Disagreement-based combinatorial pure exploration: Efficient algorithms and an analysis with localization

Tongyi Cao *1 and Akshay Krishnamurthy †1

1University of Massachusetts, Amherst, MA

December 1, 2017

Abstract

We design new algorithms for the combinatorial pure exploration problem in the multi-arm bandit framework. In this problem, we are given $K$ distributions and a collection of subsets $V \subset 2^K$ of these distributions, and we would like to find the subset $v \in V$ that has largest cumulative mean, while collecting, in a sequential fashion, as few samples from the distributions as possible. We study both the fixed budget and fixed confidence settings, and our algorithms essentially achieve state-of-the-art performance in all settings, improving on previous guarantees for structures like matchings and submatrices that have large augmenting sets. Moreover, our algorithms can be implemented efficiently whenever the decision set $V$ admits linear optimization. Our analysis involves precise concentration-of-measure arguments and a new algorithm for linear programming with exponentially many constraints.

1 Introduction

Many unsupervised learning or exploratory data analysis problems that arise across engineering and scientific disciplines involve recovering structural information from noisy data. For example, the long line of research on stochastic block models formulates graph clustering as denoising an adjacency matrix to recover a low rank binary matrix that encodes cluster membership [35, 1]. Other related structures that have seen intense theoretical investigation include submatrices [9, 32, 17], hierarchical clusterings [7], and graph-theoretic structures like matchings, spanning trees, and paths [5, 2].

In this paper we design and analyze interactive learning algorithms for these structure discovery problems. An interactive algorithm interleaves data collection with analysis, which is possible in many applications (e.g., communication network measurement [12]) and can also lead to substantially better statistical performance [11]. Our mathematical formulation is through the combinatorial pure exploration for multi-armed bandits framework [16], a recently-proposed generalization of the best-arm identification problem [34, 6] in the bandit literature. In this setting, we have access to $K$ arms, each associated with a distribution with unknown mean $\mu_a$, as well as a combinatorial decision set $V \subset 2^K$, and we would like to identify the subset $v \in V$ that has maximum mean $\mu(v) = \sum_{a \in v} \mu_a$. We can, in sequential fashion, query an arm and obtain an iid sample from that arm’s distribution, and we would like to minimize the total number of samples collected.

* tcao@cs.umass.edu
† akshay@cs.umass.edu
This model has been studied in several recent works both in the general form and with specific instantiations of the decision set \( \mathcal{V} \). The most popular examples are \( \text{TOP-K} \) and \( \text{MATROID} \), where the decision set corresponds to all \( \binom{K}{k} \) subsets and the bases of a matroid, respectively (c.f. [27, 30, 15, 13]). While near-matching upper and lower sample complexity bounds are known for these and other minimally structured examples that satisfy a matroid augmentation-type property [16], no existing algorithm achieves the optimal sample complexity in the general case despite several attempts [16, 21, 14]. Indeed, these three results can be polynomially worse than a simple non-interactive algorithm based on maximum likelihood estimation in the highly-structured setting, which informally corresponds to augmenting sets having \( \omega(1) \) size (See Proposition 2). With this in mind, our goal is to design an algorithm that is never worse than this non-interactive baseline, but that can be much better.

Since we are doing combinatorial optimization, we typically consider decision sets \( \mathcal{V} \) that are exponentially large but have small description length, so that direct enumeration of the elements in \( \mathcal{V} \) is not computationally tractable. Instead, we assume that \( \mathcal{V} \) supports efficient linear optimization, and our main algorithms only access \( \mathcal{V} \) through a linear optimization oracle. To shed further light on purely statistical issues, we also present some results for computationally inefficient algorithms.

**Our Contributions.** We make the following contributions:

1. First, we prove that in the highly-structured setting, prior results [16, 21, 14] can be polynomially worse than a simple non-interactive algorithm based on maximum likelihood estimation.

2. In the fixed confidence setting, we design an algorithm that is never worse than the non-interactive MLE, but that can adapt to heterogeneity in the problem to be substantially better. Using several novel algorithmic ideas, we show how to implement the algorithm to run in polynomial time with access to a linear optimization oracle. We also derive a computationally inefficient fixed confidence algorithm with a more refined sample complexity bound.

3. In the fixed budget setting, we design a new oracle-efficient algorithm with similar statistical improvements, improving on the non-interactive method when there is heterogeneity in the problem.

4. To demonstrate our improvements over prior work, we instantiate our results in concrete examples.

**Our Techniques.** The core of our statistical analysis is a new deviation bound for the combinatorial pure exploration problem that localizes the optimal decision set. In Theorem 1, we prove that it suffices to have a form of localized concentration, where for each \( v \in \mathcal{V} \), its mean difference to the optimal subset is controlled at a level proportional to its symmetric set difference with the optimum. On the other hand, prior work uses less-refined concentration arguments to drive the query rule, and this leads to worse guarantees. Our improvements stem from using only the localized concentration inequality in our interactive procedure.

The fixed confidence setting poses a significant challenge, since confidence bounds typically appear algorithmically, but ours is centered around the optimum, which is of course unknown! We address this difficulty with a new elimination-style algorithm that eliminates a hypothesis \( v \in \mathcal{V} \) when any other candidate is significantly better and that queries only where the survivors disagree. Using only localized concentration, we can prove that \( v^* \) is never eliminated, but also that \( v^* \) will eliminate every other \( v \in \mathcal{V} \) eventually, since it will be significantly better. This algorithm resembles approaches for disagreement-based active learning [23], but uses a much stronger elimination criteria that is crucial for obtaining our sample complexity guarantees.

Computationally, deciding if the surviving candidates disagree on an arm poses further challenges, since the description of the surviving set involves exponentially many constraints, one for each candidate \( u \in \mathcal{V} \).
This problem can be written as a linear program, which we can solve using the Plotkin-Shmoys-Tardos reduction to online learning [37]. However, since there are exponentially many constraints in the LP, the standard approach of using multiplicative weight updates fails, but exploiting further structure in the problem, we can run Follow-the-Perturbed-Leader, since the online learner’s problem is actually linear in the candidates $u$ that parametrize the constraints. Thus with a linear optimization oracle, we obtain a computationally efficient algorithm with strong sample complexity guarantee for the fixed confidence setting.

2 Preliminaries

We study the combinatorial pure exploration problem in the stochastic multi-armed bandit framework. We are given a finite set of arms $A \triangleq \{1, \ldots, K\}$, where arm $a$ is associated with a distribution $\nu_a$ with unknown mean $\mu_a \in [-1, 1]$ and support $[-1, 1]$ \footnote{Some of our results can be easily generalized to subgaussian distributions with arbitrary but known variance.}. Further, we are given a decision class $V \subseteq 2^A$. We use $d(v, v^*) \triangleq |v \ominus v^*|$ where $\ominus$ denotes the symmetric set difference. The goal is to identify a set $v \in V$ that has the largest collective mean $\sum_{a \in v} \mu_a$. With the vectorized notation $\mu \triangleq (\mu_1, \ldots, \mu_K)$ and $V \subset \{0, 1\}^K$, we seek to compute

$$
 v^* \triangleq \arg\max_{v \in V} \langle v, \mu \rangle.
$$

We are interested in learning algorithms that acquire information about the unknown $\mu$ in an interactive, iterative fashion. At the $t$th iteration, the learning algorithm selects an arm $a_t$ and receives a corresponding observation $y_t \sim \nu_{a_t}$. Importantly, the algorithm’s choice $a_t$ can depend on all previous decisions and observations $\{(a_\tau, y_\tau)\}_{\tau=1}^{t-1}$ and possibly any additional randomness.

We consider two related performance goals. In the fixed budget setting, the learning algorithm is given a budget of $T$ queries, after which it must produce an estimate $\hat{v}$ of the true optimum $v^*$, and we seek to minimize the probability of error $P[\hat{v} \neq v^*]$. In the fixed confidence setting, a failure probability parameter $\delta$ is provided as input to the algorithm, which still produces an estimate $\hat{v}$, but must further enjoy the guarantee that $P[\hat{v} \neq v^*] \leq \delta$. In this setting, we seek to minimize the number of queries issued by the algorithm.

Since we are performing combinatorial optimization over $V$, for computational efficiency, we equip our algorithms with a linear optimization oracle for $V$. Formally, we assume access to a function

$$
 \text{ORACLE}(c) \triangleq \arg\max_{v \in V} \langle v, c \rangle, \quad (1)
$$

that solves the off-line combinatorial optimization problem. This is a basic computational requirement since otherwise even if $\mu$ were known we would not be able to recover $v^*$. Technically, we allow our oracle to take one or two additional linear constraints, which poses no additional difficulty in the examples of interest (e.g., shortest paths and matchings). However, a natural question for future work is to understand the computational and statistical consequences of approximate oracles for the combinatorial exploration problem.

To fix ideas, we describe two potential applications of our results (see also Section 4).

**Example 1 (Bipartite Matching).** Consider a complete bipartite graph with $\sqrt{K}$ vertices in each partition so that there are $K$ edges, which we identify with $A$. Let $V$ denote the perfect bipartite matchings and let $\mu$ assign a weight to each edge. Here, the combinatorial exploration task amounts to finding the maximum-weight bipartite matching in a graph with edge weights that are initially unknown. Note that the linear optimization oracle (1) is available here. Such problems have applications in crowd-sourcing [36] and job scheduling, where we would like to identify the best assignment of jobs to servers or workers.
Example 2 (Biclione or Biclustering). In the same graph-theoretic setting, now let $V$ denote the set of bicliques with $\sqrt{s}$ vertices from each partition. Equivalently in a $\sqrt{K} \times \sqrt{K}$ matrix, $V$ corresponds to all submatrices of $\sqrt{s}$ rows and $\sqrt{s}$ columns. This problem is variously referred to as biclique, biclustering, or submatrix localization, and has applications in genomics [42]. Note however that the offline problem is known to be NP-hard in general, so the oracle is not available here.

A new complexity measure. We define two complexity measures that govern the performance of our algorithms. We start with the notion of a gap between the decision sets.

$$\Delta_v(\mu) \triangleq \frac{\langle v^*(\mu) - v, \mu \rangle}{d(v, v^*)}.$$  

The gap $\Delta_v(\mu)$ captures the statistical difficulty in determining if $v$ is better or worse than $v^*$. The normalization $d(v, v^*)$ accounts for the fact that the numerator is a sum of precisely this many terms. The gap for an arm $a$ is $\Delta_a(\mu) \triangleq \min_{v \in V} \Delta_v(\mu)$, which captures the difficulty of determining if $a$ is in the optimal set.

We also use a complexity measure for the decision class that is independent of $\mu$. For $v \in V$ and a natural number $k$, let $B(k, v) \triangleq \{ u \in V | d(v, u) = k \}$ be the sphere of radius $k$ centered at $v$. Then define

$$\Phi \triangleq \Phi(V) \triangleq \max_{k \in \mathbb{N}, v \in V} \frac{\log(|B(k, v)|)}{k}.$$  

Finally let $\Psi \triangleq \Psi(V) \triangleq \min_{u, v \in V} d(u, v)$ denote the smallest distance. In all of these definitions, we omit the dependence on $\mu$ when it is clear from context.

A non-interactive baseline and comparisons. As a reference point and to foreshadow our results, it is instructive to study the non-interactive setting. A non-interactive algorithm queries each arm $T/K$ times and then outputs an estimate $\hat{v}$ of $v^*$

2. Adapting fairly standard arguments (see e.g., [33]), it is not hard to prove the following result about the maximum likelihood estimator (MLE), which outputs

$$\hat{v} = \arg\max_{v \in V} \langle v, \hat{\mu} \rangle$$  

where $\hat{\mu}$ is the vector of sample averages.

Theorem 1 (Non-interactive upper bound). For any $\mu \in [-1, 1]^K$ and $\delta$ the non-interactive MLE guarantees

$$\mathbb{P}_\mu[\hat{v} \neq v^*] \leq \delta$$  

whenever

$$T = \Omega\left(\frac{K}{\min_v \Delta^2_v} \left(\Phi + \frac{\log(K/\delta)}{\Psi}\right)\right).$$

Observe that $\Phi \leq \log(K)$, $\Psi \geq 1$ and hence the bound is at most $\Omega\left(\frac{K \log(K/\delta)}{\min_v \Delta^2_v}\right)$, but it can be smaller if $B(k, v^*)$ shrinks rapidly around $v^*$. This dependence on $\Phi$ replaces a $\log |V|$ factor that would arise with a naive analysis and reflects our localized concentration inequality. Our first observation is that all prior combinatorial pure exploration bounds can be polynomially worse than Theorem 1.

Proposition 2. For the bipartite matching problem, the bound of [16] can be $\Omega(K)$ larger than Theorem 1, while the bound in [14] can be $\Omega(\sqrt{K})$ larger. For the biclique problem the bound of Gabillon et al. [21] can be $\Omega(\sqrt{s})$ larger than in Theorem 1.

2For simplicity we do not implement a stopping rule, since this has a negligible $\log(1/\Delta_v)$ dependence.
See Appendix A for the proof of Theorem 1 and Proposition 2, as well as a matching non-interactive lower bound. These comparisons are more subtle and require a deeper discussion that we defer to Section 4, since, for example, these algorithms can also outperform uniform sampling with maximum likelihood estimation. Nevertheless, Proposition 2 reflects a clearly undesirable property of these interactive algorithms. Our goal is to remedy this, and our interactive algorithm has sample complexity that is at most logarithmically worse than Theorem 1, but that can also be much better.

Related work. The closest related work to ours are the three recent papers on combinatorial pure exploration [16, 21, 14], that we have already mentioned. We discuss these results in more detail in Section 4.

Combinatorial pure exploration generalizes the best arm identification problem, which has been extensively studied (c.f., [20, 34, 6, 28, 39, 22, 10, 13, 40] for some classical and recent results). This problem is much simpler both computationally and statistically than our setting, and, accordingly, the results are much more precise. For example, in best arm identification, verifying that the optimal solution is correct is roughly as hard as finding the optimal solution, which motivates many algorithms and lower bounds based on Le Cam’s method [31, 29, 22, 14]. However, for combinatorial problems discovering the optimal solution often dominates the sample complexity, and hence these techniques do not immediately produce near-optimal results in the combinatorial setting. Nevertheless our algorithms are inspired by some ideas from this literature, namely elimination and successive-reject techniques [20, 6].

The subset selection problem, also called Top-K, is a special case of combinatorial exploration where $V$ corresponds to all $\binom{K}{k}$ subsets [27, 8, 30]. This case is minimally structured, and, in particular, there is little to be gained from our localized analysis since $\Phi = \Theta(\log(K))$. A related effect occurs when the decision set corresponds to the basis of a matroid [13].

Structure discovery has also been studied in related mathematical disciplines like signal processing, information theory, and statistics. Research on adaptive sensing from the signal processing community studies a similar setup but with assumptions on the unknown mean $\mu$, which lead to more specialized algorithms [11]. Information theorists and statisticians study the non-interactive version of this problem, which can be viewed as simply a channel coding or multiple hypothesis testing problem [33, 2]. However, most results study special combinatorial structures and few results here concern interactive algorithms [17, 7, 5, 9].

Our fixed confidence algorithm is inspired by disagreement-based active learning algorithms like CAL, that eliminate inconsistent hypotheses and query where the surviving ones disagree [18, 24, 23]. Our fixed confidence algorithm has a similar flavor, but uses a much stronger elimination criteria that enables our localized concentration guarantee and improved sample complexity bounds.

Lastly, we use an oracle for the offline optimization problem as a computational primitive. This abstraction has been used in prior work on combinatorial pure exploration [16, 14], but also in many other information acquisition problems like active learning [24, 25] and contextual bandits [3, 41, 38].

3 Results

Pseudocode for our fixed confidence algorithm is given in Algorithm 1. The algorithm proceeds in rounds, and at each round it issues queries to a judiciously chosen subset of the arms. These arms are chosen by implicitly maintaining a version space of plausibly optimal hypotheses and checking for disagreement among the version space. If there is no disagreement among an arm $a$, rather than sample from $\nu_a$, we instead hallucinate a sample that favors the surviving hypotheses.

The key ingredient is the definition of the version space. For a vector $\hat{\mu}$ and a radius parameter $\Delta$, define

$$V(\hat{\mu}, \Delta) = \{ v \in \text{conv}(V) \mid \forall u \in V, \langle \hat{\mu}, u - v \rangle \leq \Delta \| u - v \|_1 \}$$

(2)
Algorithm 1: Fixed Confidence Algorithm

1: Input: Class $V$, failure probability $\delta \in (0, 1)$
2: Set $\Delta_t = \min \{1, \sqrt{\frac{8}{t} (\Phi + \log(K\pi^2t^2/\delta))/\Psi)\}$
3: Sample each arm once $y_0(a) \sim \nu_a$
4: compute $\hat{\mu}_0 = y_0$
5: for $t = 1, 2, \ldots$, do
6: Compute $\hat{v}_t = \arg\max_{v \in V} \langle v, \hat{\mu}_t \rangle$
7: for $a \in [K]$ do
8: if $\text{DIS}(a, 1 - \hat{v}_t(a), \Delta_t, \hat{\mu}_t, \frac{\delta}{\pi^2t^2})$ then
9: Query $a$, set $y_t(a) \sim \nu_a$
10: else
11: Set $y_t(a) = 2\hat{v}_t(a) - 1$
12: end if
13: end for
14: Update $\hat{\mu}_{t+1} \leftarrow \frac{1}{t+1} \sum_{i=0}^t y_i$
15: If no queries issued this round, output $\hat{v}_t$
16: end for

Algorithm 2: Oracle-based Disagreement (DIS)

1: Input: $a, b, \Delta, \hat{\mu}, \delta$
2: $T = \frac{144K^3}{\Delta^2}, m = \frac{18 \log(2K/\delta)}{\Delta^2}, \epsilon = \sqrt{\frac{1}{9KT}}$
3: for $t = 1, \ldots, T$ do
4: for $i = 1, \ldots, m$ do
5: Sample $\sigma_{t,i} \sim \text{Unif}(0, 1/e)^K$
6: $u_{t,i} = \text{ORACLE}(V, \sum_{i=0}^{t-1} \ell_t + \sigma_{t,i})$
7: end for
8: Let $s, x_t$ be the value and optimum of
9: $\max \sum_{i=1}^m \Delta \langle v, 1 - 2u_{t,i} \rangle + \langle v, \hat{\mu} \rangle$
10: s.t. $v \in \text{conv}(V), v(a) = b$
11: if $s + \epsilon < 0$ return $\text{False}$
12: Set $\ell_t = \Delta 1 - 2\Delta x_t - \hat{\mu}$
13: end for
14: return $\text{True}$

Here $\|u - v\|$ is the distance between two sets, which reduces to the size of the symmetric set difference for integral $u, v$. At round $t$, the version space we use is $V_t = V(\hat{\mu}_t, \Delta_t)$ where $\hat{\mu}_t$ is the empirical mean using all previous samples and $\Delta_t$ is defined in the algorithm and scales like $1/\sqrt{t}$.

This version space is used by the disagreement computation (Algorithm 2), which, with parameters $a \in [K], b \in \{0, 1\}, \Delta, \hat{\mu}, \delta$ solves the feasibility problem

$$\exists v \in V(\hat{\mu}, \Delta) \text{ s.t. } v(a) = b. \quad (3)$$

At round $t$, we use $\hat{\mu}_t, \Delta_t$ and the value for $b$ that we use in Line 8 is $1 - \hat{v}_t(a)$. Since $\hat{v}_t$, being the empirical best hypothesis, is always in $V_t$, this computation amounts to checking whether there exists two hypothesis $u, v \in V_t$ with $u(a) \neq v(a)$. As such we are checking for disagreement among the surviving hypotheses in the version space, and we use this criteria to drive the query strategy.

Before turning to computational considerations, a few other details warrant some discussion. First, if at any round we detect that there is no disagreement about some arm $a$, then we use a hallucinated observation $y_t(a) = 2\hat{v}_t(a) - 1 \in \{\pm 1\}$. While this leads to bias in our estimates, since all surviving hypotheses $v \in V_t$ agree with $\hat{v}_t$ on arm $a$, this bias favors the survivors. As in related work on disagreement-based active learning, this helps enforces monotonicity of the version space [19]. Finally, we terminate once there are no remaining arms with disagreement, at which point we output the empirically best hypothesis.

**Efficient implementation of disagreement computation.** Computationally, the main bottleneck is the feasibility problem (3) required for the disagreement computation. All other computations in Algorithm 1 can be done in polynomial time or with access to a linear optimization oracle (1). Therefore, to derive a oracle-efficient algorithm, we now show how to solve problem (3), with pseudocode in Algorithm 2.

It is not hard to see that problem (3) is a linear feasibility problem, but it has $|V|$ constraints, which could be exponentially large. This precludes standard linear programming approaches, and instead we use a
reduction to online learning inspired by the Plotkin-Shmoys-Tardos technique [37]. The idea is to run an online learner to compute distributions over the constraints and solve simpler feasibility problems to generate the losses. In our case, we can express each generated loss as a linear function of the constraint parameter $u \in V$, which enables us to use Follow-The-Perturbed-Leader (FTPL) as the online learning algorithm. Importantly FTPL can be implemented here using only the linear optimization oracle. As a technical detail, we must use an empirical distribution based on repeated oracle calls to approximate the true FTPL distribution, since in our reduction the loss function is generated after and based on the random decision of the learner.

First we provide the guarantee for the disagreement routine.

**Theorem 3 (Efficient Disagreement Computation).** Algorithm 2 with parameters $a, b, \Delta, \hat{\mu}, \delta$ runs in polynomial time with $O(K^5 \log(K/(\Delta \delta))/\Delta^4)$ calls to ORACLE. If it reports FALSE then Program (3) is infeasible. If it reports TRUE then with probability at least $1 - \delta$, $\exists v \in \text{conv}(V), v(a) = b$ and $\forall u \in V, \langle \hat{\mu}, u - v \rangle \leq \Delta \|u - v\|_1 + \Delta$.

This result proves that Algorithm 2 can approximate the feasibility problem in (3) in polynomial time using the optimization oracle. The approximation is one-sided and since we do not query when the algorithm returns FALSE, the one-sided approximation only affects the sample complexity of Algorithm 1, but never the correctness. However, the following theorem, which is the correctness and sample complexity guarantee for Algorithm 1, shows that this approximation has a negligible effect.

**Theorem 4 (Fixed confidence sample complexity bound).** For any distribution, parametrized by $\mu$, and any $\delta \in (0, 1)$, Algorithm 1 guarantees that $\mathbb{P}_\mu[\hat{v} \neq v^*(\mu)] \leq \delta$. Moreover, it runs in polynomial time with access to the optimization oracle, and the total number of samples is at most

$$\sum_{a \in K} 144 \frac{\Delta^2_n (\Phi + 2 \log(144/(\Delta^2 \Psi)) + 2 \log(K \pi^2/\delta))}{\Psi}.$$

We provide the overview of the proof for this result and Theorem 3 in Section 5, with details in the appendix. The bound replaces the worst case gap in Theorem 1 with a less pessimistic notion that accounts for heterogeneity in the problem. Thus, the bound is never worse by more than a logarithmic factor, but it can be much better. Based on Proposition 2, Algorithm 1 can therefore be polynomially better than the prior results [16, 21, 14]. While comparing to these prior results is delicate, we view Theorem 4 as representing a favorable trade-off since it is never worse than the non-interactive algorithm, a property that distinguishes it from the others. This property arises from using the localized concentration inequality to introduce the instance-independent complexity measure $\Phi$. See Section 4 for a more in-depth discussion of these comparisons, with specific examples.

### 3.1 Deferred Results

In this section we state two related results: a guarantee for a disagreement-based algorithm in the fixed budget setting, and a more refined sample complexity bound for a computationally inefficient fixed confidence algorithm. Both algorithms and all proof details are deferred to the appendices.

#### 3.1.1 A fixed budget algorithm

Recall that in the fixed budget setting the learning algorithm is given a budget of $T$ queries and after issuing these queries, it must output an estimate $\hat{v}$. Our goal is to minimize the probability $\mathbb{P}[\hat{v} \neq v^*]$. As is common

---

3Technically we do have a separation oracle here, so we could use the Ellipsoid algorithm, but a standard application would certify feasibility or approximate infeasibility. Our reduction instead certifies infeasibility or approximate feasibility, which is more convenient.
in the best arm identification literature, the fixed budget setting requires a modified definition of the instance complexity, which for our fixed confidence result was $H = \sum_a \Delta_a^{-2}$. To this end, recall the definition of the arm gaps $\Delta_a$ and let $\Delta^{(j)}$ denote the $j^{th}$ largest of these values, breaking ties arbitrarily. The complexity measure for the fixed budget setting is

$$\tilde{H} = \max_j (K + 1 - j)(\Delta^{(j)})^{-2}.$$ 

It is not hard to see that $\tilde{H} \leq H \leq \tilde{\log}(K) \tilde{H}$, where $\tilde{\log}(t) = \sum_{i=1}^{t} 1/i$ is the partial harmonic sum. With these new definitions, we can state our fixed budget guarantee.

**Theorem 5** (Fixed Budget Guarantee). Given budget $T \geq K$, there is an oracle-efficient fixed budget algorithm with

$$\Pr[\hat{v} \neq v] \leq K^2 \exp \left\{ \Psi \left( \Phi - \frac{(T - K)}{9 \log(K) \tilde{H}} \right) \right\}.$$ 

The algorithm and proof are presented in Appendix C. At a high level the savings are similar to the fixed confidence setting. By using a concentration inequality that localizes around $v^*$, we obtain an improved dependence on the hypothesis complexity, replacing $\log |V|$ with $\Phi$. Obtaining an oracle-efficient algorithm is much easier here since the version space need not be maintained even implicitly.

### 3.1.2 A refined fixed confidence guarantee

We also derive a more refined sample complexity bound for the fixed confidence setting. First, define the symmetrized volume:

$$D(v, v') = \max\{ \log |B(d(v, v'), v)|, \log |B(d(v, v'), v')| \}.$$ 

We use two new instance-dependent complexity measures:

$$H_a^{(1)} = \max_{v \in \mathcal{V}, v^*} \frac{d(v_a, v^*)}{\langle \mu, v^* - v_a \rangle^2}, \quad H_a^{(2)} = \max_{v \in \mathcal{V}, v^*} \frac{d(v, v^*) D(v, v^*)}{\langle \mu, v^* - v \rangle^2}.$$ 

The two definitions here provide more refined control on the two terms in Theorem 4. Specifically $H^{(1)}$ replaces the dependence on the minimum distance $\Psi$ with the distance of the hypothesis that achieves the maximum in the complexity measure. Similarly $H^{(2)}$ replaces the volume measure $\Phi$ with a notion particular to the maximizing hypothesis. Using these definitions, in Appendix D, we derive an algorithm with the following guarantee for the fixed confidence setting.

**Theorem 6** (Refined fixed confidence guarantee). There exists a fixed confidence algorithm that guarantees

$$\Pr[\hat{v} \neq v^*(\mu)] \leq \delta$$

with sample complexity

$$T \leq 64 \sum_{a \in [K]} H_a^{(1)} \left( 2 \log(64 H_a^{(1)}) + \log \frac{\pi^2 K}{\delta} \right) + H_a^{(2)}.$$ 

This bound is always better than Theorem 4 since it essentially replaces the worst case $\Phi, \Psi$ with problem and hypothesis specific variants. However, the algorithm is not oracle-efficient.
Sample complexity | TOP-K | Matching | Biclique
--- | --- | --- | ---
Theorem 4 | $\mathcal{O}(K/\Delta^2)$ | $\mathcal{O}(K/\Delta^2)$ | $\mathcal{O}(K/(\sqrt{s}\Delta^2))$
Chen et al. [16] | $\Theta(K/\Delta^2)$ | $\Theta(K^2/\Delta^2)$ | $\Theta(K/s/\Delta^2)$
Chen et al. [14] | $\Theta(K/\Delta^2)$ | $\Omega(K^3/2/\Delta^2)$ | $\Theta(K/\Delta^2)$
Gabillon et al. [21] | $\Theta(K/\Delta^2)$ | $\Theta(K/\Delta^2)$ | $\Theta(K/\Delta^2)$

Table 1: Leading terms in the sample complexity bounds of four combinatorial pure exploration results on three classes, in the homogeneous setting where $\mu = \Delta(2v^* - 1)$. Theorem 4 is never worse than the prior results, and can be polynomially better.

### 4 Examples and Comparisons

Comparing our sample complexity bound to the prior work is delicate since in general results are incomparable. To help with the discussion, we focus on three examples: (1) the TOP-K problem, where $V$ corresponds to all $\binom{K}{s}$ subsets, (2) the bipartite matching problem in Example 1, and (3) the $\sqrt{s}$-Biclique problem in Example 2. In the first two of these examples, we have $\Phi = \tilde{O}(1)$, $\Psi = \Omega(1)$ and in the third we have $\Phi = \tilde{O}(1/\sqrt{s})$ and $\Psi = \Omega(\sqrt{s})$ (See Appendix A). We also often consider the simplified homogeneous setting where $\mu = \Delta(2v^* - 1)$. For us, this means that $\Delta_s = \Delta$. Our sample complexity bounds for the homogeneous case, along with prior results are in Table 4. We now turn to the comparisons.

#### Comparison to Chen et al. [16]
In the sample complexity bound of Chen et al. [16], the main combinatorial term is called the width, which is related to the matroid augmentation property. The three examples have width $\Theta(1)$, $\Theta(K)$ and $\Theta(s)$ respectively. On the other hand in the homogeneous case, their notion of arm complexity is $\Theta(\Delta)$ in the first two examples and $\Theta(\sqrt{s}\Delta)$ in the third. Plugging in these bounds into their result produces the second row of Table 4, where our bound matches for TOP-K and improves on theirs for both Matchings and Bicliques. However outside of the homogeneous case, their bound can be better than ours when the maximum distance $\max_{u,v} d(u,v)$ is proportional to the width, which roughly corresponds to the size of exchange sets needed to traverse the hypothesis class.

#### Comparison to Gabillon et al. [21]
Gabillon et al. [21] instead introduce a gap parameter which compares each hypothesis $v$ to its complement $C_v \in V$ where $C_v = \text{argmax}_{v \neq v'} \langle \mu, v' - v \rangle / d(v', v)$. They use complements to define an arm complexity which is always smaller than ours. However, they are not able to exploit favorable localization properties of the hypothesis classes (e.g., $\Phi$ is small and $\Psi$ is large) like we are able to. In the homogeneous case, our arm complexity agrees with theirs, and as such we obtain a polynomial improvement in problems like Biclique where $\Phi \approx 1/\Psi \ll 1$ is small. However, since their gap is never larger than ours, their result can also be better, particularly when $\Phi = \Theta(1)$. Additionally, it is worth emphasizing that their algorithm requires explicit enumeration of $V$ and can not use a linear optimization oracle.

#### Comparison to Chen et al. [14]
Finally, Chen et al. [14] introduces a third arm complexity parameter based on the solution to an optimization problem. In the homogeneous case (with enough symmetry), the solution to this program is $\Omega(K/(\Delta^2 \Psi))$ but their sample complexity bound also depends on $\log |V|$. Since $\Phi \leq \log(|V|)/\Psi$, this shows that our bound is never worse than theirs in the homogeneous case. Moreover, when $\Psi = \Theta(1)$ and $\Phi$ is small, but $|V|$ is exponentially large, our bound can be polynomially better than

---

4It is challenging, and not particularly illuminating to instantiate the sample complexity of Chen et al. [14] in the Biclique problem.
their, as is the case in the matching problem (See Appendix A for a detailed derivation). On the other hand, with heterogeneous parameter, their arm complexity is incomparable to ours, so their result can be better. We believe that their optimization-based measure (without the log |V| dependence) corresponds to the sample complexity for verifying that a proposed v is optimal, while ours corresponds to the price of exploration to find such a candidate. In addition, our result shows that log(|V|) is not necessary for many structured classes.\(^5\)

5 Proofs

In this section we provide the proofs of Theorems 3 and 4, with lemmas in Appendix B.

Proof of Theorem 3. We repeatedly use the following identity for the \(\ell_1\) norm: For any \(u \in \{0,1\}^K\) and any \(x \in [0,1]^K\),

\[
\|x - u\|_1 = \langle x + u, 1 \rangle - 2 \langle x, u \rangle.
\]  

(5)

This identity reveals that the disagreement region, \(V_t\) is polyhedral and hence Program (3) is just a linear feasibility problem. Now suppose that Program (3) is feasible and that \(x^* \in \text{conv}(V)\) is a feasible point. Then for every distribution \(p \in \Delta(V)\), \(x^*\) satisfies the mixture constraint, which is precisely what we check by solving the problem (4) and examining the objective value in Line 10 in each iteration of the algorithm. Hence by contraposition, if the algorithm ever detects infeasibility, it must be correct.

For the other direction, we use the regret bound for Follow-the-Perturbed Leader [26]. Succinctly, when the learner makes decisions \(d_t \in D \subset \mathbb{R}^d\) and the adversary chooses losses \(\ell_t \in S \subset \mathbb{R}^d\), FTPL with parameter \(\epsilon \leq 1\) guarantees

\[
\mathbb{E} \sum_{t=1}^{T} \langle d_t, \ell_t \rangle - \min_{d \in D} \sum_{t=1}^{T} \langle d, \ell_t \rangle \leq \epsilon \text{RAT} + D/\epsilon,
\]

where \(D = \max_{d,d' \in D} \|d - d'\|_1\), \(R = \max_{d \in D, \ell \in S} |\langle d, \ell \rangle|\), and \(A = \max_{\ell \in S} \|\ell\|_1\). Setting \(\epsilon = \sqrt{D/(\text{RAT})}\) gives \(2\sqrt{D \text{RAT}}\) regret. The algorithm chooses \(d_t\) by sampling \(\sigma_t \sim \text{Unif}([0,1/\epsilon]^d)\) and playing \(d_t = \arg\min_{d \in D} \langle d, \sigma_t + \sum_{\tau=1}^{t-1} \ell_{\tau} \rangle\). This induces a distribution over decisions \(d_t\), which we denote by \(p_t \in \mathbb{R}^d\) and the expectation accounts for this randomness. It will be important for us that FTPL can accommodate adaptive adversaries, and hence the loss \(\ell_t\) can depend on \(p_t\) but not on the random decision \(d_t\).

In our case, we have \(D = \text{conv}(V)\), and we write \(\ell_t = \Delta 1 - 2\Delta x_t - \hat{\mu}\) where \(x_t\) is the solution to Program (4) in the \(t\)th iteration. This makes \(D \leq K, R \leq 3K\), and \(A \leq 3K\) in our reduction so with \(\epsilon = 1/(9KT)\) the regret is \(2\sqrt{9K^2T}\). Note that while \(x_t\) and hence \(\ell_t\) depends on the random choices of the learner through \(\hat{\mu}\), we will actually apply the regret bound only on the expectation, which we denote by \(p_t\), which can be equivalently viewed as the adversary sampling to generate \(\hat{p}_t\) and \(\ell_t\). Before turning to the proof, we need one final lemma, which we defer to Appendix B.

Lemma 7. Let \(p_t = \mathbb{E}_u \hat{p}_t\) and let \(\ell_t\) be any vector, which may depend on \(\hat{\mu}\). Then with probability at least \(1 - \delta\), simultaneously for all rounds \(t \in [T]\)

\[
\sum_{u \in V} (\hat{p}_t(u) - p_t(u)) \langle u, \ell_t \rangle \leq 3K \sqrt{\frac{\log(2KT/\delta)}{2m}}.
\]

\(^5\)This does not contradict their lower bound, which constructs certain pathological classes \(V\).
To prove Theorem 3, we condition on the event in Lemma 7 and use that for distribution \( \hat{p}_t \) defining Program (4), \( x_t \) is optimal and passes the check in Line 10. Applying the regret bound for FTPL, we get

\[
0 \leq \sum_{t=1}^{T} \sum_{u \in V} \hat{p}_t(u) \left( \Delta \| u - x_t \|_1 - (u - x_t, \hat{\mu}) \right)
\]

\[
\leq \sum_{t=1}^{T} \langle x_t, \Delta \mathbf{1} + \hat{\mu} \rangle + \min_u \sum_{t=1}^{T} \langle u, \ell_t \rangle + 2\sqrt{9K^3T} + 3TK\sqrt{\frac{\log(2KT/\delta)}{2m}}.
\]

Note that we apply the regret bound on \( p_t \), the expected decision of the algorithm, rather than on \( \hat{p}_t \), the randomized one. Re-arranging, dividing through by \( T \), and using (5), we get

\[
\langle u - \bar{x}, \hat{\mu} \rangle \leq \Delta \| \bar{x} - u \|_1 + 2\sqrt{9K^3/T} + 3K \sqrt{\frac{\log(2KT/\delta)}{2m}}.
\]

We conclude the proof with our choices for \( T = 144K^3/\Delta^2 \) and \( m = \frac{18K^2 \log(2KT/\delta)}{\Delta^2} \).

**Proof of Theorem 4** The key lemma in the proof of Theorem 4 is a uniform concentration inequality on the empirical mean \( \hat{\mu} \) used by the algorithm. To state the inequality let \( \hat{\mu}_t(a) \in \mathbb{R}^d \) be the conditional mean of \( y_t(a) \), conditioning on all randomness up to round \( t \), including the execution of \textsc{Disagree}. This means that \( \hat{\mu}_t(a) \) is either \( \mu(a) \) or \( 2\hat{y}_t(a) - 1 \), depending on the outcome of the disagreement check. Recall the definition of \( \Delta_t \) in Algorithm 1. We first derive a concentration inequality relating \( \hat{\mu}_t \) to the empirical means \( \bar{\mu}_t \).

**Lemma 8.** With the above definitions, for any \( \delta \in (0, 1) \), with probability at least \( 1 - \delta/2 \)

\[
\forall t > 0, \forall v \in V, \left| \frac{1}{t} \sum_{i=1}^{t} \langle v^* - v, \bar{\mu}_t - y_i \rangle \right| \leq d(v^*, v) \Delta_t.
\]

This concentration inequality is not challenging to prove, but is much weaker than the concentration arguments used in prior work. The key difference is that our inequality only bounds differences with the true optimum \( v^* \), while the prior results bound differences between all pairs of hypotheses. Our definition of the version space \( V(\hat{\mu}, \Delta) \) with many more constraints enables using this substantially weaker concentration inequality, which leads to our sample complexity guarantees.

Define the event \( E \) to be the event that Lemma 8 holds and also that the disagreement computation succeeds at all rounds for all arms, which by Theorem 3 happens with probability \( 1 - \sum_{t>0} \frac{\delta}{\pi^2T^2} \geq 1 - \delta/2 \).

By a union bound, we see that \( P(E) \geq 1 - \delta \). Under this event, we establish two facts:

1. \( \forall t, v^* \in V_t \) where \( V_t = V(\hat{\mu}_t, \Delta_t) \) is the version space at round \( t \) (Lemma 10).
2. If \( \Delta_t \leq \Delta_a/3 \), then arm \( a \) will never be queried again (Lemma 12).

The correctness of the algorithm follows from the first fact. In detail, the algorithm only terminates at round \( t \) if it detects no disagreement on all coordinates, which means that Algorithm 2 reports infeasible for all coordinates. By Theorem 3, this means that \( V_t = \{ v^* \} \), and, by the definition of \( V_t \), we must have \( \check{v}_t \in V_t \).

Thus conditioned on the \( 1 - \delta \) event, the algorithm returns \( v^* \).

For the sample complexity, from the second fact and the definition of \( \Delta_t \), arm \( a \) will not be sampled once

\[
t \geq \frac{72}{\Delta_a^2} \left( \Phi + \frac{\log(K\pi^2T^2/\delta)}{\Psi} \right).
\]
A sufficient condition for this transcendental inequality to hold is (see Fact 13):

\[ T_a \geq \frac{144}{\Delta_a^2} \left( \Phi + \frac{2 \log(144/(\Delta_a^2\Psi)) + 2 \log(K\pi^2/\delta)}{\Psi} \right). \]

The sample complexity is at most \( \sum_a T_a \), which proves the theorem.

6 Discussion

This paper derives new algorithms for the combinatorial pure exploration problem. The algorithms represent a new sample complexity trade-off and importantly are never worse than the naïve algorithm based on uniform sampling, contrasting with the prior results. Moreover, our algorithms can be efficiently implemented whenever the combinatorial family supports efficient linear optimization.

We close with some open problems. A first natural question is understanding if there is a uniformly dominant algorithm, where one plausible approach may be via the explore-then-verify approach of Karnin [29]. Another direction involves accommodating approximate optimization oracles. We hope to study these questions in future work.

Acknowledgements

We thank Sivaraman Balakrishnan for formative and insightful discussion.
A Non-interactive analysis and Comparisons

A.1 Proof of Theorem 1

Let \( \hat{\mu} \) denote vector of sample averages from the \( T/K \) pulls on each arm. Thus \( \hat{\mu}_a \sim \nu(\mu_a, K/T) \). The non-interactive algorithm outputs

\[
\hat{v} = \arg\max_{v \in V} \langle v, \hat{\mu} \rangle
\]

Clearly, by the union bound and Hoeffding’s inequality, we get

\[
P[\hat{v} \neq v^*] \leq P[\exists v \in V(\hat{\mu}, v - v^*) \geq 0] = P[\exists v \in V(\hat{\mu} - \mu, v - v^*) \geq (\mu, v^* - v)]
\]

\[
\leq \sum_v \exp \left( \frac{-T(\mu, v^* - v)}{2Kd(v^*, v)} \right) \leq \sum_v \exp \left( \frac{-T\Delta_0^2 d(v^*, v)}{2K} \right)
\]

\[
\leq \sum_{k=1}^K |B(k, v^*)| \exp \left( \frac{-Tk \min_v \Delta_0^2}{2K} \right)
\]

\[
= \sum_{k=1}^K \exp \left( \log |B(k, v^*)| - \frac{Tk \min_v \Delta_0^2}{2K} \right)
\]

\[
\leq K \exp \left( \max_{k \in [K]} \log |B(k, v^*)| - \frac{Tk \min_v \Delta_0^2}{2K} \right)
\]

Setting this to be at most \( \delta \) and solving for \( T \) reveals

\[
T \geq \max_{k \in [K]} \frac{2K}{k\Delta_0^2} \left( \log |B(k, v^*)| + \log(K/\delta) \right).
\]

This right hand side is upper bounded by the sample complexity in the theorem statement.

A.2 A non-interactive lower bound

We now prove a lower bound for non-interactive algorithms, which reveals that Theorem 1 is tight.

**Theorem 9.** Any non-interactive must have \( \sup_{v^* \in V} P_{\mu=\Delta(2v^*-1)}[\hat{v} \neq v^*] \geq 1/2 \) as long as

\[
T \leq \frac{K}{\Delta^2} (\Phi - \log \log 3).
\]

Before turning to the proof, observe that first term in this bound matches the upper bound in Theorem 1, which is typically the leading term in combinatorial identification problems. Indeed, we always have \( \Psi \geq 1 \) and often have \( \Phi = \Theta(\log(K)) \) so that for any \( \delta = \frac{1}{\poly(K)} \) the terms coincide. More generally, we often have \( \Phi = \log(K)/\Psi \), e.g., in the Biclique problem, so the two terms coincide for polynomially small \( \delta \). However, obtaining a the optimal \( \delta \) dependence, even for non-interactive algorithms is an intriguing technical question for future work.

Note also that this lower bound applies only for non-interactive algorithms and also only for the homogeneous case where \( \mu = \Delta(2v^*-1) \) for some \( v^* \in V \). A more refined instance-dependent bound is possible with our technique but is not particularly illuminating.
Proof of Theorem 9. The proof here is based of Fano’s inequality and follows the analysis of Krishnamurthy [33]. Let us simplify notation and define $P_v = \mathbb{P}_{\mu = \Delta(2v - 1)}$ to be the distribution where $T/K$ samples are drawn from each arm and $\mu = \Delta(2v - 1)$. For any distribution $\pi$ supported on $V$ let $P_\pi$ denote the mixture distribution where first $v^* \sim \pi$ and then the samples are drawn from $P_{v^*}$. With this notation, Fano’s inequality shows that for any algorithm

$$\sup_{v^* \in V} \mathbb{P}_{v^*}[\hat{v} \neq v^*] \geq \mathbb{E}_{v^* \sim \pi} \mathbb{P}_{\mu = \Delta(2v^* - 1)}[\hat{v} \neq v^*] \geq 1 - \frac{\mathbb{E}_{v^* \sim \pi} KL(P_v || P_\pi) + \log 2}{H(\pi)}$$

Let $\hat{v} \in V$ denote the candidate that achieves the maximum in the definition of $\Phi$ and define the prior

$$\pi(v) \propto \exp \left( -\frac{T\Delta^2}{K} d(v, \hat{v}) \right).$$

With this definition, the entropy term becomes

$$H(\pi) = \log \left( \sum_v \exp \left( -\frac{T\Delta^2}{K} \frac{d(v, \hat{v})}{2} \right) \right) + \sum_v \pi(v) \log \left( \frac{d(v, \hat{v})}{2} \right) + 2 \sum_v \pi(v) KL(P_v || P_{\hat{v}}).$$

Here in the last step we use the definition of the Gaussian KL, and the tensorization property for iid sampling. As for the Kullback-Leibler term in the numerator, it is not too hard to see that

$$\sum_v \pi(v) KL(P_v || P_{\pi}) \leq \sum_v \pi(v) KL(P_v || P_{\pi}) + KL(P_{\pi} || P_{\hat{v}}) = \sum_v \pi(v) KL(P_v || P_{\hat{v}}).$$

Thus, we have proved the lower bound if

$$\sum_v \pi(v) KL(P_v || P_{\pi}) + \log(2) \leq \frac{1}{2} \log \left( \sum_v \exp \left( -\frac{T\Delta^2}{K} \frac{d(v, \hat{v})}{2} \right) \right) + \sum_v \pi(v) KL(P_v || P_{\hat{v}}).$$

After simple algebraic manipulations, we get

$$\log(2 \log(2)) \leq \sum_v \exp \left( -\frac{T\Delta^2}{K} d(v, \hat{v}) \right) = \sum_k \exp \left( \log |B(k, \hat{v})| - \frac{T\Delta^2}{K} \right)$$

Since the sum is always larger than the max, $\hat{v}$ realizes the definition of $\Phi$, and since $2 \log(2) \leq 3$, we get the result. More formally, if

$$\frac{T}{\Delta^2} (\Phi - \log \log 3)$$

Then,

$$\sum_k \exp \left( \log |B(k, \hat{v})| - \frac{T\Delta^2}{K} \right) \geq \max_k \exp (\log |B(k, \hat{v})| - \Phi k + \log 3)$$

$$= \exp(\log 3) = 3.$$

Thus if $T$ is smaller than above, the minimax probability of error is at least $1/2$. \qed
A.3 Proof of Proposition 2

Comparison with Chen et al. [16]. To compare with [16], we must introduce some of their definitions. Translating to our terminology, they define

\[
\Delta_a^{(C)} = \max_{v:a \in v \cup v^*} \langle \mu, v^* - v \rangle,
\]

which differs from our definition since it is not normalized. They also define exchange classes and a notion of width of the decision set. An exchange class is a collection of patches \( b = (b_+, b_-) \) where \( b_+, b_- \subseteq [K] \) and \( b_+ \cup b_- = \emptyset \), with several additional properties. To describe them further define the operator \( v \oplus b = (v \setminus b_-) \cup b_+ \) and \( v \ominus b = (v \setminus b_+) \cup b_- \) where \( v \) is interpreted as a subset of \([K]\). Then a set of patches \( B \) is an exchange class for \( V \) if for every pair \( v \neq v' \in V \) and every \( a \in v \setminus v' \), there exists a patch \( b \in B \) such that (1) \( a \in b_- \), (2) \( b_+ \subseteq v' \setminus v \), (3) \( b_- \subseteq v \setminus v' \), (4) \( v \oplus b \in V \), and (5) \( v' \ominus b \in V \). Then they define the width

\[
\text{width}(V) = \min_{\text{exchange classes } B} \max_{b \in B} |b_-| + |b_+|
\]

With these definitions, the fixed-confidence bound of Chen et al. [16] is

\[
\tilde{O} \left( \text{width}(V)^2 \sum_a \frac{1}{(\Delta_a^{(C)})^2} \log(K/\delta) \right)
\]

where we have omitted a logarithmic dependence on the arm complexity parameter \( \Delta_a^{(C)} \).

Now consider a bipartite matching problem with \( \sqrt{K} \) vertices on each side of the partition, so there are \( K \) edges in total. Number the vertices on one side \( a_1, \ldots, a_{\sqrt{K}} \) and on the other side \( b_1, \ldots, b_{\sqrt{K}} \). Let \( v^* \) be the matching with edges \( \{(a_i, b_i)\}_{i=1}^{\sqrt{K}} \). In the homogeneous case where \( \mu = \Delta(2v^* - 1) \), it is easy to see that \( \Delta_a^{(c)} = \Theta(\Delta) \) since for every edge \( e \) (which correspond to the arms in the bandit problem), there exist a matching that contains this edge, that disagrees with \( v^* \) on exactly two edges. Specifically, if \( e = (a_i, b_j) \) then the matching that has edge \( (a_k, b_k) \) for all \( k \neq i, j \) and edges \( (a_i, b_j) \) and \( (a_j, b_i) \) has symmetric set difference exactly 4.

On the other hand we argue that the width is \( \Theta(\sqrt{K}) \). This is by the standard augmenting path property of the matching polytope. In particular if \( v^* \) is as above and we define another matching \( v = \{(a_i, b_{i+1 \mod \sqrt{K}})\}_{i=1}^{\sqrt{K}} \), then the only patch for \( v^* \), \( v \) is to swap all edges. Hence the bound of [16], in this instance is

\[
\tilde{O} \left( \frac{K^2}{\Delta^2} \log(K/\delta) \right)
\]

which is a factor of \( K \) worse than the non-interactive algorithm in this setting.

Comparison with [14]. As for [14], their guarantee is

\[
\tilde{O} \left( \text{Low}(V)(\log(1/\delta) + \log |V|) \right),
\]

ignoring some logarithmic factors. Here \( \text{Low}(V) \) is the solution to the optimization problem

\[
\text{minimize } \sum_a \tau_a \text{ s.t. } \sum_{a \in v \oplus v^*} \frac{1}{\tau_a} \leq \langle \mu, v^* - v \rangle^2, \forall v \neq v^* \text{ and } \tau_a \geq 0, \forall a \in [K].
\]

(6)
In the homogeneous case for bipartite matching, we show that \( \text{Low}(\mathcal{V}) = \Theta(K/\Delta^2) \). This proves what we want since \( \log(\mathcal{V}) = \sqrt{K} \log K \) and hence the bound is a factor of \( \sqrt{K} \) worse than Theorem 1.

The proof here is by passing to the dual of Program 6. First we construct the Lagrangian

\[
\mathcal{L}(\tau, \alpha) = \sum \tau_a + \sum_v \alpha_v \left( \sum_{a \in v \not\to v} \frac{1}{\tau_a} - \langle \mu, v^* - v \rangle^2 \right).
\]

By weak duality, the solution of the primal problem is always lower bounded by the solution of the dual problem

\[
\min_\tau \max_\alpha \mathcal{L}(\tau, \alpha) \geq \max_\alpha \min_\tau \mathcal{L}(\tau, \alpha).
\]

Taking the derivative with respect to \( \tau \) we have

\[
\frac{\partial \mathcal{L}}{\partial \tau_a} = 1 - \sum_{v: a \in v \not\to v^*} \alpha_v \left( \frac{1}{\tau_a^2} \right) = 0 \Rightarrow \tau_a = \sqrt{\sum_{v: a \in v \not\to v^*} \alpha_v},
\]

and plugging back into the Lagrangian gives

\[
\max_{\alpha_v \geq 0} \sum_a \sqrt{\sum_{v: a \in v \not\to v^*} \alpha_v} + \sum_v \alpha_v \left( \sum_{v' \in v^*} \frac{1}{\sqrt{\sum_{v': a \in v' \not\to v'} \alpha_v'}} - \langle \mu, v^* - v \rangle^2 \right)
\]

\[
= \max_{\alpha_v \geq 0} 2 \sum_a \sqrt{\sum_{v: a \in v \not\to v^*} \alpha_v} - \sum_v \alpha_v \langle \mu, v^* - v \rangle^2.
\]

By weak duality, any feasible solution here provides a lower bound on \( \text{Low}(\mathcal{V}) \). We construct a feasible solution in a similar way to the construction we used to analyze the bound of Chen et al. [16]. Let \( v^* \) be the matching \( \{(a_i, b_i)\}_{i=1}^{\sqrt{K}} \). For every edge \( (a_i, b_j) \), there is a unique matching \( v \) that disagrees with \( v^* \) on exactly 4 edges, and for these matchings we will set \( \alpha_v \) to some constant value \( \alpha \). We set \( \alpha_v = 0 \) otherwise. This ensures that for every \( a \not\in v^*, \sum_{v: a \in v \not\to v^*} \alpha_v = \alpha \). On the other hand, for \( a \in v^* \), we get

\[
\sum_{v: a \in v \not\to v^*} \alpha_v = (\sqrt{K} - 1)\alpha \geq \alpha,
\]

since we can swap out this edge with one \( \sqrt{K} - 1 \) other edges, iterating over all other nodes on the other side of the partition. In other words, for every arm \( a \in [K] \), the first term is at least \( \sqrt{\alpha} \), while no more than \( K \) \( \alpha_s \)s are non-zero. In total, a lower bound on the dual program is given by

\[
\max_{\alpha \geq 0} 2K \sqrt{\alpha} - 4K \Delta^2 \alpha.
\]

This simpler program is optimized with \( \alpha = 1/(16\Delta^4) \) and plugging back in reveals that

\[
\text{Low}(\mathcal{V}) = \Omega(K/\Delta^2).
\]

This is all we need for our comparison, since \( \text{Low}(\mathcal{V}) \log(|\mathcal{V}|) = \Omega(K^{3/2}/\Delta^2) \) in this case.

**Comparison with [21].** In [21], the authors introduce a improved gap by defining the complement of a set. Intuitively the complement is the easiest set to compare with. For any set \( v \neq v^* \), the gap is

\[
\Delta_v^{(C)} = \max_{v', \langle \mu, v' - v \rangle > 0} \frac{\langle \mu, v' - v \rangle}{d(v', v)},
\]

\[16\]
and the set that achieves this maximum is called the complement of \( v \). A tie breaks in favor of the sets that are closer to \( v \). The gap of an arm \( a \) is

\[
\Delta_a^{(G)} = \min_{v, a \in v \otimes v^*} \Delta_v^{(G)},
\]

and their sample complexity is

\[
O \left( \sum_a \frac{1}{(\Delta_a^{(G)})^2} \log(K/\delta) \right),
\]

which is similar to the sample complexity of Chen et al. [16] except the width parameter is absorbed into the new gap definition. As a consequence, this bound is never worse than [16].

In the homogeneous biclique example, it is easy to see \( \Delta_a^{(G)} = \Delta \), since taking \( v' = v^* \) will always achieve the maximum. Hence the bound becomes \( O \left( \frac{K}{\sqrt{s}} \log(K/\delta) \right) \), due to the fact that \( \log |B(k, v^*)| = O(k/\sqrt{s} \log(K)) \), which we now prove.

The idea is that for every vertex we swap into the biclique, we switch \( \Theta(\sqrt{s}) \) edges, formally at least \( \sqrt{s}/2 \) edges but no more than \( \sqrt{s} \). Then rather than optimizing over the radius in the decision set, we optimize over the number of vertices swapped in on both sides of the partition, which we denote \( s_L, s_R \).

\[
\max \frac{1}{K} \left( \log |B(k, v^*)| + \log(K/\delta) \right) \leq \max_{s_L, s_R} \frac{2}{\sqrt{s}(s_L + s_R)} \left( \log \left( \frac{\sqrt{K}}{s_L} \right) \left( \frac{\sqrt{K}}{s_R} \right) + \log(K/\delta) \right)
\]

\[
= O \left( \frac{1}{\sqrt{s}} \log(K/\delta) \right),
\]

using standard bounds on the binomial coefficient. Thus the bound of Gabillon et al. [21] is \( \Omega(\sqrt{s}) \) worse than the bound in Theorem 1, in the homogeneous biclique problem.

## B Proofs for the lemmas

**Proof of Lemma 7.** Let \( V \) be a \( \mathbb{R}^{K \times |V|} \) matrix whose columns are the vectors \( v \in V \). Recall that \( p_t \in \Delta(V) \) is a distribution over the perturbed leader at round \( t \). Let \( S_i \in \{0, 1\}^{|V|} \) be the indicator vector of the \( i \)-th sample. Clearly, \( E[S_i] = p_t \) and \( \tilde{p}_t = \frac{1}{m} \sum_{i=1}^m S_i \). We have

\[
\sum_{u \in V} (\tilde{p}_t(u) - p_t(u)) \langle u, \ell_t \rangle = \| V \tilde{p}_t - V p_t \ell_t \|_\infty \leq \| V \tilde{p}_t - V p_t \|_\infty \| \ell_t \|_1.
\]

Let \( (\cdot)_j \) denote the \( j \)-th coordinate of a vector. By Hoeffding’s inequality and union bound we have

\[
P \left[ \forall t \in [T], \forall j \in [K], \| (V \tilde{p}_t)_j - (V p_t)_j \| \geq \epsilon \right] \leq 2KT \exp(-2m \epsilon^2),
\]

so that with probability at least \( 1 - \delta \)

\[
\forall t \in [T], \| V \tilde{p}_t - V p_t \|_\infty \leq \sqrt{\frac{\log(2KT/\delta)}{2m}}.
\]

This proves the lemma. \( \Box \)
Proof of Lemma 8. Let $F_t$ be the $\sigma$-algebra conditioning on all randomness up to and including the execution of DISAGREE for all arms $a \in [K]$ at round $t$. Thus $y_t(a)$ is $F_t$ measurable and with $Z_t = \sum_{i=1}^{t} (\bar{\mu}_i - y_i)$ it is not hard to see that $\{Z_t\}_{t=0}^T$ forms a vector-valued martingale adapted to the filtration $\{F_t\}_{t=0}^T$.

$$\mathbb{E}[Z_t|F_t] = \mathbb{E}[(\bar{\mu}_t - y_t) + Z_{t-1}|Z_{t-1}] = Z_{t-1}. $$

Observe also that $|\bar{\mu}_t(a) - y_t(a)| \leq 2$. Thus, for any $v \neq v^*$ the Azuma-Hoeffding inequality gives

$$\mathbb{P}\left[ \left| \sum_{a \in \mathcal{V}} Z_t(a)/|t| \right| \geq \epsilon \right] \leq 2 \exp\left\{ - \frac{t \epsilon^2}{8d(v,v^*)}\right\}. $$

With a union bound, we get

$$\mathbb{P}\left[ \exists t, \exists v \in \mathcal{V}, \sum_{a \in \mathcal{V}} Z_t(a)/|t| \geq \epsilon (v,v^*,\delta) \right] \leq 2 \sum_{t>0} \sum_{v \in \mathcal{V}} \exp\left\{ - \frac{t \epsilon (v,v^*,\delta)^2}{8d(v,v^*)}\right\}. $$

Following the argument in the proof of Theorem 1, this right hand side will be at most $\delta/2$ if

$$\epsilon (v,v^*,\delta) = \sqrt{\frac{8d(v,v^*)}{t}} \log \left( \frac{Kt^2\pi^2|\mathcal{E}(v,v^*)|}{\delta} \right). $$

We set $\Delta_t = \sqrt{\frac{8}{t} (\Phi + \log(Kt^2\pi^2/\delta))}$ so that for all $v \in \mathcal{V}$, $\Delta_t d(v,v^*) > \epsilon (v,v^*,\delta)$, which concludes the proof. \(\square\)

Lemma 10. Recall the definition of $\mathcal{V}_t = \mathcal{V}(\bar{\mu}_t, \Delta_t)$ at round $t$, with $\mathcal{V}(\bar{\mu}, \Delta)$ defined in (2). Then in event $\mathcal{E}$, we have that $\forall t, v^* \in \mathcal{V}_t$.

Proof. The proof is by induction. First, we know that if $v^* \in \mathcal{V}_{t-1}$ then $\langle v^* - v, \bar{\mu}_t \rangle \geq \langle v^* - v, \bar{\mu}_t \rangle$. This follows since if arm $a$ is queried then $\bar{\mu}_t(a) = \bar{\mu}_t(a)$ and if arm $a$ is not queried, we know that $v^*(a) = \bar{v}_t(a)$ and our hallucination sets $\bar{\mu}_t(a) = 2\bar{v}_t(a) - 1 = 2v^*(a) - 1 \in \{-1,1\}$. Since $\mu(a) \in [-1,1]$ and $v(a) \in \{0,1\}$ this means that $v^*(a)\bar{\mu}_t(a) \geq v(a)\bar{\mu}_t(a)$. Thus, if $\forall i \in [t-1], v^* \in \mathcal{V}_i$ (which is our inductive hypothesis), then by Lemma 8 $\forall v \in \mathcal{V}$

$$\langle v - v^*, \bar{\mu}_t \rangle \leq \left( v - v^*, \frac{1}{t} \sum_{i=1}^{t} \bar{\mu}_t \right) + \Delta_t d(v,v^*) \leq \langle v - v^*, \mu \rangle + \Delta_t d(v,v^*).$$

By definition of $\mathcal{V}_t$, this proves that $v^* \in \mathcal{V}_t$. Clearly the base case holds since $v^* \in \mathcal{V}_0 = \mathcal{V}$. \(\square\)

Lemma 11. Let $x \in conv(\mathcal{V}) = \sum_i \alpha_i v_i$, where $v_i \in \mathcal{V}$, $\sum \alpha_i = 1$, $\alpha_i \geq 0$ and further let $v \in \mathcal{V}$. We have

$$\|x - v\|_1 = \sum_i \alpha_i \|v_i - v\|_1. $$

Proof. This follows by integrality of $v \in \mathcal{V}$ and (5). In particular, for integral $v, \|x - v\|$ is actually linear so we can bring the $\sum \alpha_i$ outside the $\ell_1$ norm. \(\square\)

Lemma 12. Under event $\mathcal{E}$, once $t$ is such that $\Delta_t < \Delta_0/3$, arm $a$ will not be sample again.
Proof. We consider here the case where \( \nu^*(a) = 1 \). For \( \nu^*(a) = 0 \) the analysis is similar. Assume for the sake of contradiction that \( a \) is sampled, which means that \( \text{DIS}(a, 1 - \hat{v}_t(a), \Delta_t, \hat{\mu}_t) \) returns TRUE. If \( \nu^*(a) = 1 \), then \( \forall v \in \mathcal{V} \) with \( \nu(a) = 0 \) we have

\[
\langle \nu^* - v, \hat{\mu}_t \rangle \geq \langle \nu^* - v, \sum_{t=1}^{T} \hat{\mu}_e \rangle - \Delta_t d(\nu^*, v) \geq \langle \nu^* - v, \mu \rangle - \Delta_t d(\nu^*, v) > 2d(\nu^*, v) \Delta_t
\]

The first inequality is Lemma 8, the second uses the property of the hallucinated samples that we used in Lemma 10. The last inequality is due to \( \Delta_a \leq \frac{d(\nu^*, v)}{\alpha} \) and our assumption that \( \Delta_t < \Delta_a/3 \). This implies that \( \hat{v}_t(a) = 1 \), which means that we execute \text{DISAGREE} to check if any surviving hypothesis \( v \in \mathcal{V} \) has \( \nu(a) = 0 \). Since we sampled arm \( a \), this means there exists \( x \in \text{conv}(\mathcal{V}) \) such that

\[
\forall u \in \mathcal{V} \langle u - x, \hat{\mu}_t \rangle \leq \Delta_t \|u - x\|_1 + \Delta_t.
\]

This follows by Theorem 3 which holds under the event \( \mathcal{E} \). Now write \( x = \sum_i \alpha_i v_i \) where \( \alpha \) is a distribution and \( v_i \in \mathcal{V} \). Since \( x(a) = 0 \), we must have \( v_i(a) = 0 \) for all \( i \). This means that

\[
\langle \nu^* - x, \hat{\mu}_t \rangle = \sum_i \alpha_i \langle \nu^* - v_i, \hat{\mu}_t \rangle + 2 \sum_i \alpha_i d(\nu^*, v_i) \Delta_t \geq \Delta_t \|\nu^* - x\|_1 + \Delta_t.
\]

The last inequality is due to Lemma 11 and the fact that \( \forall i, d(\nu^*, v_i) \geq 1 \). This contradicts the guarantee in Theorem 3, which means that \( \text{DIS}(a, 1 - \hat{v}_t(a), \Delta_t, \hat{\mu}_t) \) cannot return TRUE.

We use the Lemma 8 from Antos et al. [4].

Fact 13 (Lemma 8 from Antos et al. [4]). Let \( a > 0 \), for any \( t \geq \frac{2}{a} \max\{\log \frac{1}{a} - b, 0\} \), we have \( at + b \geq \log t \).

C Proof of Theorem 5

In the fixed budget setting, we follow a classic rejection strategy used by many algorithms in other settings (e.g., Successive Rejects Audibert and Bubeck [6], SAR Bubeck et al. [8], CSAR Chen et al. [16] and also the algorithm of [21]).

We require several new definitions. First recall that our definition of the gap for arm \( a \) is \( \Delta_a \). Let \( \Delta^{(j)} \) be the \( j \)th largest element in \( \{\Delta_a\}_{a \in [K]} \). Then the main complexity measure is \( H = \max_j (K + 1 - j)(\Delta^{(j)})^{-2} \). For short hand we define the partial harmonic sum \( \log(t) = \sum_{i=1}^{t} 1/i \). Assume that the total budget is \( T \), and define

\[
n_t = \left[ \frac{T - K}{\log(K)(K + 1 - t)} \right], \quad n_0 = 0
\]

which will be related to the number of queries issued in each round of our algorithm. As before, let \( \hat{\mu}_t \) be the empirical mean at round \( t \) of the algorithm and let \( \hat{v}_t = \arg\max_{v \in \mathcal{V}} \langle v, \hat{\mu}_t \rangle \) be the empirical maximizer. Define the empirical gaps at round \( t \) for hypotheses and arms respectively as

\[
\hat{\Delta}_{t,v} = \frac{(\hat{\mu}_t, \hat{v}_t - v)}{d(\hat{v}_t, v)}, \quad \hat{\Delta}_{t,a} = \min_{a \in \hat{v}_t \Delta_v} \hat{\Delta}_{t,v}.
\]
Algorithm 3: Fixed budget algorithm for combinatorial identification

1: Input: \( V \), set of arm \([K] \), \( \{n_t\}_d \)
2: Set \( t \leftarrow 1, A_1 \leftarrow \emptyset, R_1 \leftarrow \emptyset \)
3: for \( t = 1, 2, 3, \ldots, K \) do
4: Sample arms in \([K] \setminus (A_t \cup R_t)\). For \( n_t - n_{t-1} \) times, for \( a \in A_t \) use sample value 1 and for \( a \in R_t \) use sample value \(-1\) (i.e., hallucinate samples).
5: Update \( \hat{\mu}_t \).
6: for \( a \in [K] \setminus (A_t \cup R_t) \) do
7: for \( k = 1, \ldots, 2K \) do
8: Compute \( g_{t,k} = \text{ORACLE-FB}(\hat{\mu}_t, \hat{v}_t, a, k) \)
9: end for
10: Compute \( g_t(a) = \min_{k \in [2K]} g_{t,k} \).
11: end for
12: \( \hat{a}_t = \arg \max_{a \in [K] \setminus (A_t \cup R_t)} g_t(a) \).
13: if \( \hat{a}_t \in \hat{v}_t \) then
14: \( A_{t+1} = A_t \cup \hat{a}_t \)
15: else
16: \( R_{t+1} = R_t \cup \hat{a}_t \)
17: end if
18: end for
19: return \( A_{K+1} \)

With these definitions, we are now ready to describe the fixed budget algorithms, with pseudocode in 3. The algorithm maintains a set of “accepted” and “rejected” arms, \( A_t \) and \( R_t \) in the pseudocode at round \( t \), and once an arm is marked “accept” or “reject” it is never queried again. At each round \( t \) we issue several queries to all surviving arms, ensuring that each arm has \( n_t \) total queries, and then we find the arm with the largest empirical gap \( \hat{\Delta}_{t,a} \) and accept it if it is included in the ERM \( \hat{v}_t \). Otherwise we reject.

In lines 7 to 13, we use the linear optimization oracle to find the arm with the largest empirical gap. To do this, we first compute \( \hat{v}_t \) and then, for each arm \( a \) and each \( k \in [K] \), we use the oracle to find the set \( v \) that (1) disagrees with \( \hat{v}_t \) on arm \( a \), (2) has \( d(v, v^*) = k \) and (3) minimizes \( \langle \hat{\mu}, v - \hat{v}_t \rangle \). Using 5 this can be written as a linear optimization problem with just two constraints. Specifically, we define the subroutine \( \text{ORACLE-FB}(\hat{\mu}, \hat{v}, a, k) \) as

\[
\text{ORACLE-FB} \triangleq \min_{v \in \text{conv}(V)} \langle \hat{\mu}, \hat{v} - v \rangle \\
\text{s.t.} \quad \langle 1, \hat{v} + v \rangle - 2\langle \hat{v}, v \rangle = k \\
\langle v, e_a \rangle = 1 - \hat{v}(a).
\]

This subroutine requires a single call to our linear optimization oracle. \( \text{ORACLE-FB} \) outputs the value of the optimization problem if it is feasible, and \(+\infty\) otherwise. Fixing arm \( a \), we compute \( \hat{\Delta}_{t,a} \) by solving this optimization problem for each value of \( k \), dividing by \( k \) and taking the minimum value. Since for integral \( \hat{v} \) (which we have), \( d(\hat{v}, v) = \langle 1, \hat{v} + v \rangle - 2\langle \hat{v}, v \rangle \), this clearly computes \( \hat{\Delta}_{t,a} \). At this point finding the arm with the largest empirical gap can be done by enumeration.

We restate the theorem and then turn to the proof.
Theorem 14 (Theorem 5 restated). Given budget $T \geq K$, Algorithm 3 guarantees

$$
P[\hat{v} \neq v] \leq K^2 \exp \left\{ \Psi \left( \Phi - \frac{(T - K)}{9 \log(K)H} \right) \right\}.
$$

Proof. First, note that in each round we eliminate one arm and sample the rest for $n_t$ times. Thus after round $t$ we have sampled each surviving arm $n_t$ times, and exactly one arm is sampled $n_t$ times for each $i \in [K]$. Thus the total number of samples is

$$
\sum_{t=1}^{K} n_t = \sum_{t=1}^{K} \left[ \frac{T - K}{\log(K)(K + 1 - t)} \right] \leq \sum_{t=1}^{K} \frac{T - K}{\log(K)(K + 1 - t)} + 1 = T.
$$

Second, define $\bar{\mu}_t$ as before to be the mean of the all samples up to and including round $t$, taking into account the hallucination. $\bar{\mu}_t(a)$ is an average of $n_t$ terms where if at round $i \leq t$ we place $a \in A_i$, then the last $n_t - n_i$ terms are just 1. Similarly if at round $n_t$ we place $a \in R_t$ then the last $n_t - n_i$ terms are $-1$. Otherwise all terms are simply $\mu(a)$. Formally,

$$
\bar{\mu}_t(a) = \frac{1}{n_t} \sum_{t=1}^{K} (n_t - n_{t-1}) \mu 1\{a \not\in R_t \cup A_t\} + 1\{a \in A_t\} - 1\{a \in R_t\}.
$$

Note that this is different but related to our definition in the fixed confidence proof. We define the high probability event:

$$
E \triangleq \{ \forall t \in [K], \forall v \in V, |(v - v^*, \bar{\mu}_t - \bar{\mu}_t)| < c(d(v, v^*)\Delta)^t\},
$$

where $c < 1$ is a constant that we will set later. Now we show that $E$ holds with high probability:

$$
P[E] \leq \sum_{t} \sum_{v \in V} \exp \left\{ -\frac{c^2(d(v, v^*)\Delta^2(t)^2)(T - K)}{\log(K)(K + 1 - t)} \right\}
$$

$$
\leq K \sum_{v \in V} \exp \left\{ -\frac{c^2(T - K)d(v, v^*)}{\log(K)H} \right\}
$$

$$
\leq K \sum_{k \in [K]} \exp \left\{ -\frac{c^2(T - K)k}{\log(K)H} + \log |B(k, v^*)| \right\}
$$

$$
\leq K^2 \exp \left\{ \Psi \left( \Phi - \frac{(T - K)c^2}{\log(K)H} \right) \right\}.
$$

Line 7–13 of the algorithm computes $\hat{a}_t = \arg\max_a \Delta_{\hat{a}_t,a}$ efficiently using the linear optimization oracle as we have discussed. Then the algorithm decides to accept or reject $\hat{a}_t$ based on whether it is in the ERM $\hat{v}_t$ at round $t$. We proceed to show that, conditioned on event $E$, $A_{K+1} = v^*$. At round $t$, define

$$
a_t^* = \arg\max_{a \in [K] \setminus (A_t \cup R_t)} \Delta_a,
$$

where $A_t$ and $R_t$ are the currently accepted and reject arms at the beginning of round $t$ and $\Delta_a$ is the true arm complexity, toward $v^*$. Further assume (inductively) that $A_t \subset v^*$ and $R_t \cup v^* = \emptyset$. We establish five facts:
**Fact 1.** At the beginning of round $t$, $a_t^*$ satisfies $\Delta_{a_t^*} \geq \Delta^{(t)}$. If this statement does not hold at round $t$, then we must have eliminated all of the the $t$ arms $\Delta(1), \ldots, \Delta^{(t)}$. However, since we eliminate exactly one arm in each round, we can only eliminate $t - 1$ arms before round $t$, which produces a contradiction since $a_t^*$ is the maximizer.

**Fact 2.** Under the inductive hypothesis, for all $v \in \mathcal{V}$, we have $\langle \hat{\mu}_t, v^* - v \rangle \geq \langle \mu, v^* - v \rangle$. This is similar to the argument we used in the fixed confidence proof. For any arm $a$, if $a \notin A_t \cup R_t$ then the corresponding terms are equal. If $a \in A_t$ then since by induction we know $a \in v^*$, the term for $v^*$ is as high as possible and analogously if $a \in R_t$ the term for $v^*$ is as low as possible.

**Fact 3.** $a_t^* \in \hat{v}_t \iff a_t^* \in v^*$. Assume for the sake of contradiction that $a_t^* \in \hat{v}_t$ and $a_t^* \notin v^*$. The proof is the same for the other case. We have

$$
\Delta_{a_t^*} = \min_{a_t^* \in v^* \ominus v} \frac{\langle \mu, v^* - v \rangle}{d(v^*, v)} \leq \frac{\langle \mu, \hat{v}_t - v \rangle}{d(\hat{v}_t, v^*)}.
$$

Thus we have $\langle \hat{\mu}, \hat{v}_t - v^* \rangle \leq -\Delta_{a_t^*}$. By the previous fact we know $\Delta_{a_t} \geq \Delta^{(t)}$ since $a_t^*$ is the maximizer. Now, conditioned on $\mathcal{E}$:

$$
\frac{\langle \hat{\mu}, \hat{v}_t - v^* \rangle}{d(\hat{v}_t, v^*)} < \frac{\langle \hat{\mu}, \hat{v}_t - v^* \rangle}{d(\hat{v}_t, v^*)} + c\Delta^{(t)} \leq \frac{\langle \mu, \hat{v}_t - v^* \rangle}{d(\hat{v}_t, v^*)} + c\Delta^{(t)} - \Delta^{(t)} - \Delta_{a_t^*} \leq 0.
$$

The first inequality is by event $\mathcal{E}$, the second is by Fact 2 and the final one is by Fact 1 and the definition of $a_t^*$. This results in a contradiction.

**Fact 4.** Let $\hat{v}_t,a_t^*$ be the set that witnesses $\hat{\Delta}_{t,a_t^*}$, i.e. $\hat{v}_t,a_t^* = \arg\min_{v \ominus \hat{v}_t} \hat{\Delta}_{t,v}$. We have that $\langle \hat{\mu}, v^* - \hat{v}_t,a_t^* \rangle > 0$. To see why, note that $a_t^* \in \hat{v}_t \ominus \hat{v}_t,a_t^*$ and by Fact 3 we have $a_t^* \in v^* \ominus \hat{v}_t,a_t^*$. Conditioning on $\mathcal{E}$ and using the fact that the true gap $\Delta_{a_t^*}$ involves minimizing over $v \in \mathcal{V}$ we get

$$
\frac{\langle \hat{\mu}, v^* - \hat{v}_t,a_t^* \rangle}{d(v^*, \hat{v}_t,a_t^*)} \geq \frac{\langle \mu, v^* - \hat{v}_t,a_t^* \rangle}{d(v^*, \hat{v}_t,a_t^*)} - c\Delta^{(t)} \geq \frac{\langle \mu, v^* - \hat{v}_t,a_t^* \rangle}{d(v^*, \hat{v}_t,a_t^*)} - c\Delta^{(t)} - \Delta_{a_t^*} \geq 0.
$$

The last step here uses Fact 1.

**Fact 5.** $\hat{a}_t \in \hat{v}_t \iff \hat{a}_t \in v^*$. Assume for the sake of contradiction that $\hat{a}_t \in \hat{v}_t, \hat{a}_t \notin v^*$. We have

$$
\hat{\Delta}_{t,a_t} = \min_{a_t \in \hat{v}_t \Delta v} \frac{\langle \hat{\mu}_t, \hat{v}_t - v \rangle}{d(\hat{v}_t, v)} \leq \frac{\langle \hat{\mu}_t, \hat{v}_t - v^* \rangle}{d(\hat{v}_t, v^*)}.
$$

As above, let $\hat{v}_t,a_t^*$ be the set that witnesses $\hat{\Delta}_{t,a_t^*}$. Since $\hat{a}_t$ maximizes $\hat{\Delta}_{t,a}$ over all surviving arms $a$ and since $a_t^*$ is surviving by definition, we have

$$
\hat{\Delta}_{t,a_t} \geq \min_{a_t^* \in \hat{v}_t \ominus v} \frac{\langle \hat{\mu}_t, \hat{v}_t - v \rangle}{d(\hat{v}_t, v)} = \frac{\langle \hat{\mu}_t, \hat{v}_t - \hat{v}_t,a_t^* \rangle}{d(\hat{v}_t, \hat{v}_t,a_t^*)}
$$

$$
\geq \frac{\langle \hat{\mu}_t, \hat{v}_t - v^* \rangle + \langle \hat{\mu}_t, v^* - \hat{v}_t,a_t^* \rangle}{d(\hat{v}_t, v^*) + d(v^*, \hat{v}_t,a_t^*)}
$$

$$
\geq \min \left\{ \frac{\langle \hat{\mu}_t, \hat{v}_t - v^* \rangle}{d(\hat{v}_t, v^*)}, \frac{\langle \hat{\mu}_t, v^* - \hat{v}_t,a_t^* \rangle}{d(v^*, \hat{v}_t,a_t^*)} \right\}
$$

$$
\leq \min\{a, b\}.
$$

The last inequality holds since both terms in the numerator are non-negative as we have shown above in Fact 4. Since we previously upper bounded $\hat{\Delta}_{t,a_t}$ by what we are now calling $a$, we have $a \geq \min\{a, b\}$. If $a \leq b$,
then all of the inequalities are actually equalities, so we must have \( a = b \). The other case is that \( a > b \), so we can address both cases by considering \( a \geq b \). Expanding the definition and applying the concentration inequality, we have

\[
\begin{align*}
 b & \equiv \frac{\langle \hat{\mu}_t, v^* - \hat{v}_t, a_t \rangle}{d(v^*, \hat{v}_t, a_t)} \geq \frac{\langle \mu, v^* - \hat{v}_t, a_t \rangle}{d(v^*, \hat{v}_t, a_t)} - c\Delta(t) \geq \Delta_a; - c\Delta(t).
\end{align*}
\]

On the other hand,

\[
\begin{align*}
 a & \equiv \frac{\langle \hat{\mu}_t, \hat{v}_t - v^* \rangle}{d(\hat{v}_t, v^*)} \leq \frac{\langle \mu, \hat{v}_t - v^* \rangle}{d(\hat{v}_t, v^*)} + c\Delta(t) \leq c\Delta(t).
\end{align*}
\]

Both of these calculations also require Fact 2. Setting \( c = 1/3 \), we have

\[
\Delta_a; \leq 2c\Delta(t) < \Delta(t),
\]

which contradicts Fact 1 and the definition of \( a_t \).

Wrapping up. To conclude the proof, we proceed by induction. Clearly the base case that \( A_0 \subset v^* \) and \( R_0 \cap v^* = \emptyset \) is true. Now conditioning on \( \mathcal{E} \) and assuming the inductive hypothesis, we have that by Fact 5, the arm \( \hat{a}_t \in \hat{v}_t \iff \hat{a}_t \in v^* \). This directly proves the inductive step since the algorithm’s rule for accepting an arm agrees with \( v^* \).

\( \Box \)

D Proof of Theorem 6

Ignoring computational efficiency, we show how to obtain a more refined sample complexity bound for the fixed confidence setting. Recall that in the main concentration argument in Lemma 8, we proved that

\[
P[\exists t \in \mathbb{N}, \exists v \in \mathcal{V}, |\langle v^* - v, \hat{\mu}_t - \sum_{i=1}^t \hat{\mu}_i \rangle| \geq \epsilon_t(v, v^*, \delta)] \leq 2 \sum_{t \in \mathbb{N}} \sum_{v \in \mathcal{V}} \exp \left\{ -\frac{t\epsilon_t(v, v^*, \delta)^2}{8d(v, v^*)} \right\}.
\]

Setting

\[
\epsilon_t(v, v^*, \delta) = \sqrt{\frac{8d(v, v^*)}{t} \log \frac{|B(d(v, v^*), v)|}{\pi^2 Kt^2}},
\]

we have that the probability of this event is at most \( \delta \). Previously we set each arm to have the same confidence interval

\[
\Delta_t = \sqrt{\frac{8}{t} \left( \Phi + \frac{\log(\pi^2 Kt^2/(3\delta))}{\Psi} \right)},
\]

which enabled us to write the disagreement region as a polyhedral set in \( \mathcal{V} \). To obtain a more refined sample complexity bound, we would like to use \( \epsilon_t(v, v^*, \delta) \) directly. However, note that \( \epsilon_t(v, v^*, \delta) \neq \epsilon_t(v', v, \delta) \) unless the hypothesis space is \( \mathcal{V} \) is symmetric. We symmetrize \( \epsilon_t \) by defining

\[
D(v, v') \equiv \max \{ \log |B(d(v, v'), v)|, \log |B(d(v, v'), v')| \} = D(v', v),
\]

23
Algorithm 4: Inefficient fixed confidence algorithm

1: Input: $\mathcal{V}$, set of arms $[K]$, $\delta$
2: Set $\mathcal{V}_1 = \mathcal{V}$
3: for $t = 1, 2, 3, \ldots$ do
4: $\mathcal{A}_t = \emptyset$
5: for $a \in [K]$ do
6: if $\exists v, v' \in \mathcal{V}_t$ such that $v(a) \neq v'(a)$ then
7: $\mathcal{A}_t = \mathcal{A}_t \cup a$, query $a$, set $y_t(a) \sim \mathcal{N}(\mu(a), 1)$
8: end if
9: end for
10: Update $\hat{\mu}_t = \frac{1}{t} \sum_{\tau=1}^{t} y_{\tau}$.
11: $\mathcal{R}_t \leftarrow \{ v \in \mathcal{V}_t \mid \exists u \in \mathcal{V}_t, u \neq v, \langle u - v, \hat{\mu}_t \rangle > \epsilon'_t(u, v, \delta) \}$$
12: Update $\mathcal{V}_{t+1} \leftarrow \mathcal{V}_t \setminus \mathcal{R}_t$
13: if $|\mathcal{V}_{t+1}| = 1$ then
14: return the single element $v \in \mathcal{V}_{t+1}$.
15: end if
16: end for

and the symmetric confidence interval

$$\epsilon'_t(v, v', \delta) \triangleq \sqrt{\frac{8d(v, v')}{t} \left( \log \frac{\pi^2 K t^2}{3\delta} + D(v, v') \right)}.$$ (8)

Define the complexity measures, for $v \neq v^*$

$$H^{(1)}_v = \frac{d(v, v^*)}{\langle \mu, v^* - v \rangle^2}, \quad H^{(1)}_a = \max_{a \in [v \neq v^*]} H^{(1)}_v,$$

$$H^{(2)}_v = \frac{d(v, v^*)D(v, v^*)}{\langle \mu, v^* - v \rangle^2}, \quad H^{(2)}_a = \max_{v: a \in [v \neq v^*]} H^{(2)}_v.$$ (9)

The main difference here is that we are not normalizing by $d(v, v^*)^2$ as we did in the proof of Theorem 4 but rather just $d(v, v^*)$. In some sense we replace the term depending on $\Psi$ with $H^{(1)}_a$ and the term depending on $\Phi$ with $H^{(2)}_a$.

To prove Theorem 6, we construct an inefficient fixed confidence algorithm, with pseudocode in Algorithm 4. The algorithm is essentially identical to Algorithm 1, except we use the new definition $\epsilon'$ in the confidence bounds defining the version space, which forces us to do explicit enumeration. One other minor difference is that we are now explicitly enforcing monotonicity of the version space, so we need not use hallucination as we did before.

We restate the theorem and the proceed with the proof.

Theorem 15 (Theorem 6 restated). Algorithm 4 satisfies $\mathbb{P}[\hat{v} \neq v^*] \leq \delta$ and has sample complexity

$$T \leq 64 \sum_{a \in [K]} H^{(1)}_a \left( 2 \log(64H^{(1)}_a) + \log \frac{\pi^2 K}{3\delta} \right) + 64H^{(2)}_a$$

24
Proof. In a similar way to Lemma 8 we can prove that

\[
P\{\forall t, \forall v \in V_t, |\langle v^* - v, \mu_t - \mu \rangle > \epsilon'_t(v^*, v, \delta)\} \leq 2 \sum_{v \in V} \exp \left\{ - \frac{t \epsilon'_t(v^*, v, \delta)^2}{8d(v, v^*)} \right\}.
\]

The important thing here is that if \( v \in V_t \) then we must query every \( a \in v \ominus v^* \) and moreover since we are explicitly enforcing monotonicity (i.e. \( V_t \subset V_t-1 \)), we also queried all of these arms in all previous rounds. Thus we are obtaining unbiased samples to evaluate these mean differences. Using the definition of \( \epsilon'_t \) in (8), this probability is at most \( \delta \).

Next we prove that when the algorithm terminates, the output is \( v^* \). We work conditional on the \( 1 - \delta \) event that the concentration inequality holds. We argue that \( v^* \) is never eliminated, or formally \( v^* \notin R_t \) for all \( t \). To see why observe that by the concentration inequality \( \forall v \in V_{t-1} \neq v^* \), we have

\[
\langle \mu_t, v - v^* \rangle \leq \langle \mu, v - v^* \rangle + \epsilon'_t(v, v^*, \delta).
\]

By the definition of the set \( R_t \), this means that no surviving \( v \in V_t \) can eliminate \( v^* \). The proof of the claim now follows by induction since \( v^* \in V_1 \). Thus, if \( |V_t| = 1 \) the only element must be \( v^* \), which proves the correctness of the algorithm.

We now turn to the sample complexity. We argue here that if \( t > 32H^{(1)}_a \log(\pi^2 Kt^2/(3\delta)) + 32H^{(2)}_a \) then from round \( t \) onwards, arm \( a \) will not be sampled again. This condition on \( t \) implies that for all \( v \in V \) such that \( a \in v \ominus v^* \), we have

\[
\epsilon'_t(v^*, v, \delta) \leq \sqrt{\frac{8d(v, v^*)}{t}} \left( \log(\pi^2 Kt^2/(3\delta)) + D(v, v^*) \right) < \langle \mu, v - v^* \rangle / 2,
\]

by the definitions of \( H^{(1)}_a \) and \( H^{(2)}_a \). Using this simpler fact we argue that \( a \) cannot be sampled again. Working toward a contradiction, assume that \( a \) is sampled at round \( t+1 \), which means there exists two hypotheses \( v_1, v_2 \in V_{t+1} \) such that \( v_1(a) \neq v_2(a) \). We now consider several cases.

**Case 1.** If \( v_1 = v^* \) then we clearly have

\[
\langle v^* - v_2, \mu_t \rangle \geq \langle v^* - v_2, \mu \rangle - \epsilon'_t(v^*, v_2, \delta) > \epsilon'_t(v^*, v_2, \delta)
\]

which is a contradiction since \( v_2 \) must have been eliminated at round \( t \). A similar argument applies if \( v_2 = v^* \).

**Case 2.** If neither \( v_1, v_2 \) are \( v^* \) let us assume without loss of generality that \( a \in v_1 \setminus v_2 \). Recall that \( v^* \in V_t \) always. Now, suppose that \( a \notin v^* \), which means that \( a \in v_1 \ominus v^* \) based on our assumptions. This means

\[
\langle v^* - v_1, \mu_t \rangle \geq \langle v^* - v_1, \mu \rangle - \epsilon'_t(v^*, v, \delta) > \epsilon'_t(v^*, v_1, \delta)
\]

This is a contradiction since it implies that \( v_1 \) was eliminated at round \( t - 1 \). On the other hand, if \( a \in v^* \) then \( a \in v^* \ominus v_2 \) in which case we can use the exact same argument on \( v_2 \).

This proves that \( a \notin A_{t+1} \) and since \( V_t \) is monotonic, so is \( A_t \), which means that \( a \) is never sampled again.

To summarize, we have now shown that for each arm \( a \), the arm will be sampled at most \( t_a \) times, where \( t_a \) is the smallest integer satisfying

\[
t_a \geq 32H^{(1)}_a \log(\pi^2 Kt_a^2/(3\delta)) + 32H^{(2)}_a.
\]

The final result now follows from an application of Fact 13.
References

[1] Emmanuel Abbe, Afonso S Bandeira, and Georgina Hall. Exact recovery in the stochastic block model. *IEEE Transactions on Information Theory*, 2016.

[2] Louigi Addario-Berry, Nicolas Brounin, Luc Devroye, and Gábor Lugosi. On combinatorial testing problems. *The Annals of Statistics*, 2010.

[3] Alekh Agarwal, Daniel Hsu, Satyen Kale, John Langford, Lihong Li, and Robert E. Schapire. Taming the monster: A fast and simple algorithm for contextual bandits. In *International Conference on Machine Learning*, 2014.

[4] András Antos, Varun Grover, and Csaba Szepesvári. Active learning in heteroscedastic noise. *Theoretical Computer Science*, 2010.

[5] Ery Arias-Castro and Emmanuel J. Candès. Searching for a trail of evidence in a maze. *The Annals of Statistics*, 2008.

[6] Jean-Yves Audibert and Sébastien Bubeck. Best arm identification in multi-armed bandits. In *Conference on Learning Theory*, 2010.

[7] Sivaraman Balakrishnan, Min Xu, Akshay Krishnamurthy, and Aarti Singh. Noise Thresholds for Spectral Clustering. In *Advances in Neural Information Processing Systems*, 2011.

[8] Sébastien Bubeck, Tengyao Wang, and Nitin Viswanathan. Multiple identifications in multi-armed bandits. In *International Conference on Machine Learning*, 2013.

[9] Cristina Butucea and Yuri I. Ingster. Detection of a sparse submatrix of a high-dimensional noisy matrix. *Bernoulli*, 2013.

[10] Alexandra Carpentier and Andrea Locatelli. Tight (lower) bounds for the fixed budget best arm identification bandit problem. In *Conference on Learning Theory*, 2016.

[11] Rui Castro and Ervin Tánczos. Adaptive sensing for estimation of structured sparse signals. *IEEE Transactions on Information Theory*, 2015.

[12] Rui Castro, Mark Coates, Gang Liang, Robert Nowak, and Bin Yu. Network tomography: Recent developments. *Statistical science*, 2004.

[13] Lijie Chen, Anupam Gupta, and Jian Li. Pure exploration of multi-armed bandit under matroid constraints. In *Conference on Learning Theory*, 2016.

[14] Lijie Chen, Anupam Gupta, Jian Li, Mingda Qiao, and Ruosong Wang. Nearly optimal sampling algorithms for combinatorial pure exploration. In *Conference on Learning Theory*, 2017.

[15] Lijie Chen, Jian Li, and Mingda Qiao. Nearly instance optimal sample complexity bounds for top-k arm selection. In *Artificial Intelligence and Statistics*, 2017.

[16] Shouyuan Chen, Tian Lin, Irwin King, Michael R Lyu, and Wei Chen. Combinatorial pure exploration of multi-armed bandits. In *Advances in Neural Information Processing Systems*, 2014.
[17] Yudong Chen and Jiaming Xu. Statistical-computational tradeoffs in planted problems and submatrix localization with a growing number of clusters and submatrices. *Journal of Machine Learning Research*, 2016.

[18] David Cohn, Les Atlas, and Richard Ladner. Improving generalization with active learning. *Machine Learning*, 1994.

[19] Sanjoy Dasgupta, Daniel Hsu, and Claire Monteleoni. A general agnostic active learning algorithm. In *Advances in Neural Information Processing Systems*, 2007.

[20] Eyal Even-Dar, Shie Mannor, and Yishay Mansour. Action elimination and stopping conditions for the multi-armed bandit and reinforcement learning problems. *Journal of machine learning research*, 2006.

[21] Victor Gabillon, Alessandro Lazaric, Mohammad Ghavamzadeh, Ronald Ortner, and Peter Bartlett. Improved learning complexity in combinatorial pure exploration bandits. In *Artificial Intelligence and Statistics*, 2016.

[22] Aurélien Garivier and Emilie Kaufmann. Optimal best arm identification with fixed confidence. In *Conference on Learning Theory*, 2016.

[23] Steve Hanneke. Theory of disagreement-based active learning. *Foundations and Trends in Machine Learning*, 2014.

[24] Daniel Hsu. *Algorithms for Active Learning*. PhD thesis, University of California at San Diego, 2010.

[25] Tzu-Kuo Huang, Alekh Agarwal, Daniel Hsu, John Langford, and Robert E. Schapire. Efficient and parsimonious agnostic active learning. In *Advances in Neural Information Processing Systems*, 2015.

[26] Adam Kalai and Santosh Vempala. Efficient algorithms for online decision problems. *Journal of Computer and System Sciences*, 2005.

[27] Shivaram Kalyanakrishnan, Ambuj Tewari, Peter Auer, and Peter Stone. Pac subset selection in stochastic multi-armed bandits. In *International Conference on Machine Learning*, 2012.

[28] Zohar Karnin, Tomer Koren, and Oren Somekh. Almost optimal exploration in multi-armed bandits. In *Proceedings of the 30th International Conference on Machine Learning (ICML-13)*, 2013.

[29] Zohar S Karnin. Verification based solution for structured mab problems. In *Advances in Neural Information Processing Systems*, 2016.

[30] Emilie Kaufmann and Shivaram Kalyanakrishnan. Information complexity in bandit subset selection. In *Conference on Learning Theory*, 2013.

[31] Emilie Kaufmann, Olivier Cappé, and Aurélien Garivier. On the complexity of a/b testing. In *Conference on Learning Theory*, 2014.

[32] Mladen Kolar, Sivaraman Balakrishnan, Alessandro Rinaldo, and Aarti Singh. Minimax localization of structural information in large noisy matrices. *Advances in Neural Information Processing Systems*, 2011.

[33] Akshay Krishnamurthy. Minimax structured normal means inference. *IEEE International Symposium on Information Theory*, 2016.
[34] Shie Mannor and John N Tsitsiklis. The sample complexity of exploration in the multi-armed bandit problem. *Journal of Machine Learning Research*, 2004.

[35] Elchanan Mossel, Joe Neeman, and Allan Sly. Belief propagation, robust reconstruction and optimal recovery of block models. In *Conference on Learning Theory*, 2014.

[36] Barzan Mozafari, Purna Sarkar, Michael Franklin, Michael Jordan, and Samuel Madden. Scaling up crowd-sourcing to very large datasets: a case for active learning. *Proceedings of the VLDB Endowment*, 2014.

[37] Serge A. Plotkin, David B. Shmoys, and Éva Tardos. Fast approximation algorithms for fractional packing and covering problems. *Mathematics of Operations Research*, 1995.

[38] Alexander Rakhlin and Karthik Sridharan. Bistro: An efficient relaxation-based method for contextual bandits. In *International Conference on Machine Learning*, 2016.

[39] Daniel Russo. Simple bayesian algorithms for best arm identification. In *Conference on Learning Theory*, 2016.

[40] Max Simchowitz, Kevin Jamieson, and Benjamin Recht. The simulator: Understanding adaptive sampling in the moderate-confidence regime. In *Conference on Learning Theory*, 2017.

[41] Vasilis Syrgkanis, Haipeng Luo, Akshay Krishnamurthy, and Robert E Schapire. Improved regret bounds for oracle-based adversarial contextual bandits. In *Advances in Neural Information Processing Systems*, 2016.

[42] Shu Wang, Robin R Gutell, and Daniel P Miranker. Biclustering as a method for rna local multiple sequence alignment. *Bioinformatics*, 2007.