -BESTARM is ℓ -list repli*cable if there is a list* $L \subseteq [k]$ *of size* ℓ *so that (1) for every* $i \in L$, $\mu^* - \mu_i < \epsilon$ (2) $Pr[\mathcal{A}$ *outputs a arm from* $L] \geq 1 - \delta$.

427 428 429 Lemma 6.4. If there is an (ℓ, δ) -list replicable algorithm for k-MAB that has $o(T)$ regret with *probability* $\geq 1 - \delta$ *then there is a l-list replicable algorithm for* $(k, \epsilon, 2\delta)$ *-BESTARM for any constant* ϵ *and* δ .

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⁴³¹ The above Lemma formalizes Step (1). The proof of the lemma is based on the observation that any $o(T)$ -regret algorithm for k-MAB should not play a bad arm too frequently. Thus, we could use

432 433 434 k-MAB algorithm with $o(T)$ regret to tell us an approximate best arm by simply looking at the most frequently played arm.

435 436 Therefore, to prove Theorem [6.1](#page-7-2) it suffices to show that there is no $(k-1, \frac{1}{k+1})$ -list replicable algorithm for (k, ϵ, δ) -BESTARM (Step (2)).

437 438 439 440 441 Following is a sketch of the proof. Suppose there is a $(k - 1, \delta)$ -list replicable algorithm A for (k, ϵ, δ) -BESTARM. Let C be a $(k-1)$ -dimensional cuboid. For each point $\vec{p} = (\alpha_1, \dots, \alpha_{k-1}) \in \mathcal{C}$, we associate k arms with means $(\alpha_1, \ldots, \alpha_{k-1}, \frac{1}{2})$. Each point $\vec{p} \in \mathcal{C}$ is assigned a color from $[k]$ as follows: Consider the behavior of the algorithm A on the k arms associated with the point \vec{p} . If arm $i \in [k]$ is the most likely output of A, then color the point \vec{p} with color i.

442 443 444 445 446 447 448 449 450 451 It can be shown that the above coloring is a "proper coloring" (known as Sperner/KKM coloring) of C. Thus by Sperner/KKM lemma, there exists a point $\vec{p} \in C$, such that for every $\nu > 0$, the v-neighborhood of p (points that are v close in ℓ_{∞} -norm sense) contains k points $\vec{p}_1, \ldots, \vec{p}_k$ with distinct colors. Without loss of generality, let the most likely output of A on the arms associated with the point \vec{p}_i be i. The crucial observation is that since A is $(k - 1, \delta)$ -list replicable, the probability of the most likely output is at least $\frac{1-\delta}{k-1}$. On the other hand, since the points $\vec{p}_1,\ldots,\vec{p}_k$ are arbitrarily close, by data processing inequality, it can be argued that the behavior of the algorithm A must be very similar on each of these inputs. This would imply that the algorithm A on instance associated with \vec{p}_1 must output each arm in [k] with probability at least $\frac{1-\delta}{k-1}$. This leads to contradictions as the sum of these probabilities is more than 1, for the choice of δ .

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Remark. We make a few remarks. Consider Algorithm [3](#page-6-2) with $B = 2$. With a slight modification (play the best estimate arm in the second batch), this is a $(k, 0)$ -list replicable algorithm with regret $\tilde{O}(T^{2/3})$. Thus, by Theorem [6.1,](#page-7-2) in the sub-linear regret regime, the list size of k is optimal. We also point out that $\delta \leq \frac{1}{k+1}$ is necessary due to the following: Consider the $(k, 0)$ -list replicable algorithm as discussed. Since there are only k-traces, there is a trace with probability $\leq \frac{1}{k}$. The remaining $k-1$ traces have probability at least $(1-\frac{1}{k})$. Thus this is a $(k-1, \frac{1}{k})$ list-replicable algorithm.

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7 LINEAR BANDITS

In this section, we provide the algorithm for list-replicable linear bandit. In the linear bandit setting, we are given a set of actions $A \subset \mathbb{R}^d$ for some dimension d. Similar to the MAB setting, an agent is allowed to take one action a_t from A at each time t and receive a reward r_t . The assumption is that r_t satisfies a linear structure.

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7.1 ALGORITHM

472 473 474 475 We now introduce our algorithm. The algorithm takes a phase-elimination batched structure, in each batch b, the algorithm maintains a set of surviving actions A_b such that for all $a \in A_b$, $\mu_{a^*} \le$ $\mu_a + \epsilon_{b-1}$ for some ϵ_{b-1} depending on the previous batch. Given a target regret bound R_T , we choose the current batch size, T_b , so that $\epsilon_{b-1} T_b \lesssim R_T$ and $\sum_{b=1}^B T_b \lesssim T$.

476 477 478 479 480 481 482 483 484 485 Similar to the MAB analysis, B is either constant or log-logarithmic in T . The critical component to maintain the regret bound is that we need to eliminate the arms with error smaller than the previous batch. We first choose a small set of arms from the survival set A_b . These arms are chosen such that they can be "good" representatives (in terms of linear regression) of the survival set. More specifically, we choose the G -optimal design (specified shortly), which contains $2d$ arms. Our algorithm plays each arm a specific number of times to obtain a sufficient number of samples about its mean. With these samples, we call the ReplicableMeans (Theorem [5.10\)](#page-6-1) estimator to produce $a(2d+1)$ -list-replicable for their means. We then solve linear regression for these estimated means to obtain θ^* for this batch and eliminate the arms with sub-optimality below the accuracy level. We will show that the algorithm halts in at most B batches and achieves the desired regret bound. The list-complexity is therefore $(2d + 1)^{B-1}$.

Initialize: $A_1 = A$, $\epsilon_0 = 1$, $\nu \leftarrow \frac{1}{2^{B+1}-2}$, $\alpha \leftarrow \frac{1}{2} + \nu$

 $\mathrm{Let}\, \bar{\mu}_{(b)} \leftarrow \mathrm{ReplicableMeans}(\mu'_{(b)})$

Solve for estimated mean by: $\hat{\theta} \leftarrow (\Phi_b^{\top} \Phi_b)^{\dagger} \Phi_b^{\top} \bar{\mu}_{(b)}$

 $\mathcal{A}_{b+1} \leftarrow \{a \in \mathcal{A}_{b} : \max_{a' \in \mathcal{A}_{b}} \langle a', \hat{\theta} \rangle - \langle a, \hat{\theta} \rangle \le \epsilon_{b}/2\}$

Algorithm 4: $(2d+1)^{B-1}$ -List Replicable Linear Bandit Algorithm **Input:** Horizon T, Number of batches $B > 1$, Failure probability $\delta > 0$

 $\mu'_{(b)} = (\mu'_{a,(b)})_{a \in \text{supp}(\pi_b)}$ (halt the algorithm if T arms are played)

Let $\Phi_b = [a]_{a \in \text{supp}(\pi_b)}^{\top}$ be the matrix of stacking all actions in $\text{supp}(\pi_b)$

Denote error parameter: $\epsilon_b \leftarrow \sqrt{\frac{cd^4 \log \frac{d'B}{\delta}}{T_b}}$, where $T_b = |\text{supp}(\pi_b)| N_b$ Eliminate actions $a \in A_b$ with sub-optimality below the accuracy level:

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end

for $b=1,\ldots,B$ do

506 507 508 Definition 7.1. For any compact set $A \subset \mathbb{R}^d$, let $\pi : A \to [0,1]$ be a distribution on A. Denote $V(\pi) = \sum_a \pi(a)aa^\top$ *and* $g(\pi) = \sup_{a \in \mathcal{A}} \lim_{\lambda \to 0} ||a||_{(\lambda I + V(\pi))^{-1}}$ *.* π *is a c-G-optimal design for* A, if $g(\pi) \leq cd$.

 $b=1,...,b$ do
Find a $\sqrt{2}$ -*G*-optimal design π_b for \mathcal{A}_b using Corollary [7.3](#page-9-1) with $d' = |\text{supp}(\pi_b)| \leq 2d$. For $a \in \text{supp}(\pi_b)$, play a for $N_b \leftarrow \lceil T^{\alpha(2-\frac{1}{2^{b-1}})}/d' \rceil$ times and obtain empirical mean

509 510 Theorem 7.2 (G-optimal design [Kiefer & Wolfowitz](#page-10-16) [\(1960\)](#page-10-16)). *For any compact subset* $A \subset \mathbb{R}^d$, *there exists a* 1-G-optimal design π , $G \subset A$ *such that* $|\text{supp}(\pi)| = d$.

511 512 513 Corollary 7.3. *For any compact subset* $A \subset \mathbb{R}^d$, *there exists a* $\sqrt{2}$ -G-optimal design π , $G \subset A$, *such that* $|\text{supp}(\pi)| \leq 2d$ *and* π *is a uniform distribution over* supp (π) *.*

514 515 516 517 Theorem 7.4 (Guarantee of Algorithm [4\)](#page-9-2). *For every* $\delta \in (0,1]$ *, and integer* $B > 1$ *, Algorithm [4,](#page-9-2) for input bandit instance satisfying Assumption [2.4,](#page-1-2) with probability at least* 1 − δ*, has list-complexity* $O[(2d+1)^{B-1}]$, and enjoys a regret bound $R_T \leq O\left(d^2T^{\nu}\sqrt{T\log{\frac{dB}{\delta}}} \right)$ *where* $\nu = \frac{1}{2^{B+1}-2}$.

8 CONCLUSION

521 522 523 524 525 526 This work introduces and initiates the study of list replicability for the Multi-Armed Bandits problem. We designed various list-replicable algorithms for k -MAB with near-optimal regret in T and list-complexity linear/polynomial in k. To complement these results, we show that we can not hope to design $(k - 1)$ -list replicable algorithms with sublinear regret. An open question is to close the gap between upper and lower bounds on the list complexity. For example, in Theorem [5.4,](#page-5-1) if we chose $\delta = \frac{1}{k}$, then the list size is $O(k^2)$. Can we prove that list complexity is $\Omega(k^2)$? A general question is to investigate trade-offs between list complexity and regret.

527 528 529 530 531 532 533 534 535 Remark about UCB. The list complexity of UCB-based algorithms is exponentially dependent on T. Consider the case when $k = 2$ and both arms have identical distributions. Let UCB₁ and $UCB₂$ represent the UCB estimates of arm 1 and arm 2, respectively. Let us assume that at some time t, $UCB_1 < UCB_2$. UCB algorithm dictates that we shall play arm 2 till the estimate of arm 1 is larger. However, because the samples are random, the time at which we start playing arm 1 is probabilistic. For each time step where a switch is possible results in a new trace. This trait makes the list complexity of UCB-based algorithms exponentially dependent on T . Note that the list complexities of our algorithms are independent of T . We leave it as open question about what changes need to be made to UCB to guarantee list replicability.

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537 538 REFERENCES

539 Shipra Agrawal and Navin Goyal. Near-optimal regret bounds for thompson sampling. *Journal of the ACM (JACM)*, 64(5):1–24, 2017.

540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 Peter Auer, Nicolo Cesa-Bianchi, and Paul Fischer. Finite-time analysis of the multiarmed bandit problem. *Machine learning*, 47:235–256, 2002. Monya Baker. 1,500 scientists lift the lid on reproducibility. *Nature*, 533(7604), 2016. C Glenn Begley and Lee M Ellis. Raise standards for preclinical cancer research. *Nature*, 483 (7391):531–533, 2012. Sebastien Bubeck, Nicolo Cesa-Bianchi, et al. Regret analysis of stochastic and nonstochastic multi- ´ armed bandit problems. *Foundations and Trends® in Machine Learning*, 5(1):1–122, 2012. Mark Bun, Roi Livni, and Shay Moran. An equivalence between private classification and online prediction. In Sandy Irani (ed.), *61st IEEE Annual Symposium on Foundations of Computer Science, FOCS 2020, Durham, NC, USA, November 16-19, 2020*, pp. 389–402. IEEE, 2020. Nicolo Cesa-Bianchi and Paul Fischer. Finite-time regret bounds for the multiarmed bandit problem. In *ICML*, volume 98, pp. 100–108. Citeseer, 1998. Nicolo Cesa-Bianchi, Ofer Dekel, and Ohad Shamir. Online learning with switching costs and other adaptive adversaries. *Advances in Neural Information Processing Systems*, 26, 2013. Jesus A. De Loera, Elisha Peterson, and Francis Edward Su. A polytopal generalization of sperner's lemma. *Journal of Combinatorial Theory, Series A*, 100(1):1–26, 2002. ISSN 0097-3165. doi: https://doi.org/10.1006/jcta.2002.3274. URL [https://www.sciencedirect.com/](https://www.sciencedirect.com/science/article/pii/S0097316502932747) [science/article/pii/S0097316502932747](https://www.sciencedirect.com/science/article/pii/S0097316502932747). Peter Dixon, A. Pavan, Jason Vander Woude, and N. V. Vinodchandran. List and certificate complexities in replicable learning. In A. Oh, T. Naumann, A. Globerson, K. Saenko, M. Hardt, and S. Levine (eds.), *Advances in Neural Information Processing Systems*, volume 36, pp. 30784–30806. Curran Associates, Inc., 2023. URL [https://proceedings.neurips.cc/paper_files/paper/2023/file/](https://proceedings.neurips.cc/paper_files/paper/2023/file/61d0a96d4a73b626367310b3ad32579d-Paper-Conference.pdf) [61d0a96d4a73b626367310b3ad32579d-Paper-Conference.pdf](https://proceedings.neurips.cc/paper_files/paper/2023/file/61d0a96d4a73b626367310b3ad32579d-Paper-Conference.pdf). Eric Eaton, Marcel Hussing, Michael Kearns, and Jessica Sorrell. Replicable reinforcement learning. In Alice Oh, Tristan Naumann, Amir Globerson, Kate Saenko, Moritz Hardt, and Sergey Levine (eds.), *Advances in Neural Information Processing Systems 36: Annual Conference on Neural Information Processing Systems 2023, NeurIPS 2023, New Orleans, LA, USA, December 10 - 16, 2023*, 2023. Hossein Esfandiari, Alkis Kalavasis, Amin Karbasi, Andreas Krause, Vahab Mirrokni, and Grigoris Velegkas. Replicable bandits. In *The Eleventh International Conference on Learning Representations*, 2023. URL <https://openreview.net/forum?id=gcD2UtCGMc2>. Badih Ghazi, Ravi Kumar, and Pasin Manurangsi. User-level differentially private learning via correlated sampling. In Marc'Aurelio Ranzato, Alina Beygelzimer, Yann N. Dauphin, Percy Liang, and Jennifer Wortman Vaughan (eds.), *Advances in Neural Information Processing Systems 34: Annual Conference on Neural Information Processing Systems 2021, NeurIPS 2021, December 6-14, 2021, virtual*, pp. 20172–20184, 2021. Russell Impagliazzo, Rex Lei, Toniann Pitassi, and Jessica Sorrell. Reproducibility in learning. In *Proceedings of the 54th Annual ACM SIGACT Symposium on Theory of Computing*, pp. 818–831, 2022. John PA Ioannidis. Why most published research findings are false. *PLoS medicine*, 2(8):e124, 2005. Amin Karbasi, Grigoris Velegkas, Lin Yang, and Felix Zhou. Replicability in reinforcement learning. *Advances in Neural Information Processing Systems*, 36, 2024. Emilie Kaufmann, Olivier Cappé, and Aurélien Garivier. On bayesian upper confidence bounds for bandit problems. In *Artificial intelligence and statistics*, pp. 592–600. PMLR, 2012. Jack Kiefer and Jacob Wolfowitz. The equivalence of two extremum problems. *Canadian Journal of Mathematics*, 12:363–366, 1960.

A.2 PROOFS OF SECTION [5.2](#page-4-0)

Proof of Lemma [5.6.](#page-5-2) Following a similar analysis for the proof of Lemma [5.2](#page-4-2)

We first prove, for all $i \in [k]$, $Pr(X_i \ge m_i | E) = 1$.

645 Let $i \in [k],$ for each $b \leq m_i-1$

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$$
\hat{\Delta}_{i,(b)} \leq \Delta_i + 2\epsilon_b \leq \tau_{m_i-1} + 2\epsilon_b \leq \tau_b + \frac{3(\sqrt{2}-1)}{2C}\tau_b \leq 3\tau_b \leq \mathfrak{D}_b
$$

We now prove, For all $i \in [k]$, $Pr(X_i \le m_i + 2|E) = 1$. Note that $\epsilon_b < \tau_b$. Let $i \in [k]$, for $b = m_i + 2$, $\hat{\Delta}_{i,(b)} \geq \Delta_i - 2\epsilon_b > \tau_{m_i} - 2\tau_b = 5\tau_{b-1} - 2\cdot \frac{\tau_{b-1}}{\epsilon}$ $\frac{b-1}{5} > 3\tau_{b-1} > \mathfrak{D}_b$ \Box

Proof of Lemma [5.9.](#page-6-3) Ignoring constants.

$$
R_T \le T_1 \cdot 1 + \sum_{b=2}^{B} T_b \mathfrak{D}_{b-1} \le \sum_{b=2}^{B} 5^{2b} C^2 \cdot \sqrt{\frac{k}{5^{2b}} \log \frac{1}{\theta}} = C^2 \sqrt{k \log \frac{1}{\theta}} \cdot 25^{\frac{B}{2}} = \frac{k}{\delta} \sqrt{k \log \frac{k \log T}{\delta}}.
$$

A.3 PROOFS OF SECTION [5.3](#page-6-0)

Proof of Lemma [5.13.](#page-7-3) Let $\theta = \frac{\delta}{B}$, we have, ignoring constants

$$
R_T \leq T_1 \cdot 1 + \sum_{b=2}^{B} T_b \cdot \epsilon_b = T^{\alpha} + \sum_{b=2}^{B} T_b \cdot \sqrt{\frac{k^3}{T_{b-1}} \log \frac{k}{\theta}} = T^{\alpha} + \sqrt{k^3 \log \frac{k}{\theta}} \sum_{b=2}^{B} \frac{T_b}{\sqrt{T_{b-1}}}
$$

= $T^{\alpha} + \sqrt{k^3 \log \frac{k}{\theta}} \sum_{b=2}^{B} T^{\alpha} = T^{\alpha} + BT^{\alpha} \sqrt{k^3 \log \frac{kB}{\delta}}$
= $O\left(kT^{\nu} \sqrt{kT \log \frac{kB}{\delta}}\right)$

 \Box

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Proof of Lemma [5.8.](#page-6-4) We first prove

Claim A.2. *Let* $i \in [k]$ *and* $b = m_i, m_i + 1, m_i + 2$ *, there are at most two b-bad rs for i*.

Proof. Let $b = m_i, m_i + 1, m_i + 2$. Firstly, observe that the decision boundaries $\mathfrak{D}_{b,1}, \mathfrak{D}_{b,2}, \ldots, \mathfrak{D}_{b,C}$ are spaced by $4\epsilon_b$. The estimate interval $[\Delta_i - 2\epsilon_b, \Delta_i + 2\epsilon_b]$ has length $4\epsilon_b$ and can contain at most two $\mathfrak{D}_{b,r}$, $\mathfrak{D}_{b,r+1}$. See Figure [1.](#page-5-0) П

Let $i \in [k]$. Fix $b = m_i$ or $m_i + 1$ or $m_i + 2$, the number of b-bad r's for i at most 2 via Claim [A.2.](#page-12-1) **683** In the worst case, there are 2 bad rs for each of m_i , $m_i + 1$, and $m_i + 2$, and all of them are different. **684** Therefore, there can be at most $3 \times 2 = 6$ for *i*. Therefore, there can be at most $k \times 6$ bad *rs*. ⊔ **685**

687 A.4 PROOFS OF SECTION [6](#page-7-0)

688 689 690 691 692 693 694 *Proof of Lemma* [6.4.](#page-7-4) Let M be a (ℓ, δ) -list replicable algorithm for k-MAB that has a regret $o(T)$ with probability $\geq 1 - \delta$. We design a ℓ -list replicable algorithm A for $(k, \epsilon, 2\delta)$ -BESTARM using M. A works as follows: Simulate M for T steps and let N_i be the number of times arm i was played. Output the arm that is most frequently played: That is, output $\arg \max_i N_i$, breaking ties by outputting the smallest numbered arm. The list replicability of $\mathcal A$ follows due to the ℓ -list replicability M. It suffices to show that A outputs an arm ϵ -close to the best arm with probability $\geq 1-\delta.$

695 696 697 698 Let Ω be the sample space of the algorithm M. Each sample point $\omega \in \Omega$ is a sequence of alternating actions and rewards. We say that a sample point ω is *good* if the regret of M along ω is $o(T)$ and the trace associated with ω is in the list. By union, it follows that Pr[ω is good] $\geq 1 - 2\delta$.

699 700 701 Consider a good $\omega \in \Omega$ Let $a = \mathcal{A}(\omega)$ be the output in this sample point. We now claim the $\mu_a \geq$ $\mu^* - \epsilon$. Assume for contradiction's sake, that the output $\mu_a < \mu^* - \epsilon$. We know that $N_a(\omega) \geq \frac{T}{k}$ because A outputs most frequently played arm. Hence the regret along ω is $\geq N_a(\omega)\epsilon \geq \frac{T\epsilon}{k}$. Since ϵ and k are constants, this is a contradiction. Thus Pr[A outputs ϵ -best arm] $\geq 1 - \delta$.

702 703 A.4.1 LOWERBOUND ON THE LIST COMPLEXITY OF (k, ϵ, δ) -BESTARM

704 705 706 In this section, we will prove that there is no $(k-1, \frac{1}{k+1})$ -list replicable algorithm for (k, ϵ, δ) -BESTARM. We first introduce the necessary definitions and notation and then state Sperner/KKM Lemma.

707 708 709 710 711 712 Definition A.3 (Sperner/KKM Coloring). Let $d \in \mathbb{N}$ and let C be a d-dimensional cuboid and let V *be the vertex set (corners) of C. For a face* F *of* C (*of any dimension*) let V_F *be the set of vertices of* F. A coloring function color : $C \rightarrow [d+1]$ of C is called a Sperner/KKM coloring if (1) ${color(v) \mid v \in V} = [d+1]$ *(intuitively, all colors are used on the corners) (2) for any face* F of C, for any point $p \in F$, it holds that $color(p) = color(v)$ for some $v \in V_F$ (informally, the color of p *is color of one of the vertices in the face* F*).*

713 714 715 716 Theorem A.4 (Cubical Sperner/KKM lemma [De Loera et al.](#page-10-15) [\(2002\)](#page-10-15)). Let $d \in \mathbb{N}$ and let C be a d-dimensional cuboid. Let $color : \mathcal{C} \to [d+1]$ be a Sperner/KKM coloring of C. Then there is a *point* p such that for every $\nu > 0$, ν -neighbourhood of p, $\mathcal{B}_{\nu}^{\infty}(p)$ that contains $d + 1$ points with *distinct colors.*

717 718 Theorem A.5. Let $\epsilon \leq \frac{1}{2k}$ and $\delta \leq \frac{1}{k+1}$. There is no $(k-1)$ -list replicable algorithm for (k, ϵ, δ) -BESTARM*.*

719 720 721 *Proof of Theorem [A.5.](#page-13-1)* Let A be a $(k-1)$ -list replicable algorithm for the (k, ϵ, δ) -BESTARM where the total number of times arms are played is n .

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722 723 724 725 726 727 728 We will use Sperner/KKM Lemma on the $(k - 1)$ -dimensional cuboid to arrive at a contradiction. The cuboid C is defined as $[0, 1] \times [0, 1 - \epsilon] \times [0, 1 - 2\epsilon] \times \cdots \times [0, (1 - (k - 2)\epsilon)]$. For each point $p = \langle \alpha_1, \cdots \alpha_{k-1} \rangle \in \mathcal{C}$, associate an instance $I(p) = \langle \alpha_1, \alpha_2, \cdots, \alpha_{k-1}, \frac{1}{2} \rangle$ of the (k, ϵ, δ) -BESTARM. We assign a color from [k] to each point of the cuboid C as follows: Color of a point p is the arm whose output probability is the largest when the algorithm \overline{A} is run on input $I(p)$ (breaking the ties arbitrarily). More formally, $color(p) = \arg \max_{a \in [k]} \{Pr[A(I(p)) = a]\}.$ We first claim that the above coloring is a valid Sperner/KKM coloring.

730 731 732 733 734 Coloring of the vertices of C. A vertex (corner) v of C is specified by $\langle \alpha_1, \alpha_2, \ldots, \alpha_{k-1} \rangle$ where α_i is either 0 or $(1 - (i - 1)\epsilon)$. Let i^{*} be the *first index* i where α_i is non-zero if such an i exists otherwise (when all α_i 's are 0) $i^* = k$. Note that the $color(v) = i^*$. This is because for any $i \neq i^*$, $a_{i^*} - a_i \geq \epsilon$ and A should output the arm i^* with probability $\geq 1 - \delta$. Note that all k colors are used while coloring the vertices of C. Figure [2](#page-15-0) for the case $k = 3$.

736 737 738 739 Coloring of any face F. For an ℓ ($0 < \ell < k - 2$), consider a $(k - 1 - \ell)$ dimensional face F of C. Face F is specified specifying ℓ coordinates $i_1 < i_2 < \cdots < i_\ell$ and fixing them to be α_{i_j} , where α_{i_j} is either 0 or $(1-(i_j-1)\epsilon)$. We claim that the color of any point on F is one of the colors of \mathcal{V}_F .

740 741 742 743 744 745 Case 1. All α_i s are 0 in F: In this case the $color(V_F) = [k] \setminus \{i_1, \ldots, i_l\}$. This is because of the following. Fix $i \in [k] \setminus \{i_1, \dots, i_\ell\}$. Consider a point p whose ith co-ordinate is $(1 - (i - 1)\epsilon)$ and all other co-ordinates are zero. This point belongs to V_F and gets color i. Note that the kthcoordinate of $I(p)$ is $1/2$ for every p. Thus the color of a point p can not belong to $\{i_1, i_2, \dots, i_\ell\}$. By a very similar reasoning, it follows that for any point p on F cannot have color from $\{i_1, \ldots, i_l\}$ and hence the coloring is proper.

747 748 749 750 751 Case 2. At least one α_{i_j} is non-zero: Let j^* be the smallest index such that among $\{1, \dots, \ell\}$ such $\alpha_{i_{j^*}} \neq 0$. In this case, we claim that the $color(V_F) = \{1, \cdots i_{j^*}\} \setminus \{i_1, \cdots, i_{j^*-1}\}$. Fix a vertex $v \in$ $V(F)$. Color of this vertex cannot be any of i_1, \dots, i_{j^*-1} as all these co-ordinates in $I(v)$ are zero. Let $i > i_{j^*}$, note that $\alpha_{i_{j^*}} - \alpha_i \ge \epsilon$. Thus i can not be the color of v. We can apply a very similar reasoning to conclude that for any point p on F, its color belongs to $\{1, \dots, i_{j^*}\}\setminus \{i_1, \dots, i_{j^*-1}\}.$

752 753 754 To finish the proof, we need the following *distance lemma* that can be proved by Data Processing inequality.

755 Lemma A.6 (Distance Lemma). Let p and q be the two points of the cuboid C such that $||p-q||_{\infty} \leq$ *v*. Then, for any $a \in [k]$, $|\Pr[A(I(p)) = a] - \Pr[A(I(q)) = a]| \leq n \cdot k \cdot \nu$

756 757 758 759 760 761 762 Now we are ready to complete the proof. Let $\nu = \frac{1}{k^5 n}$. By the Sperner/KKM Lemma, there is ν neighborhood in C (in ℓ_{∞} -norm) with points p_1, \cdots, p_k such that each point gets a distinct color. Let $a_i = \arg \max_{a \in [k]} \{ \Pr[\mathcal{A}(I(p_i)) = a] \}.$ Note that all a_i 's are distinct as colors of p_i 's are distinct. By definition of list replicability $Pr[A(I(p_i) = a_i] \ge \frac{1-\delta}{k-1} \ge \frac{k}{(k-1)(k+1)} = \frac{k}{k^2-1}, 1 \le i \le k$. We have the following $Pr[A(I(p_1) = a_1] \ge \frac{k}{k^2-1}]$ and for $2 \le i \le k$, $Pr[A(I(p_1) = a_i] \ge k]$ $\frac{k}{k^2-1} - n \cdot k \cdot \nu = \frac{k}{k^2-1} - \frac{1}{k^4}$ by distance lemma.

763 764 765 Thus, the following leads to a contradiction, $Pr[A(I(p_1)) \in \{a_1, \dotsb a_k\}] \ge \frac{k}{k^2-1} + \frac{k(k-1)}{k^2-1} - \frac{k-1}{k^4} >$ 1.

A.5 PROOFS OF SECTION [7](#page-8-0)

768 769 770 771 *Proof of Corollary* [7.3.](#page-9-1) Let π ^{init} be a 1-G-optimal design whose existence is guaranteed by Theo-rem [7.2.](#page-9-3) For each $a \in \text{supp}(\pi^{\text{init}})$, we add $\lceil d\pi^{\text{init}}(a) \rceil$ copies of a into the support of π . Note that this implies supp(π) is a multiset. We define π to be the uniform distribution over all actions on its support.

Clearly,

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$$
|\text{supp}(\pi)| \le \sum_{a \in \text{supp}(\pi^{\text{init}})} \lceil d\pi^{\text{init}}(a) \rceil \le |\text{supp}(\pi^{\text{init}})| + d \sum_{a \in \text{supp}(\pi^{\text{init}})} \pi^{\text{init}}(a) = 2d.
$$

Moreover,

$$
V(\pi) = \frac{1}{|\text{supp}(\pi)|} \sum_{a \in \text{supp}(\pi)} a a^{\top} \succeq \frac{1}{2d} \sum_{a \in \text{supp}(\pi)} a a^{\top} \succeq \frac{1}{2} \sum_{a' \in \text{supp}(\pi^{\text{init}})} \pi^{\text{init}}(a') a a^{\top} = \frac{1}{2} V(\pi^{\text{init}}).
$$

Therefore, π is a $\sqrt{2}$ -G-optimal design.

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782 783 *Proof of Theorem [7.4.](#page-9-4)* We first show correctness. For each batch b, let $\mu = (\mu_a)_{a \in \text{supp}(\pi_b)}$. By Hoeffding bound and a union bound, for each batch b, with probability at least $1 - \delta/B$,

$$
\forall a \in \text{supp}(\pi_b): \quad |\mu'_{a,(b)} - \mu_a| \le O\left(\frac{\epsilon_b}{\sqrt{d^3}}\right)
$$

where μ' is the empirical mean and ϵ_b is error parameter defined in Algorithm [4.](#page-9-2) Thus, by The-orem [5.10,](#page-6-1) we have that with probability at least $1 - \delta/B$, the estimated mean $\bar{\mu}_{(b)}$ satisfies $(|\text{supp}(\pi_b)| + 1)$ -list replicablity and

$$
\forall a \in \text{supp}(\pi_b): \quad |\bar{\mu}_{a,(b)} - \mu_a| \le O\left(\frac{\epsilon_b}{\sqrt{d}}\right)
$$

Let $V = \sum_{a \in \text{supp}(\pi_b)} aa^{\top}$. We have

$$
\forall a \in \mathcal{A}_b : \langle a, (\theta^* - \hat{\theta}) \rangle \le \langle a(V^{\dagger})^{1/2}, V^{1/2}(\theta - \hat{\theta}) \rangle
$$

$$
\le \sqrt{a^{\top} V^{\dagger} a} \cdot \sqrt{(\theta^* - \hat{\theta})^{\top} V(\theta^* - \hat{\theta})}
$$

$$
\le \sqrt{g(\pi_b) / |\text{supp}(\pi_b)|} \sqrt{(\theta^* - \hat{\theta})^{\top} \Phi^{\top} \Phi(\theta^* - \hat{\theta})}
$$

$$
\le O(\epsilon_b)
$$

where we use

$$
\|\Phi(\theta^* - \hat{\theta})\|_2 = \|\bar{\mu}_{a,(b)} - \mu_a\|_2 \le O(\epsilon_b).
$$

Hence, the overall regret of the algorithm is with probability at least $1 - \delta$ bounded by,

$$
R_T \le T_1 \cdot 1 + \sum_{b=2}^B T_b \cdot \epsilon_b = T^{\alpha} + \sum_{b=2}^B T_b \cdot \sqrt{\frac{d^4}{T_{b-1}} \log \frac{dB}{\delta}} = T^{\alpha} + \sqrt{d^4 \log \frac{dB}{\delta}} \sum_{b=2}^B \frac{T_b}{\sqrt{T_{b-1}}} = T^{\alpha} + \sqrt{d^4 \log \frac{dB}{\delta}} \sum_{b=2}^B T^{\alpha} = T^{\alpha} + BT^{\alpha} \sqrt{d^4 \log \frac{dB}{\delta}} = \tilde{O} \left(d^2 T^{\nu} \sqrt{T} \right).
$$

 where we ignore constant factors and $\alpha = \frac{1}{2} + \nu$. We also note that $T_B \leq T$ and $\sum_{i=1}^B T_b = T$ Thus, with probability at least $1 - \delta$, the list complexity is bounded by $(2d+1)^{B-1}$. \Box μ_2 $(0, 1 - \epsilon)$ $(1, 1 - \epsilon)$ (0, 0) $(1, 0)$ μ_1 Figure 2: Coloring of 2-dimensional cuboid for $k = 3$. Colors blue, red, and green are identified with coloring with arms 1,2, and 3 respectively. Point (x, y) is associated with instance $(x, y, 1/2)$.