Polynomial-time Algorithms for Multiple-arm Identification with Full-bandit Feedback

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Abstract

We study the problem of stochastic multiple-arm identification, where an agent sequentially explores a size-$k$ subset of arms (a.k.a. a super-arm) from given $n$ arms and tries to identify the best super-arm. Most existing work has considered the semi-bandit setting, where the agent can observe the reward of each pulled arm, or assumed each arm can be queried at each round. However, in real-world applications, it is costly or sometimes impossible to observe a reward of individual arms. In this study, we tackle the full-bandit setting, where only a noisy observation of the total sum of a super-arm is given at each pull. Although our problem can be regarded as an instance of the best arm identification in linear bandits, a naive approach based on linear bandits is computationally infeasible since the number of super-arms $K$ is exponential. To cope with this problem, we first design a polynomial-time approximation algorithm for a 0-1 quadratic programming problem arising in confidence ellipsoid maximization. Based on our approximation algorithm, we propose a bandit algorithm whose computation time is $O(\log K)$, thereby achieving an exponential speedup over linear bandit algorithms. We provide a sample complexity upper bound that is still worst-case optimal. Finally, we conduct experiments on large-scale datasets with more than $10^{10}$ super-arms, demonstrating the superiority of our algorithms in terms of both the computation time and the sample complexity.

1 Introduction

The stochastic multi-armed bandit (MAB) is a classical decision making model, which characterizes the trade-off between exploration and exploitation in stochastic environments [33]. While the most well-studied objective is to minimize the cumulative regret or maximize the cumulative reward [7] [11], another popular objective is to identify the best arm with the maximum expected reward from given $n$ arms. This problem, called pure exploration or best arm identification in the MAB, has received much attention recently [4] [14] [16] [17] [24] [29].

An important variant of the MAB is the multiple-play MAB problem (MP-MAB), in which the agent pulls $k$ ($\geq 1$) different arms at each round [1] [2] [31] [32]. In many application domains, we need to make a decision to take multiple actions among a set of all possible choices. For example, in online advertisement auctions, companies want to choose multiple keywords to promote their products to consumers based on their search queries [18]. From millions of available choices, a company aims to find the most effective set of keywords by observing the historical performance of the chosen keywords. This decision making is formulated as the MP-MAB, where each arm corresponds to each keyword. In addition, MP-MAB has
In this paper, we study the multiple-arm identification problem, which corresponds to the pure exploration in the MP-MAB. In this problem, the goal is to find the size-$k$ subset (a.k.a. a super-arm) with the maximum expected rewards. The problem is also called the top-$k$ selection or $k$-best arm identification, and has been extensively studied recently. The above prior work has considered the semi-bandit setting, in which we can observe a reward of each single-arm in the pulled super-arm, or assumed that a single-arm can be queried. However, in many application domains, it is costly to observe a reward of individual arms, or sometimes we cannot access feedback from individual arms. For example, in crowdsourcing, we often obtain a lot of labels given by crowdworkers, but it is costly to compile labels according to labelers. Furthermore, in software projects, an employer may have complicated tasks that need multiple workers, in which the employer can only evaluate the quality of a completed task rather than a single worker performance. In such scenarios, we wish to extract expert workers who can perform the task with high quality, only from a sequential access to the quality of the task completed by multiple workers.

In this study, we tackle the multiple-arm identification with full-bandit feedback, where only a noisy observation of the total sum of a super-arm is given at each pull, rather than a reward of each pulled single-arm. This setting is more challenging since estimators of expected rewards of single-arms are no longer independent of each other. We can see our problem as an instance of the pure exploration in linear bandits, which has received increasing attention. In linear bandits, each arm has its own feature $x \in \mathbb{R}^n$, while in our problem, each super-arm can be associated with a vector $x \in \{0, 1\}^n$. Most linear bandit algorithms have, however, the time complexity at least proportional to the number of arms. Therefore, a naive use of them is computationally infeasible since the number of super-arms $K = \binom{n}{k}$ is exponential. A modicum of research on linear bandits addressed the time complexity; Jun et al. proposed efficient algorithms for regret minimization, which results in the sublinear time complexity $O(K^\rho)$ for $\rho \in (0, 1)$. Nevertheless, in our setting, they still have to spend $O(\rho k)$ time, where $\rho \in (0, 1)$ is a constant, which is exponential. Thus, to perform multiple-arm identification with full-bandit feedback in practice, the computational infeasibility needs to be overcome since fast decisions are required in real-world applications.

Our Contribution. In this study, we design algorithms, which are efficient in terms of both the time complexity and the sample complexity. Our contributions are summarized as follows:

(i) We propose a polynomial-time approximation algorithm (Algorithm 1) for an NP-hard 0-1 quadratic programming problem arising in confidence ellipsoid maximization. In the design of the approximation algorithm, we utilize algorithms for a classical combinatorial optimization problem called the densest $k$-subgraph problem (D$k$S) [13]. Importantly, we provide a theoretical guarantee for the approximation ratio of our algorithm (Theorem 1).

(ii) Based on our approximation algorithm, we propose a bandit algorithm (Algorithm 2) that runs in $O(\log K)$ time (Theorem 2), and provide an upper bound of the sample complexity (Theorem 3) that is still worst-case optimal. This result means that our algorithm achieves an exponential speedup over linear bandit algorithms while keeping the statistical efficiency. Moreover, we propose another algorithm (Algorithm 3) that employs the first-order approximation of confidence ellipsoids, which empirically performs well.

(iii) We conduct a series of experiments on both synthetic and real-world datasets. First, we run our proposed algorithms on synthetic datasets and verify that our algorithms give good approximation to an exhaustive search algorithm. Next, we evaluate our algorithms on large-scale crowdsourcing datasets with more than $10^{10}$ super arms, demonstrating the superiority of our algorithms in terms of both the time complexity and the sample complexity. Note that the multiple-arm identification problem is a special class of the combinatorial pure exploration, where super-arms follow certain combinatorial constraints such as paths, matchings, or matroids. We can also design a simple algorithm (Algorithm 1 in Appendix A) for the combinatorial pure exploration under general constraints with full-bandit feedback, which results in looser but general sample complexity bound. For details, see Appendix A. Owing to space limitations, all proofs in this paper
are given in Appendix F.

2 Preliminaries

Problem definition. Let \([n] = \{1, 2, \ldots, n\}\) for an integer \(n\). For a vector \(x \in \mathbb{R}^n\) and a matrix \(B \in \mathbb{R}^{n \times n}\), let \(\|x\|_B = \sqrt{x^T B x}\). For a vector \(\theta \in \mathbb{R}^n\) and a subset \(S \subseteq [n]\), we define \(\theta(S) = \sum_{e \in S} \theta(e)\). Now, we describe the problem formulation formally. Suppose that there are \(n\) single-arms associated with unknown reward distributions \(\{\phi_1, \ldots, \phi_n\}\). The reward from \(\phi_e\) for each single-arm \(e \in [n]\) is expressed as \(X_t(e) = \theta(e) + \epsilon_t(e)\), where \(\theta(e)\) is the expected reward and \(\epsilon_t(e)\) is the zero-mean noise bounded in \([-R, R]\) for some \(R > 0\). The agent chooses a size-\(k\) subset from \(n\) single-arms at each round \(t\) for an integer \(k > 0\). In the well-studied semi-bandit setting, the agent pulls a subset \(M_t\), and then she can observe \(X_t(e)\) for each \(e \in M_t\) independently sampled from the associated unknown distribution \(\phi_e\). However, in the full-bandit setting, she can only observe the sum of rewards \(r_{M_t} = \theta(M_t) + \sum_{e \in M_t} \epsilon_t(e)\) at each pull, which means that estimators of expected rewards of single-arms are no longer independent of each other.

We call a size-\(k\) subset of single-arms a super-arm. We define a decision class \(M\) as a finite set of super-arms that satisfies the size constraint, i.e., \(M = \{M \subseteq 2^{[n]} : |M| = k\}\); thus, the size of the decision class is given by \(K = \binom{n}{k}\). Let \(M^* \subseteq M\) be the optimal super-arm in the decision class \(M\), i.e., \(M^* = \arg \max_{M \in M} \theta(M)\). In this paper, we focus on the \((\varepsilon, \delta)\)-PAC setting, where the goal is to design an algorithm to output the super-arm \(\text{Out} \in M\) that satisfies for \(\delta \in (0, 1)\) and \(\varepsilon > 0\), \(\Pr[\theta(\text{Out}) - \theta(\text{Out})] \geq 1 - \delta\). An algorithm is called \((\varepsilon, \delta)\)-PAC if it satisfies this condition. In the fixed confidence setting, the agent’s performance is evaluated by her sample complexity, i.e., the number of rounds until the agent terminates.

Technical tools. In order to handle full-bandit feedback, we utilize approaches for best arm identification in linear bandits. Let \(M_t = (M_{t1}, M_{t2}, \ldots, M_{tn}) \in \mathcal{M}^t\) be a sequence of super-arms and \((r_{M_{t1}}, \ldots, r_{M_{tn}}) \in \mathbb{R}^t\) be the corresponding sequence of observed rewards. Let \(\chi_M \in \{0, 1\}^n\) denote the indicator vector of super-arm \(M \in \mathcal{M}\); for each \(e \in [n]\), \(\chi_M(e) = 1\) if \(e \in M\) and \(\chi_M(e) = 0\) otherwise. We define the sequence of indicator vectors corresponding to \(M_t\) as \(x_t = (\chi_{M_{t1}}, \ldots, \chi_{M_{tn}})\). An unbiased least-squares estimator for \(\theta \in \mathbb{R}^n\) can be obtained by \(\hat{\theta}_t = A_{x_t}^{-1} b_{x_t} \in \mathbb{R}^n\), where \(A_{x_t} = \sum_{i=1}^t \chi_{M_{t_i}}\chi_{M_{t_i}}^T \in \mathbb{R}^{n \times n}\) and \(b_{x_t} = \sum_{i=1}^t \chi_{M_{t_i}} r_{M_{t_i}} \in \mathbb{R}^n\). It suffices to consider the case where \(A_{x_t}\) is invertible, since we shall exclude a redundant feature when any sampling strategy cannot make \(A_{x_t}\) invertible. We define the empirical best super-arm as \(\hat{M}_t^* = \arg \max_{M \in \mathcal{M}} \hat{\theta}_t(M)\).

Computational hardness. The agent continues sampling a super-arm until a certain stopping condition is satisfied. In order to check the stopping condition, existing algorithms for best arm identification in linear bandits involve the following confidence ellipsoid maximization:

\[
\text{CEM: } \max \|\chi_M\|_{A_{x_t}^{-1}} \quad \text{s.t. } M \in \mathcal{M},
\]

where recall that \(\|\chi_M\|_{A_{x_t}^{-1}} = \sqrt{\chi_M^T A_{x_t}^{-1} \chi_M}\). Existing algorithms in linear bandits implicitly assume that an optimal solution to CEM can be exhaustively searched (e.g., \(\text{LS} \ [50]\)). However, since the number of super-arms \(K\) is exponential in our setting, it is computationally intractable to exactly solve it. Therefore, we need its approximation or a totally different approach for solving the multiple-arm identification with full-bandit feedback.

3 Confidence Ellipsoid Maximization

In this section, we design an approximation algorithm for confidence ellipsoid maximization CEM. In the combinatorial optimization literature, an algorithm is called an \(\alpha\)-approximation algorithm if it returns a solution that has an objective value greater than or equal to the optimal value times \(\alpha \in (0, 1]\) for any instance. Let \(W \in \mathbb{R}^{n \times n}\) be a symmetric matrix. CEM introduced above can be naturally represented by
the following 0-1 quadratic programming problem:

\[
\text{QP: } \max \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} x_i x_j \quad \text{s.t.} \quad \sum_{i=1}^{n} x_i = k, \quad x_i \in \{0, 1\}, \quad \forall i \in [n].
\]

Notice that QP can be seen as an instance of the uniform quadratic knapsack problem, which is known to be NP-hard [7], and there are few results of polynomial-time approximation algorithms even for a special case (see Appendix C for details).

In this study, by utilizing algorithms for a classical combinatorial optimization problem, called the densest k-subgraph problem (DkS), we design an approximation algorithm that admits theoretical performance guarantee for QP with positive definite matrix W. The definition of the DkS is as follows. Let \( G = (V, E, w) \) be an undirected graph with nonnegative edge weight \( w = (w_e)_{e \in E} \). For a vertex set \( S \subseteq V \), let \( E(S) = \{ (u, v) \in E : u, v \in S \} \) be the subset of edges in the subgraph induced by \( S \). We denote by \( w(S) \) the sum of the weights in the subgraph induced by \( S \), i.e., \( w(S) = \sum_{e \in E(S)} w_e \). In the DkS, given \( G = (V, E, w) \) and positive integer \( k \), we are asked to find \( S \subseteq V \) with \( |S| = k \) that maximizes \( w(S) \). Although the DkS is NP-hard, there are a variety of polynomial-time approximation algorithms [3][5][18]. The current best approximation result for the DkS has an approximation ratio of \( \Omega(1/|V|^{1/4+\epsilon}) \) for any \( \epsilon > 0 \) [1]. The direct reduction of QP to the DkS results in an instance that has arbitrary weights of edges. Existing algorithms cannot be used for such an instance since these algorithms need an assumption that the weights of all edges are nonnegative.

Now we present our algorithm for QP, which is detailed in Algorithm 1. The algorithm operates in two steps. In the first step, it constructs an \( n \)-vertex complete graph \( \tilde{G} = (V, E, \tilde{w}) \) from a given symmetric matrix \( W \in \mathbb{R}^{n \times n} \). For each \( \{i, j\} \in E \), the edge weight \( \tilde{w}_{ij} \) is set to \( w_{ij} + w_{ii} + w_{jj} \). Note that if \( W \) is positive definite, \( \tilde{w}_{ij} \geq 0 \) holds for every \( \{i, j\} \in E \), which means that \( \tilde{G} \) is an instance of the DkS (see Lemma 4 in Appendix F). In the second step, the algorithm accesses the densest k-subgraph oracle (DkS-Oracle), which accepts \( \tilde{G} \) as input and returns in polynomial time an approximate solution for the DkS. Note that we can use any polynomial-time approximation algorithm for the DkS as the DkS-Oracle. Let \( \alpha_{DkS} \) be the approximation ratio of the algorithm employed by the DkS-Oracle. By sophisticated analysis on the approximation ratio of Algorithm 1 we have the following theorem.

**Theorem 1.** For QP with any positive definite matrix \( W \in \mathbb{R}^{n \times n} \), Algorithm 1 with \( \alpha_{DkS} \)-approximation DkS-Oracle is a \( \left( \frac{1}{k-1} \frac{\lambda_{\min}(W)}{\lambda_{\max}(W)} \right)^{\alpha_{DkS}} \)-approximation algorithm, where \( \lambda_{\min}(W) \) and \( \lambda_{\max}(W) \) represent the minimum and maximum eigenvalues of \( W \), respectively.

Notice that we prove \( \frac{\lambda_{\min}(W)}{\lambda_{\max}(W)} = O(1/k) \) for any round \( t > n \) in our bandit algorithm (see Lemma 7 in Appendix F).

### 4 Main Algorithm

Based on the approximation algorithm proposed in the previous section, we propose two algorithms for the multiple-arm identification with full-bandit feedback. Note that we assume that \( k \geq 2 \) since the multiple-arm identification with \( k = 1 \) is the same as best arm identification problem of the MAB.
Algorithm 2: Static allocation algorithm with approximate quadratic maximization (SAQM)

\begin{algorithm} 
\begin{algorithmic}
  \State \textbf{Input}: Accuracy $\epsilon > 0$, confidence level $\delta \in (0,1)$, allocation strategy $p$
  \For{$t=1,\ldots, n$ do}
    \State $t \leftarrow t + 1$ and pull $M_t \in \text{supp}(p)$;
    \State Observe $r_{M_t}$, and update $A_t$ and $b_t$;
  \EndFor
  \While{stopping condition (4) is not true do}
    \State $t \leftarrow t + 1$;
    \State Pull $M_t \leftarrow \arg\min_{M \in \text{supp}(p)} \frac{T_M(t)}{p_M}$;
    \State Observe $r_{M_t}$, and update $A_t$ and $b_t$;
    \State $\hat{\theta}_t \leftarrow A_{x_t}^{-1} b_t$;
    \State $\hat{M}_t^* \leftarrow \arg\max_{M \in M} \hat{\theta}_t(M)$;
    \State $M_t^* \leftarrow \text{Quadratic Maximization}(A_{x_t}^{-1})$;
    \State $Z_t \leftarrow C_t \|x_t\|_{A_{x_t}^{-1}}$
  \EndWhile
  \State return $\hat{M}^* \leftarrow \hat{M}_t^*$
\end{algorithmic}
\end{algorithm}

Static algorithm. We deal with static allocation strategies, which sequentially sample a super-arm from a fixed sequence of super-arms. In general, adaptive strategies will perform better than static ones, but due to the computational hardness, we focus on static ones to analyze the worst-case optimality [45]. For static allocation strategies, where $x_t$ is fixed beforehand, Soare et al. [45] provided the following proposition on the confidence ellipsoid for $\hat{\theta}_t$.

Proposition 1 (Soare et al. [45], Proposition 1). Let $\epsilon_t$ be a noise variable bounded as $\epsilon_t \in [-\sigma, \sigma]$ for $\sigma > 0$. Let $c = 2\sqrt{2}\sigma$ and $c' = 6/\pi^2$ and fix $\delta \in (0,1)$. Then, for any fixed sequence $x_t$, with probability at least $1 - \delta$, the inequality

$$|x^T \theta - x^T \hat{\theta}_t| \leq C_t \|x\|_{A_{x_t}^{-1}}$$

holds for all $t \in \{1, 2, \ldots\}$ and $x \in \mathbb{R}^n$, where $C_t = c\sqrt{\log(c' t^2 K/\delta)}$.

In our problem, the proposition holds for $\sigma = kR$. Two allocation strategies named as G-allocation and $\mathcal{X}\mathcal{Y}$-allocation are discussed in Soare et al. [45]. Approximating the optimal G-allocation can be done via convex optimization and efficient rounding procedure, and $\mathcal{X}\mathcal{Y}$-allocation can be computed in similar manner (see Appendix D). In static algorithms, the agent pulls a super-arm from a fixed set of super-arms until a certain stopping condition is satisfied. Therefore, it is important to construct a stopping condition guaranteeing that the estimate $\hat{\theta}_t$ belongs to a set of parameters that admits the empirical best super-arm $M_t^*$ as an optimal super-arm $M^*$ as quickly as possible.

Proposed algorithm. Now we propose an algorithm named SAQM, which is detailed in Algorithm 2. Let $\mathcal{P}$ be a $K$-dimensional probability simplex. We define an allocation strategy $p$ as $p = (p_M)_{M \in M} \in \mathcal{P}$, where $p_M$ prescribes the proportions of pulls to super-arm $M$, and let $\text{supp}(p) = \{M \in M: p_M > 0\}$ be its support. Let $T_M(t)$ be the number of times that $M$ is pulled before $(t+1)$-th round. At each round $t$, SAQM samples a super-arm $M_t = \arg\min_{M \in \text{supp}(p)} \frac{T_M(t)}{p_M}$, and updates statistics $A_{x_t}, b_t$ and $\hat{\theta}_t$. Then, the algorithm computes the empirical best super-arm $\hat{M}_t^*$, and approximately solves CEM in (1), using Algorithm 1 as a subroutine. Note that any $\alpha$-approximation algorithm for QP is a $\sqrt{\alpha}$-approximation algorithm for CEM. SAQM employs the following stopping condition:

$$\hat{\theta}_t(M_t^*) - C_t \|x_t\|_{A_{x_t}^{-1}} \geq \max_{M \in M_t \setminus \{\hat{M}_t^*\}} \hat{\theta}_t(M) + \frac{1}{\alpha_t} C_t Z_t - \epsilon,$$

where $Z_t$ denotes the objective value of an approximate solution $M_t^*$ for CEM, and $\alpha_t$ denotes the approximation ratio of our algorithm for CEM at round $t$. Note that we can compute the value of $\alpha_t$...
(Algorithm 2) runs in polynomial time. If we employ the algorithm by Feige, Peleg, and Kortsarz, the running time of SAQM becomes $O(n^3)$, where the exponent $\omega \leq 2.373$ is equal to that of the computation time of matrix multiplication (e.g., see [35]).

Let $\Lambda_p = \sum_{M \in \mathcal{M}} P_M X_M \chi^{\top}_M$ be a design matrix. We define the problem complexity as $H_2 = \frac{\rho(p)}{\Delta_{min}^{2\alpha}}$, where $\rho(p) = \max_{M \in \mathcal{M}} \|X_M\|^2_{\Lambda_p^{-1}}$ and $\Delta_{min} = \arg\min_{M \in \mathcal{M} \setminus \{M^*\}} \theta(M^*) - \theta(M)$, which is also appeared in Soare et al. [45]. The next theorem shows that SAQM is $(\varepsilon, \delta)$-PAC and gives a problem-dependent sample complexity bound.

**Theorem 3.** Given any instance of the multiple-arm identification with full-bandit feedback, with probability at least $1 - \delta$, SAQM (Algorithm 2) returns an $\varepsilon$-optimal super-arm $\hat{M}^*$ and the total number of samples $T$ is bounded as follows:

\[ T = O \left( k^2H_z \left( n^{3.5} \log \left( \frac{n}{\varepsilon} \right) \right) + \log \left( n^{3.5} H_z \left( n^{3.5} H_z + \log \left( \frac{n}{\delta} \right) \right) \right) \right). \]

It is worth mentioning that if we have an $\alpha$-approximation algorithm for CEM with a more general decision class $\mathcal{M}$ (such as paths, matchings, matroids), we can extend Theorem 3 for the combinatorial pure exploration (CPE) with general constraints as follows.

**Corollary 1.** Given any instance of CPE with a decision class $\mathcal{M}$ in the full-bandit setting, with probability at least $1 - \delta$, SAQM (Algorithm 2) with $\alpha$-approximation of CEM returns an $\varepsilon$-optimal set $\hat{M}^*$, and the total number of samples $T$ is bounded as follows:

\[ T \leq 8 \left( 3 + \frac{1}{\alpha} \right)^2 k^2H_z \log \left( \frac{e' K}{\delta} \right) + C(H_z, \delta), \]

where $C(H_z, \delta) = O \left( k^2H_z \log \left( \frac{kH_z}{\delta} \left( kH_z + \log \left( \frac{k}{\delta} \right) \right) \right) \right)$.

Theorem 3 corresponds to the case where $\alpha = O(1/kn^2)$ in Corollary 1. Soare et al. [45] considered the oracle sample complexity of a linear best-arm identification problem. The oracle complexity, which is based on the optimal allocation strategy $p$ derived from the true parameter $\theta$, is $O(\rho(p) \log(1/\delta))$. Soare et al. [45] showed that the sample complexity with G-allocation strategy matches the oracle sample complexity up to constants in the worst case. The sample complexity of SAQM is also worst-case optimal in the sense that it matches $O(\rho(p) \log(1/\delta))$, while SAQM runs in polynomial time.

**Heuristic algorithm.** In SAQM, we compute an upper confidence bound of the expected reward of each super-arm. However, in order to reduce the number of required samples, we wish to directly construct a tight confidence bound for the gap of the reward between two super-arms. For this reason, we propose another algorithm SA-FOA. The procedure of SA-FOA is shown in Algorithm 3. Given an allocation strategy $p$, this algorithm continues sampling until the stopping condition $\frac{1}{2} \geq Z_i' - \hat{\theta}_i(M_i^*)$ is satisfied, where $Z_i'$ denotes the objective value of an approximate solution of the following maximization problem:

\[ \max_{M \in \mathcal{M} \setminus \{M_i^*\}} \left( \hat{\theta}(M) + C_i \|X_M - X_{M_i^*}\|_{A_i^{-1}} \right). \]

The second term of (5) can be regarded as the confidence interval of the estimated gap $\hat{\theta}_i(M) - \hat{\theta}_i(M_i^*)$. We employ a first-order approximation technique, in order to simultaneously maximize the estimated reward $\hat{\theta}_i(M)$ and the matrix norm $\|X_M - X_{M_i^*}\|_{A_i^{-1}}$. For a fixed super-arm $M_i$, we approximate $\|X_M - X_{M_i^*}\|_{A_i^{-1}}$.
We can approximately solve it by Algorithm 1, and choose the best approximate solution that maximizes the which follows from real-world datasets. We conduct the experiments on small synthetic datasets and large-scale compare our algorithms with an exhaustive search algorithm namely diagonal approximation of confidence ellipsoids. Note that in this section, we evaluate the empirical performance of our algorithms, namely SAQM (Algorithm 3) and SA-FOA (Algorithm 4 in Appendix A) as a naive algorithm that works in polynomial-time. SA-FOA employs simplified confidence bounds obtained by diagonal approximation of confidence ellipsoids. Note that ICB can solve the combinatorial pure exploration problem with general constraints and results in another sample complexity (see Lemma 3 in Appendix A). We compare our algorithms with an exhaustive search algorithm namely Exhaustive, which runs in exponential time (see Appendix E for details). We conduct the experiments on small synthetic datasets and large-scale real-world datasets.

### Algorithm 3: Static allocation algorithm with first-order approximation (SA-FOA)

**Input**: Accuracy $\epsilon > 0$, confidence level $\delta \in (0, 1)$, allocation strategy $p_f$

```plaintext
for $t = 1, \ldots, n$ do
  \begin{align*}
    t &\leftarrow t + 1 \text{ and pull } M_t \in \text{supp}(p_f); \\
    \text{Observe } r_{M_t}, \text{ and update } A_t \text{ and } b_t;
  \end{align*}

while $\frac{c_t}{\gamma} \geq Z_t^* - \hat{\theta}_t(M_t^*)$ is not true do
  \begin{align*}
    &t \leftarrow t + 1; \\
    \text{Pull } M_t \leftarrow \arg\min_{M \in \text{supp}(p_f)} T_M(t); \\
    \text{Observe } r_{M_t}, \text{ and then update } A_t, b_t \text{ and } \hat{\theta}_t \leftarrow A_{x_t}^{-1}b_t; \\
    \hat{M}_t &\leftarrow \arg\max_{M \in \mathcal{M}} \hat{\theta}_t(M); \\
    m &\leftarrow \ell n \text{ for some positive integer } \ell;
  \end{align*}

for $i = 1, \ldots, m$ do
  \begin{align*}
    F &\leftarrow \{\emptyset\}; \\
    \text{Choose a super arm } M_i \in \text{supp}(p_f) \text{ at uniformly random}; \\
    \gamma &\leftarrow \frac{2\|x_M - \hat{x}_{\hat{M}_t}\|_{A_{x_t}^{-1}}}{C_t}; \\
    B_t &\leftarrow \gamma A_{x_t}^{-1} - \text{Diag}(2\gamma(A_{x_t}^{-1}, \hat{x}_{\hat{M}_t})) + \text{Diag}(\hat{\theta}_t); \\
    F &\leftarrow F \cup \{\text{QuadraticMaximization}(B_t)\}; \\
    Z_t^* &\leftarrow \max_{M \in F} \left(\hat{\theta}_t(M) + C_t\|x_M - \hat{x}_{\hat{M}_t}\|_{A_{x_t}^{-1}}\right);
  \end{align*}

return $\hat{M}^* \leftarrow \hat{M}_t^*$
```

Using the following bound:

$$
\|x_M - \hat{x}_{\hat{M}_t}\|_{A_{x_t}^{-1}} \leq \frac{\|x_M - \hat{x}_{\hat{M}_t}\|_{A_{x_t}^{-1}}^2}{2\|x_M - \hat{x}_{\hat{M}_t}\|_{A_{x_t}^{-1}}} + \frac{\|x_M - \hat{x}_{\hat{M}_t}\|_{A_{x_t}^{-1}}}{2}.
$$

which follows from $\sqrt{a + x} \leq \sqrt{a} + \frac{x}{2\sqrt{a}}$ for any $a, x > 0$. For any $y \in \mathbb{R}^n$, let Diag($y$) be a matrix whose $i$-th diagonal component is $y(i)$ for $i \in [n]$. The above first-order approximation allows us to transform the original problem to QP, where the objective function is

$$
x_M^\top \left(\gamma A_{x_t}^{-1} - \text{Diag}(2\gamma(A_{x_t}^{-1}, \hat{x}_{\hat{M}_t})) + \text{Diag}(\hat{\theta}_t)\right)x_M,
$$

with a positive constant $\gamma = \frac{C_t}{2\|x_M - \hat{x}_{\hat{M}_t}\|_{A_{x_t}^{-1}}^2}$. We can approximately solve it by Algorithm 1 and choose the best approximate solution that maximizes the original objective among $\ell n$ super arms. Notice that SA-FOA is an $(\epsilon, \delta)$-PAC algorithm since we compute the upper bound of the objective function in (5) and thus it will not stop earlier. In our experiments, it works well although we have no theoretical results on the sample complexity. We will also observe in the experiments that the approximation error of SA-FOA for (5) becomes smaller as the number of rounds increases.

### 5 Experiments

In this section, we evaluate the empirical performance of our algorithms, namely SAQM (Algorithm 2) and SA-FOA (Algorithm 3). We also implement another algorithm namely ICB (Algorithm 4 in Appendix A) as a naive algorithm that works in polynomial-time. ICB employs simplified confidence bounds obtained by diagonal approximation of confidence ellipsoids. Note that ICB can solve the combinatorial pure exploration problem with general constraints and results in another sample complexity (see Lemma 3 in Appendix A). We compare our algorithms with an exhaustive search algorithm namely Exhaustive, which runs in exponential time (see Appendix E for details). We conduct the experiments on small synthetic datasets and large-scale real-world datasets.
Synthetic datasets. To see the dependence of the performance on the minimum gap $\Delta_{\text{min}}$, we generate synthetic instances as follows. We first set the expected rewards for the top-$k$ single-arms uniformly at random from $[0,1]$. Let $\theta_{\text{min},k}$ be the the minimum expected reward in the top-$k$ single-arms. We set the expected reward of the $(k+1)$-th best single-arm to $\theta_{\text{min},k} - \Delta_{\text{min}}$ for the predetermined parameter $\Delta_{\text{min}} \in [0,1]$. Then, we generate the expected rewards of the rest of single-arms by uniform samples from $[-1, \theta_{\text{min},k} - \Delta_{\text{min}}]$ so that expected rewards of the best super-arm is larger than those of the rest of super-arms by at least $\Delta_{\text{min}}$. We set the additive noise distribution $\mathcal{N}(0,1)$ and $\delta = 0.05$. All algorithms employ G-allocation strategy.

First, we examine the approximation precision of our approximation algorithms. The results are reported in Figure 1. $\text{SAQM}$ and $\text{SA-FOA}$ employ some approximation mechanisms to test the stopping condition in polynomial time. Recall that $\text{SAQM}$ approximately solves CEM in (1) to attain an objective value of $Z_t$, and $\text{SA-FOA}$ approximately solves the maximization problem in (1) to attain an objective value of $Z'_t$. We set up the experiments with $n = 10$ single-arms and $k = 5$. We run the experiments for the small gap ($\Delta_{\text{min}} = 0.1$) and large gap ($\Delta_{\text{min}} = 1.0$). We plot the approximation ratio and the additive approximation error of $\text{SAQM}$ and $\text{SA-FOA}$ in the first 100,000 rounds. From the results, we can see that the approximation ratios of them are almost always greater than 0.9, which are far better than the worst-case guarantee proved in Theorem 1. In particular, the approximation ratio of $\text{SA-FOA}$ in the small gap case is surprisingly good (around 0.95) and grows as the number of rounds increases. This result implies that there is only a slight increase of the sample complexity caused by the approximation, especially when the expected rewards of single-arms are close to each other.

Next, we conduct the experiments to compare the running time of algorithms. We set $n = 10, 12, \ldots, 24$ and $k = n/2$ on synthetic datasets. We report the results in Figure 2. As can be seen, $\text{Exhaustive}$ is prohibitive on instances with large number of super-arms, while our algorithms can run fast even if $n$ becomes larger, which matches our theoretical analysis. The results indicate that polynomial-time algorithms are of crucial importance for practical use.

Finally, we evaluate the number of samples required to identify the best super-arm for varying $\Delta_{\text{min}}$. Based on the above observation, we set $\alpha = 0.9$. The result is shown in Figure 3 which indicates that the numbers of samples of our algorithms are comparable to that of $\text{Exhaustive}$. We observed that our
algorithms always output the optimal super-arm.

Real-world datasets on crowdsourcing. We use the crowdsourcing datasets compiled by Li et al. [36] whose basic information is shown in Table 1. The task is to identify the top-\(k\) workers with the highest accuracy only from a sequential access to the accuracy of part of labels given by some workers. Notice that the number of super-arms is more than 10^{10} and \(\Delta_{\text{min}}\) is less than 0.1 in all experiments. We set \(k = 10\) and \(\epsilon = 0.5\). Since Exhaustive is prohibitive, we compare other three algorithms. All algorithms employ uniform allocation strategy. The result is shown in Table 2 which indicates the applicability of our algorithms to the instances with a massive number of super-arms. Moreover, all three algorithms found the optimal subset of crowdworkers. In all datasets, SA-FOA outperformed the other algorithms. ICB also worked well, but it became worse especially for Science in which the number of workers is more than 100. This result implies that when the number of workers (single-arms) is large, the algorithm with simplified confidence bounds may degrade the sample complexity, while algorithms with confidence ellipsoids require less samples as SAQM and SA-FOA perform well (see Appendix A for more discussion).

| Dataset   | #task | #worker | Average | Best  |
|-----------|-------|---------|---------|-------|
| IT        | 25    | 36      | 0.54    | 0.84  |
| Medicine  | 36    | 45      | 0.48    | 0.92  |
| Chinese   | 24    | 50      | 0.37    | 0.79  |
| Pokénon   | 20    | 55      | 0.28    | 1.00  |
| English   | 30    | 63      | 0.26    | 0.70  |
| Science   | 20    | 111     | 0.29    | 0.85  |

| Dataset   | ICB   | SAQM   | SA-FOA |
|-----------|-------|--------|--------|
| IT        | 46,658| 68,328 | 3,421  |
| Medicine  | 73,337| 86,252 | 3,493  |
| Chinese   | 105,214| 110,504| 4,949  |
| Pokénon   | 20,943| 91,423 | 3,050  |
| English   | 118,587| 291,773| 9,313  |
| Science   | 362,558| 291,773| 15,611 |

6 Conclusion

We studied the multiple-arm identification with full-bandit feedback, where we cannot observe a reward of each single-arm, but only the sum of the rewards. To overcome the computational challenges, we designed a novel approximation algorithm for a 0-1 quadratic programming problem with theoretical guarantee. Based on our approximation algorithm, we proposed a polynomial-time algorithm SAQM that runs in \(O(\log K)\) time and provided an upper bound of the sample complexity, which is still worst-case optimal; the result indicates that our algorithm provided an exponential speedup over exhaustive search algorithm while keeping the statistical efficiency. We also designed a novel algorithm SA-FOA using first-order approximation that empirically performs well. Finally, we conducted experiments on synthetic and real-world datasets with more than 10^{10} super-arms, demonstrating the superiority of our algorithms in terms of both the computation time and the sample complexity. There are several directions for future research. It remains open to design adaptive algorithms with a problem-dependent optimal sample complexity. It is also interesting question to seek a lower bound of any \((\epsilon, \delta)\)-PAC algorithm that works in polynomial-time. Extension for combinatorial pure exploration with full-bandit feedback is another direction.
References

[1] R. Agrawal, M. Hegde, and D. Teneketzis. Multi-armed bandit problems with multiple plays and switching cost. *Stochastics and Stochastic Reports*, 29:437–459, 1990.

[2] V. Anantharam, P. Varaiya, and J. Walrand. Asymptotically efficient allocation rules for the multiarmed bandit problem with multiple plays-Part I: I.I.D. rewards. *IEEE Transactions on Automatic Control*, 32:968–976, 1987.

[3] Y. Asahiro, K. Iwama, H. Tamaki, and T. Tokuyama. Greedily finding a dense subgraph. *Journal of Algorithms*, 34(2):203–221, 2000.

[4] J.-Y. Audibert and S. Bubeck. Best arm identification in multi-armed bandits. In *COLT’10: Proceedings of the 23rd Annual Conference on Learning Theory*, pages 41–53, 2010.

[5] A. Bhaskara, M. Charikar, E. Chlamtac, U. Feige, and A. Vijayaraghavan. Detecting high log-densities: An $O(n^{1/4})$ approximation for densest $k$-subgraph. In *STOC’10: Proceedings of the 42nd ACM Symposium on Theory of Computing*, pages 201–210, 2010.

[6] M. Bouhtou, S. Gaubert, and G. Sagnol. Submodularity and randomized rounding techniques for optimal experimental design. *Electronic Notes in Discrete Mathematics*, 36:679–686, 2010.

[7] S. Bubeck, N. Cesa-Bianchi, et al. Regret analysis of stochastic and nonstochastic multi-armed bandit problems. *Foundations and Trends® in Machine Learning*, 5:1–122, 2012.

[8] S. Bubeck, T. Wang, and N. Viswanathan. Multiple identifications in multi-armed bandits. In *ICML’13: Proceedings of the 30th International Conference on Machine Learning*, pages 258–265, 2013.

[9] T. Cao and A. Krishnamurthy. Disagreement-based combinatorial pure exploration: Efficient algorithms and an analysis with localization. *arXiv preprint*, arXiv:1711.08018, 2017.

[10] W. Cao, J. Li, Y. Tao, and Z. Li. On top-k selection in multi-armed bandits and hidden bipartite graphs. In *NIPS’15: Proceedings of the 28th Annual Conference on Neural Information Processing Systems*, pages 1036–1044, 2015.

[11] N. Cesa-Bianchi and G. Lugosi. *Prediction, Learning, and Games*. Cambridge University Press, 2006.

[12] L. Chen, A. Gupta, and J. Li. Pure exploration of multi-armed bandit under matroid constraints. In *COLT’16: Proceedings of the 29th Annual Conference on Learning Theory*, pages 647–669, 2016.

[13] L. Chen, A. Gupta, J. Li, M. Qiao, and R. Wang. Nearly optimal sampling algorithms for combinatorial pure exploration. In *COLT’17: Proceedings of the 30th Annual Conference on Learning Theory*, pages 482–534, 2017.

[14] L. Chen and J. Li. On the optimal sample complexity for best arm identification. *arXiv preprint*, arXiv:1511.03774, 2015.

[15] S. Chen, T. Lin, I. King, M. R. Lyu, and W. Chen. Combinatorial pure exploration of multi-armed bandits. In *NIPS’14: Proceedings of the 27th Annual Conference on Neural Information Processing Systems*, pages 379–387, 2014.

[16] E. Even-Dar, S. Mannor, and Y. Mansour. PAC bounds for multi-armed bandit and Markov decision processes. In *COLT’02: Proceedings of the 15th Annual Conference on Learning Theory*, pages 255–270, 2002.

[17] E. Even-Dar, S. Mannor, and Y. Mansour. Action elimination and stopping conditions for the multi-armed bandit and reinforcement learning problems. *Journal of Machine Learning Research*, 7:1079–1105, 2006.
[18] U. Feige, D. Peleg, and G. Kortsarz. The dense \( k \)-subgraph problem. Algorithmica, 29(3):410–421, 2001.

[19] V. Gabillon, M. Ghavamzadeh, and A. Lazaric. Best arm identification: A unified approach to fixed budget and fixed confidence. In NIPS’12: Proceedings of the 25th Annual Conference on Neural Information Processing Systems, pages 3212–3220, 2012.

[20] V. Gabillon, M. Ghavamzadeh, A. Lazaric, and S. Bubeck. Multi-bandit best arm identification. In NIPS’11: Proceedings of the 24th Annual Conference on Neural Information Processing Systems, pages 2222–2230, 2011.

[21] V. Gabillon, A. Lazaric, M. Ghavamzadeh, R. Ortner, and P. Bartlett. Improved learning complexity in combinatorial pure exploration bandits. In AISTATS’16: Proceedings of the 19th International Conference on Artificial Intelligence and Statistics, pages 1004–1012, 2016.

[22] S. Huang, X. Liu, and Z. Ding. Opportunistic spectrum access in cognitive radio networks. In INFOCOM’08: Proceedings of the 27th IEEE International Conference on Computer Communications, pages 1427–1435, 2008.

[23] W. Huang, J. Ok, L. Li, and W. Chen. Combinatorial pure exploration with continuous and separable reward functions and its applications. In IJCAI’18: Proceedings of the 27th International Joint Conference on Artificial Intelligence, pages 2291–2297, 2018.

[24] K. Jamieson, M. Malloy, R. Nowak, and S. Bubeck. lil’UCB: An optimal exploration algorithm for multi-armed bandits. In COLT’14: Proceedings of the 27th Annual Conference on Learning Theory, pages 423–439, 2014.

[25] K. Jun, A. Bhargava, R. Nowak, and R. Willett. Scalable generalized linear bandits: Online computation and hashing. In NIPS’17: Proceedings of the 30th Annual Conference on Neural Information Processing Systems, pages 99–109, 2017.

[26] S. Kalyanakrishnan and P. Stone. Efficient selection of multiple bandit arms: Theory and practice. In ICML’10: Proceedings of the 27th International Conference on Machine Learning, pages 511–518, 2010.

[27] S. Kalyanakrishnan, A. Tewari, P. Auer, and P. Stone. PAC subset selection in stochastic multi-armed bandits. In ICML’12: Proceedings of the 29th International Conference on Machine Learning, pages 655–662, 2012.

[28] D. R. Karger. Random sampling and greedy sparsification for matroid optimization problems. Mathematical Programming, 82(1):41–81, 1998.

[29] E. Kaufmann, O. Cappé, and A. Garivier. On the complexity of best-arm identification in multi-armed bandit models. The Journal of Machine Learning Research, 17:1–42, 2016.

[30] E. Kaufmann and S. Kalyanakrishnan. Information complexity in bandit subset selection. In COLT’13: Proceedings of the 26th Annual Conference on Learning Theory, pages 228–251, 2013.

[31] J. Komiyama, J. Honda, and H. Nakagawa. Optimal regret analysis of thompson sampling in stochastic multi-armed bandit problem with multiple plays. In ICML’15: Proceedings of the 32nd International Conference on Machine Learning, pages 1152–1161, 2015.

[32] P. Lagrée, C. Vernade, and O. Cappe. Multiple-play bandits in the position-based model. In NIPS’16: Proceedings of the 29th Annual Conference on Neural Information Processing Systems 29, pages 1597–1605, 2016.

[33] T. Lai and H. Robbins. Asymptotically efficient adaptive allocation rules. Advances in Applied Mathematics, 6(1):4–22, 1985.
[34] T. Lattimore and C. Szepesvari. The End of Optimism? An Asymptotic Analysis of Finite-Armed Linear Bandits. In *AISTATS’17: Proceedings of the 20th International Conference on Artificial Intelligence and Statistics*, pages 728–737, 2017.

[35] F. Le Gall. Powers of tensors and fast matrix multiplication. In *ISSAC’14: Proceedings of the 39th ACM International Symposium on Symbolic and Algebraic Computation*, pages 296–303, 2014.

[36] J. Li, Y. Baba, and H. Kashima. Hyper questions: Unsupervised targeting of a few experts in crowdsourcing. In *CIKM’17: Proceedings of the 26th ACM International Conference on Information and Knowledge Management*, pages 1069–1078, 2017.

[37] P. Perrault, P. Vianney, and V. Michal. Exploiting structure of uncertainty for efficient matroid semi-bandits. In *ICML’19, to appear*, 2019.

[38] F. Pukelsheim. *Optimal Design of Experiments*. Society for Industrial and Applied Mathematics, 2006.

[39] F. Radlinski, R. Kleinberg, and T. Joachims. Learning diverse rankings with multi-armed bandits. In *ICML’08: Proceedings of the 25th International Conference on Machine Learning*, pages 784–791, 2008.

[40] D. Retelny, S. Robaszkiewicz, A. To, W. S. Lasecki, J. Patel, N. Rahmati, T. Doshi, M. Valentine, and M. S. Bernstein. Expert crowdsourcing with flash teams. In *UIST ’14: Proceedings of the 27th Annual ACM Symposium on User Interface Software and Technology*, pages 75–85, 2014.

[41] A. Roy Chaudhuri and S. Kalyanakrishnan. PAC identification of a bandit arm relative to a reward quantile. In *AAAI’17: Proceedings of the 31st AAAI Conference on Artificial Intelligence*, pages 1977–1985, 2017.

[42] A. Roy Chaudhuri and S. Kalyanakrishnan. PAC identification of many good arms in stochastic multi-armed bandits. In *ICML’19, to appear*, 2019.

[43] P. Rusmevichientong and D. P. Williamson. An adaptive algorithm for selecting profitable keywords for search-based advertising services. In *EC ’06: Proceedings of the 7th ACM Conference on Electronic Commerce*, pages 260–269, 2006.

[44] G. Sagnol. Approximation of a maximum-submodular-coverage problem involving spectral functions, with application to experimental designs. *Discrete Applied Mathematics*, 161:258–276, 2013.

[45] M. Soare, A. Lazaric, and R. Munos. Best-arm identification in linear bandits. In *NIPS’14: Proceedings of the 27th Annual Conference on Neural Information Processing Systems*, pages 828–836, 2014.

[46] C. Tao, S. Blanco, and Y. Zhou. Best arm identification in linear bandits with linear dimension dependency. In *ICML’18: Proceedings of the 35th International Conference on Machine Learning*, pages 4877–4886, 2018.

[47] R. Taylor. Approximation of the quadratic knapsack problem. *Operations Research Letters*, 44(4):495–497, 2016.

[48] L. Tran-Thanh, S. Stein, A. Rogers, and N. R. Jennings. Efficient crowdsourcing of unknown experts using bounded multi-armed bandits. *Artificial Intelligence*, pages 89 – 111, 2014.

[49] H. Whitney. On the abstract properties of linear dependence. *American Journal of Mathematics*, 57(3):509–533, 1935.

[50] L. Xu, J. Honda, and M. Sugiyama. A fully adaptive algorithm for pure exploration in linear bandits. In *AISTATS’18: Proceedings of the 21st International Conference on Artificial Intelligence and Statistics*, pages 843–851, 2018.

[51] Y. Zhou, X. Chen, and J. Li. Optimal PAC multiple arm identification with applications to crowdsourcing. In *ICML’14: Proceedings of the 31st International Conference on Machine Learning*, pages 217–225, 2014.

12
A Simplified Confidence Bounds for the Combinatorial Pure Exploration

In this appendix, we see the fundamental observation of employing a simplified confidence bound to obtain a computational efficient algorithm for the combinatorial pure exploration problem. We consider any decision class $\mathcal{M}$, in which super-arms satisfy any constraint where a linear maximization problem is polynomial-time solvable. The examples of decision class considered here are paths, matchings, or matroids (see Appendix B for the definition of matroids). The purpose of this appendix is to give a polynomial-time algorithm for solving the combinatorial pure exploration with general constraints by using the simplified confidence bound, and see the trade-off between the computational efficiency and computational efficiency. The $(\epsilon, \delta)$-PAC algorithm proposed in this section, named ICB, is also evaluated in our experiments.

For a matrix $B \in \mathbb{R}^{n \times n}$, let $B(i, j)$ denote the $(i, j)$-th entry of $B$. We construct a simplified confidence bound, named an independent confidence bound, which is obtained by diagonal approximation of confidence ellipsoids. We start with the following lemma, which shows that $\theta$ lies in an independent confidence region centered at $\hat{\theta}$ with high-probability.

**Lemma 1.** Let $c' = 6/\pi^2$. Let $\epsilon_i$ be a noise variable bounded as $\epsilon_i \in [\sigma, \sigma]$ for $\sigma > 0$. Then, for any fixed sequence $x_t$, any $t \in \{1, 2, \ldots\}$, and $\delta \in (0, 1)$, with probability at least $1 - \delta$, the inequality

$$|x^\top \theta - x^\top \hat{\theta}_t| \leq C_t \sum_{i=1}^n |x_i| \sqrt{A_{x_t}^{-1}(i, i)}$$

holds for all $x \in \{-1, 0, 1\}^n$, where

$$C_t = \sigma \sqrt{2 \log(c't^2n/\delta)}.$$

This lemma can be derived from Proposition 1 and the triangle inequality. The RHS of Proposition 1 only has linear terms of $\{x_i\}_{i \in [n]}$, whereas that of (3) in Proposition 1 has the matrix norm $\|x\|_{A_t^{-1}}$, which results in a difficult instance. As long as we assume that linear maximization oracle is available, maximization of this value can be also done in polynomial time. For example, maximization of the RHS of (1) under matroid constraints can be solved by using the simple greedy procedure [28] described in Appendix B. Based on the independent confidence bounds, we propose ICB, which is detailed in Algorithm 4. At each round $t$, ICB computes the empirical best super-arm $\hat{M}_t^*$, and then solves the following maximization problem:

$$P_1: \max \theta(M) + C_t \sum_{i=1}^n |\chi_M(i) - \chi_{\hat{M}_t^*}(i)| \sqrt{A_{x_t}^{-1}(i, i)},$$

s.t. $M \in \mathcal{M} \setminus \{\hat{M}_t^*\}.$

The second term in the objective of $P_1$ can be regarded as the confidence interval of the estimated gap $\hat{\theta}_t(M) - \hat{\theta}_t(\hat{M}_t^*)$. ICB continues sampling a super-arm until the following stopping condition is satisfied:

$$Z_t^* - \hat{\theta}_t(\hat{M}_t^*) < \epsilon,$$

where $Z_t^*$ represents the optimal value of $P_1$. Note that $P_1$ is solvable in polynomial time because $P_1$ is an instance of linear maximization problems. As the following lemma states, ICB is an efficient algorithm in terms of the computation time.

**Lemma 2.** Given any instance of combinatorial pure exploration with full-bandit feedback with decision class $\mathcal{M}$, ICB (Algorithm 4) at each round $t \in \{1, 2, \ldots\}$ runs in polynomial time.

The proof is given in Appendix F. For example, ICB runs in $O(\max\{n^2, ng(n)\})$ time for matroid constraints, where $g(n)$ is the computation time to check whether given super-arm is contained in the decision class. Note that $g(n)$ is polynomial in $n$ for any matroid constraints. For example, $g(n) = O(n)$ if we consider the case where each super-arm corresponds to a spanning tree of a graph $G = (V, E)$, and a decision class corresponds to a set of spanning trees in a given graph $G$.  

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Algorithm 4: Static allocation with independent confidence bound (ICB)

**Input**: Accuracy $\epsilon > 0$, confidence level $\delta \in (0, 1)$, allocation strategy $p$

*for* $t = 1, \ldots, n$ *
do
  $t \leftarrow t + 1$;
  Pull $M_t \in \text{supp}(p)$;
  Observe $r_t$;
  Update $A_t$ and $b_t$;
*while* stopping condition (2) is not true *
do
  $t \leftarrow t + 1$;
  Pull $M_t \leftarrow \arg\min_{M \in \text{supp}(p)} \frac{T_M(t)}{p_M}$;
  Observe $r_t$;
  Update $A_t$ and $b_t$;
  $\hat{\theta}_t \leftarrow A_{x_t}^{-1}b_t$;
  $\hat{M}_t^* \leftarrow \arg\max_{M \in \mathcal{M}} \hat{\theta}_t(M)$;
  $Z_t^* \leftarrow \max_{M \in \mathcal{M} \setminus \{\hat{M}_t^*\}} \left(\hat{\theta}_t(M) + C_t \sum_{i=1}^{n} |(\mathbf{x}_M(i) - \mathbf{x}_{\hat{M}_t^*}(i))|\sqrt{A_{x_t}^{-1}(i,i)}\right)$;
*end while*
  *return* $\hat{M}^* \leftarrow \hat{M}_t^*$

From the definition, we have $A_t = \sum_{M \in \mathcal{M}} T_M(t)\mathbf{x}_M\mathbf{x}_M^\top$, where $T_M(t)$ denotes the number of times that $M$ is pulled before the round $t + 1$. Let $\Lambda'_{p} = \sum_{M \in \mathcal{M}} p_M\mathbf{x}_M\mathbf{x}_M^\top$. We define $\rho'(p)$ as

$$\rho'(p) = \left(\max_{M,M' \in \mathcal{M}} \sum_{i=1}^{n} |\mathbf{x}_M(i) - \mathbf{x}_{M'}(i)|\sqrt{\Lambda_{p}^{-1}(i,i)}\right)^2. \tag{3}$$

Now, we give a problem-dependent sample complexity bound of ICB with allocation strategy $p$ as follows.

**Lemma 3.** Given any instance of combinatorial pure exploration with decision class $\mathcal{M}$ in full-bandit setting, with probability at least $1 - \delta$, ICB (Algorithm 4) returns an $\epsilon$-optimal super-arm $\hat{M}^*$ and the total number of samples $T$ is bounded as follows:

$$T = O\left(k^2H'\log\left(\frac{n}{\delta}\left(k^2H'_e + k^2H'_e + \log\left(\frac{n}{\delta}\right)\right)\right)\right),$$

where $H'_e = \frac{\rho'(p)}{(\Delta_{\min} + \epsilon)^2}.$

The proof is given in Appendix F. Notice that in the MAB, this diagonal approximation is tight since $A_{x_t}$ becomes a diagonal matrix. However, for combinatorial settings where the size of super-arms is $k \geq 2$, there is no guarantee that this approximation is tight; the approximation may degrate the sample complexity. Although the proposed algorithm here empirically perform well when the number of single-arms is not large, it is still unclear that using the simplified confidence bound should be desired instead of ellipsoids confidence bounds since $\rho'(p)$ is $\Omega(n)$. This is the reason why we focus on the approach with confidence ellipsoids.

### B Definition of Matroids

A *matroid* is a combinatorial structure that abstracts many notions of independence such as linearly independent vectors in a set of vectors (called the *linear matroid*) and spanning trees in a graph (called the *graphical matroid*) [49]. Formally, a matroid is a pair $J = (E, \mathcal{I})$, where $E = \{1, 2, \ldots, n\}$ is a finite set called a *ground set* and $\mathcal{I} \subseteq 2^E$ is a family of subsets of $E$ called *independent sets*, that satisfies the following axioms:

1. $\emptyset \in \mathcal{I}$;
2. $X \subseteq Y \in \mathcal{I} \implies X \in \mathcal{I}$;
3. \( \forall X,Y \in \mathcal{I} \) such that \( |X| < |Y|, \exists e \in Y \setminus X \) such that \( X \cup \{e\} \in \mathcal{I} \).

A weighted matroid is a matroid that has a weight function \( w: E \to \mathbb{R} \). For \( F \subseteq E \), we define the weight of \( F \) as \( w(F) = \sum_{e \in F} w(e) \).

Let us consider the following problem: given a weighted matroid \( J = (E, \mathcal{I}) \) with \( w: E \to \mathbb{R} \), we are asked to find an independent set with the maximum weight, i.e., \( \arg\max_{F \in \mathcal{I}} w(F) \). This problem can be solved exactly by the following simple greedy algorithm \[28\]. The algorithm initially sets \( F \) to the empty set. Then, the algorithm sorts the elements in \( E \) with the decreasing order by weight, and for each element \( e \) in this order, the algorithm adds \( e \) to \( F \) if \( F \cup \{e\} \in \mathcal{I} \). Letting \( g(n) \) be the computation time for checking whether \( F \) is independent, we see that the running time of the above algorithm is \( O(n \log n + n g(n)) \).

**C Uniform Quadratic Knapsack Problem**

Assume that we have \( n \) items, each of which has weight 1. In addition, we are given an \( n \times n \) non-negative integer matrix \( W = (w_{ij}) \), where \( w_{ii} \) is the profit achieved if item \( i \) is selected and \( w_{ij} + w_{ji} \) is a profit achieved if both items \( i \) and \( j \) are selected for \( i < j \). The uniform quadratic knapsack problem (UQKP) calls for selecting a subset of items whose overall weight does not exceed a given knapsack capacity \( k \), so as to maximize the overall profit. The UQKP can be formulated as the following 0-1 integer quadratic programming:

\[
\begin{align*}
\text{max.} \quad & \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} x_i x_j \\
\text{s.t.} \quad & \sum_{i=1}^{n} x_i \leq k.
\end{align*}
\]

The UQKP is an NP-hard problem. Indeed, the maximum clique problem, which is also NP-hard, can be reduced to it; Given a graph \( G = (V,E) \), we set \( w_{ii} = 0 \) for all \( i \) and \( w_{ij} = 1 \) for all \( \{i,j\} \in E \). Solving this problem, it allows us to find a clique of size \( k \) if and only if the optimal solution of the problem has value \( k(k-1) \) \[47\].

**D Allocation Strategies**

In this section, we briefly introduce the possible allocation strategies and describe how to implement a continuous allocation \( p \) into a discrete allocation \( x_t \) for any sample size \( t \). We report the efficient rounding procedure introduced in \[38\]. In the G-allocation strategy, we make the sequence of selection \( x_t \) to be \( x_t^G = \arg\min_{x_t \in \mathbb{R}^n} \max_{x \in X} \|x\|_{A_t}^{-1} \) for \( X \subseteq \mathbb{R}^n \), which is NP-hard optimization problem. There are massive studies that proposed approximate solutions to solve it in the experimental design literature \[6\] \[44\]. We can optimize the continuous relaxation of the problem by the projected gradient algorithm, multiplicative algorithm, or interior point algorithm. From the obtained the optimal allocation \( p \), we wish to design a discrete allocation for fixed sample size \( t \).

Given an allocation \( p \in \mathcal{P} \), recall that \( \text{supp}(p) = \{j \in [K] : p_j > 0\} \). Let \( t_i \) be the number of pulls for arm \( i \in \text{supp}(p) \) and \( s \) be the size of \( \text{supp}(p) \). Then, letting the frequency \( t_i = \lceil (t - \frac{1}{2}s) p_i \rceil \) results in \( \sum_{i \in \text{supp}(p)} t_i \) samples. If \( \sum_{i \in \text{supp}(p)} t_i = t \), this allocation is a desired solution. Otherwise, we conduct the following procedure until the \( \sum_{i \in \text{supp}(p)} t_i = n \) is 0; increase a frequency \( t_j \) which attains \( t_j/p_j = \min_{i \in \text{supp}(p)} t_i/p_i \) to \( t_j + 1 \), or decreasing some \( t_j \) with \( (t_j - 1)/p_j = \max_{i \in \text{supp}(p)} (t_i - 1)/p_i \) to \( t_j - 1 \). Then \((t_1, \ldots, t_s)\) lies in the efficient design apportionment (see \[38\]). Note that since the relaxation problem has exponential number of variables in our setting, we are restricted to the number of \( \text{supp}(p) \) instead of dealing with all super-arms.
Algorithm 5: Exhaustive Search (Exhaustive)

**Input**: Accuracy $\varepsilon > 0$, confidence level $\delta \in (0, 1)$, allocation strategy $p$

for $t = 1, \ldots, n$ do
- Pull $M_t \in \text{supp}(p)$;
- Observe $r_t$;
- Update $A_t$ and $b_t$;
while $Z^*_t \geq \varepsilon$ do
  - $t \leftarrow t + 1$;
  - Pull $M_t \leftarrow \text{argmin}_{M \in \text{supp}(p)} \frac{T_M(t)}{p_M}$;
  - Observe $r_t$;
  - Update $A_t$ and $b_t$;
  - $\hat{M}^*_t \leftarrow \text{argmax}_{M \in M} \hat{\theta}_t(M)$;
  - $Z^*_t \leftarrow \max_{M \in M \setminus \hat{M}^*} \left( \hat{\theta}_t(M) + C_t \| \chi_M - \chi_{M^*} \|_{A^{-1}_t} \right) - \hat{\theta}_t(\hat{M}^*)$;
return $\hat{M}^* \leftarrow \hat{M}^*_t$;

E Details of Experiments

All experiments were conducted on a Macbook with a 1.3 GHz Intel Core i5 and 8GB memory. All codes were implemented by using Python. The entire procedure of Exhaustive is detailed in Algorithm 5. This algorithm reduces our problem to the pure exploration problem in the linear bandit, and thus runs in exponential time, i.e., $O(n^k)$. In all experiments, we employed the approximation algorithm called the greedy peeling \cite{soda2017} as the $D_k$-Oracle. Specifically, the greedy peeling algorithm iteratively removes a vertex with the minimum weighted degree in the currently remaining graph until we are left with the subset of vertices with size $k$. The algorithm runs in $O(n^2)$.

F Proofs

First, we introduce the notation. For $M, M' \in \mathcal{M}$, let $\Delta(M, M')$ be the value gap between two super-arms, i.e., $\Delta(M, M') = |\theta(M) - \theta(M')|$. Also, let $\hat{\Delta}(M, M')$ be the empirical gap between two super-arms, i.e., $\hat{\Delta}(M, M') = |\hat{\theta}_t(M) - \hat{\theta}_t(M')|$.

F.1 Proof of Lemma 2

**Proof.** The empirical best super-arm $\hat{M}^*_t$ can be computed by the greedy algorithm under matroid constraint \cite{soda2017} (the greedy algorithm is described in Appendix B). The maximization of $P_1$ is linear maximization under matroid constraint, and thus, this is also solvable by the greedy algorithm. Letting $g(n)$ be the computation time for checking whether a super-arm satisfies the matroid constraint or not, we see that the running time of the greedy procedure is $O(n \log n + ng(n))$. Moreover, updating $A^{-1}_t$ needs $O(n^2)$ time. Therefore, we have the lemma. \qed

F.2 Proof of Lemma 3

**Proof.** First we define random event $\mathcal{E}$ as follows:

$$\mathcal{E} = \left\{ \forall t \in \{1, 2, \ldots, \}, \forall M, M' \in \mathcal{M}, \left| \hat{\theta}_t(M) - \hat{\theta}_t(M') \right| \leq C_t \sum_{i=1}^{n} |\chi_M(i) - \chi_{M'}(i)| \sqrt{A^{-1}_t(i, i)} \right\}.$$

We notice that random event $\mathcal{E}$ implies that the event that the confidence intervals of all super-arm $M \in \mathcal{M}$ are valid at round $t$. From Lemma 1, we see that the probability that event $\mathcal{E}$ occurs is at least $1 - \delta$. Under the event $\mathcal{E}$, we see that the output $\hat{M}^*$ is an $\varepsilon$-optimal super-arm. In the rest of the proof, we shall
assume that event $\mathcal{E}$ holds. Next, we focus on bounding the sample complexity $T$. By recalling the stopping condition, a sufficient condition for stopping is that for $M^*$ and for $t > n$,

$$
\varepsilon > \max_{M \in \mathcal{M} \setminus \{M^*\}} \left( \theta_t(M) + C_t \sum_{i=1}^{n} |\chi_{M}(i) - \chi_{M^*}(i)| \sqrt{A_{M}^{-1}(i, i)} \right) - \tilde{\theta}_t(M^*).
$$

Let $\overline{M} = \arg\max_{M \in \mathcal{M} \setminus \{M^*\}} \left( \tilde{\theta}_t(M) + C_t \sum_{i=1}^{n} |\chi_{M}(i) - \chi_{M^*}(i)| \sqrt{A_{M}^{-1}(i, i)} \right)$. Eq. (1) is satisfied if

$$
\tilde{\Delta}(M^*, \overline{M}) > C_t \sqrt{\frac{\rho(p)}{t}} - \varepsilon. \tag{2}
$$

From Lemma 1 with $x = \chi_{M'} - \chi_{\pi}$, with probability at least $1 - \delta$, we have

$$
\tilde{\Delta}(M^*, \overline{M}) \geq \Delta(M^*, \overline{M}) - C_t \sum_{i=1}^{n} |\chi_{M'}(i) - \chi_{\pi}(i)| \sqrt{A_{M}^{-1}(i, i)} \geq \Delta(M^*, \overline{M}) - C_t \sqrt{\frac{\rho(p)}{t}}. \tag{3}
$$

Combining (2) and (3), we see that a sufficient condition for stopping is given by $\Delta(M^*, \overline{M}) \geq \Delta_{\text{min}} \geq 2C_t \sqrt{\frac{\rho(p)}{t}} - \varepsilon$. Therefore, we have $t \geq 4C_t^2 H_{\varepsilon}$ as a sufficient condition to stop. Let $\tau > n$ be the stopping time of the algorithm. From the above discussion, we see that $\tau \leq 4C_t^2 H_{\varepsilon}$. Recalling that $C_t = \sigma \sqrt{2 \log(cT^2 n/\delta)}$, we have $\tau \leq 8\sigma^2 \log(c'\tau^2 n/\delta)H_{\varepsilon}$. Let $\tau'$ be a parameter that satisfies

$$
\tau = 8\sigma^2 \log(c'\tau^2 n/\delta)H_{\varepsilon}. \tag{4}
$$

Then, it is obvious that $\tau' \leq \tau$ holds. For $N$ defined as $N = 8\sigma^2 \log(c'n/\delta)H_{\varepsilon}$, we have

$$
\tau' \leq \tau = 16\sigma^2 \log(\tau')H_{\varepsilon} + N \leq 16\sigma^2 \sqrt{\tau^2}H_{\varepsilon} + N
$$

Transforming this inequality, we obtain

$$
\sqrt{\tau'} \leq 8\sigma^2 H_{\varepsilon} + \sqrt{64\sigma^4 H_{\varepsilon}^2 + N} \leq 2\sqrt{64\sigma^4 H_{\varepsilon}^2 + N}. \tag{5}
$$

Let $L = 2\sqrt{64\sigma^4 H_{\varepsilon}^2 + N}$, which equals the RHS of (5). We see that log $L = O \left( \log \left( \sigma H_{\varepsilon} \left( \sigma^2 H_{\varepsilon} + \log \left( \frac{n}{\delta} \right) \right) \right) \right)$. Then, using this upper bound of $\tau'$ in (4), we have

$$
\tau \leq 16\sigma^2 H_{\varepsilon} \log \left( \frac{c'n}{\delta} \right) + C(H_{\varepsilon}, \delta),
$$

where

$$
C(H_{\varepsilon}, \delta) = O \left( \sigma^2 H_{\varepsilon} \log \left( \sigma H_{\varepsilon} \left( \sigma^2 H_{\varepsilon} + \log \left( \frac{n}{\delta} \right) \right) \right) \right).
$$

Recalling that $\sigma = kR$, we obtain

$$
\tau = O \left( k^2 R^2 H_{\varepsilon} \log \left( \frac{n}{\delta} \right) \left( kR H_{\varepsilon} \left( k^2 R^2 H_{\varepsilon} + \log \left( \frac{n}{\delta} \right) \right) \right) \right).
$$

\[\square\]

F.3 Proof of Theorem 1

We begin by showing the following three lemmas.

**Lemma 4.** Let $W \in \mathbb{R}^{n \times n}$ be any positive definite matrix. Then $\tilde{G} = (V, E, \tilde{w})$ constructed by Algorithm 1 is a non-negative weighted graph.

**Proof.** For any $(i, j) \in V^2$, we have $w_{ii} \geq 0$ and $w_{jj} \geq 0$ since $W$ is a positive definite matrix. If $w_{ij} \geq 0$, it is obvious that $\tilde{w}_{ij} = w_{ij} + w_{ii} + w_{jj} \geq 0$. We consider the case $w_{ij} < 0$. In the case, we have
\( w_{ij} + w_{ii} + w_{jj} > 2w_{ij} + w_{ii} + w_{jj} \geq 0 \), where the last inequality holds from the definition of positive definite matrix \( W \). Thus, we obtain the desired result.

**Lemma 5.** Let \( W \in \mathbb{R}^{n \times n} \) be any positive definite matrix and \( \tilde{W} = (\tilde{w}_{ij}) \) be the adjacency matrix of the complete graph constructed by Algorithm 1. Then, for any subset of vertices \( S \subseteq V \) such that \( |S| \geq 2 \), we have \( w(S) \leq \tilde{w}(S) \).

**Proof.** We have

\[
  w(S) = \sum_{e \in E(S)} w_e = \sum_{\{i,j\} \in E(S): i \neq j} w_{ij} + \sum_{i \in S} w_{ii}
  \leq \sum_{\{i,j\} \in E(S): i \neq j} w_{ij} + (|S| - 1) \sum_{i \in S} w_{ii} = \tilde{w}(S),
\]

where the last inequality holds since each diagonal component \( w_{ii} \) is positive for all \( i \in V \) from the definition of the positive definite matrix.

**Lemma 6.** Let \( W \in \mathbb{R}^{n \times n} \) be any positive definite matrix and \( \tilde{W} = (\tilde{w}_{ij}) \) be the adjacency matrix of the complete graph constructed in Algorithm 1. Then, for any subset of vertices \( S \subseteq V \), we have \( \frac{w(S)}{\tilde{w}(S)} \leq (|S| - 1) \frac{\lambda_{\text{max}}(W)}{\lambda_{\text{min}}(W)} \), where \( \lambda_{\text{min}}(W) \) and \( \lambda_{\text{max}}(W) \) represent the minimum and maximum eigenvalues of \( W \), respectively.

**Proof.** We consider the following two cases: Case (i) \( \sum_{\{i,j\} \in E(S): i \neq j} w_{ij} \geq 0 \) and Case (ii) \( \sum_{\{i,j\} \in E(S): i \neq j} w_{ij} < 0 \).

**Case (i)** Since \( W = (w_{ij})_{1 \leq i,j \leq n} \) is positive definite matrix, we see that diagonal component \( w_{ii} \) is positive for all \( i \in V \). Thus, we have

\[
  \tilde{w}(S) = \sum_{\{i,j\} \in E(S): i \neq j} w_{ij} + (|S| - 1) \sum_{i \in S} w_{ii}
  \leq (|S| - 1) \left( \sum_{\{i,j\} \in E(S): i \neq j} w_{ij} + \sum_{i \in S} w_{ii} \right) = (|S| - 1) w(S).
\]

Since \( W \) is positive definite, we have \( w(S) > 0 \). That gives us the desired result.

**Case (ii)** In this case, we see that

\[
  \tilde{w}(S) = \sum_{\{i,j\} \in E(S): i \neq j} w_{ij} + (|S| - 1) \sum_{i \in S} w_{ii} \leq (|S| - 1) \sum_{i \in S} w_{ii}.
\]

For any diagonal component \( w_{ii} \) we have that \( w_{ii} \leq \max_{1 \leq i,j \leq n} w_{ij} \). For the largest component \( \max_{1 \leq i,j \leq n} w_{ij} \), we have

\[
  \max_{1 \leq i,j \leq n} w_{ij} \leq \max_{1 \leq i,j \leq n} \frac{1}{2} e_i^\top W e_i + \frac{1}{2} e_j^\top W e_j \leq \lambda_{\text{max}}(W),
\]

where the first inequality is satisfied since \( W \) is positive definite. Thus, we obtain

\[
  \tilde{w}(S) < |S|(|S| - 1) \lambda_{\text{max}}(W). \tag{6}
\]

For the lower bound of \( w(S) \), we have

\[
  w(S) = \chi_s^\top W \chi_s = \frac{\chi_s^\top W \chi_s}{\| \chi_s \|_2^2} |S| > \lambda_{\text{min}}(W) |S|. \tag{7}
\]
Combining (6) and (7), we obtain
\[
\tilde{w}(S) < \left( |S| - 1 \right) \frac{\lambda_{\text{max}}(W)}{\lambda_{\text{min}}(W)},
\]
which completes the proof.

We are now ready to prove Theorem 1.

**Proof of Theorem 1.** For any round \( t > n \), let \( x_s \) be the approximate solution obtained by Algorithm 1 and \( Z \) be its objective value. Let \( \tilde{w} : 2^n \rightarrow \mathbb{R} \) be the weight function defined by Algorithm 1. We denote the optimal value of QP by \( \text{OPT} \). Let us denote optimal solution of the DkS for \( G([n], E, \tilde{w}) \) by \( \tilde{S}_{\text{OPT}} \). Adjacency matrix \( W \) is a symmetric positive definite matrix; thus, Lemmas 4, 5 and 6 hold for \( W \). We have
\[
\tilde{w}(S_t) \geq \alpha_{\text{DkS}} \tilde{w}(\tilde{S}_{\text{OPT}}), \quad (\because \text{\( S_t \) is an } \alpha_{\text{DkS}} \text{-approximate solution for DkS}(\tilde{G}),)
\]
\[
\geq \alpha_{\text{DkS}} \tilde{w}(\tilde{S}_{\text{OPT}}), \quad (\because \text{Lemma 5}). \quad (8)
\]
Thus, we obtain
\[
Z = x_s^\top A^{-1}_x x_s = w(S_t)
\]
\[
\geq \frac{1}{|S| - 1} \frac{\lambda_{\text{min}}(W)}{\lambda_{\text{max}}(W)} \tilde{w}(S_t) \quad (\because \text{Lemma 6})
\]
\[
\geq \frac{1}{|S| - 1} \frac{\lambda_{\text{min}}(W)}{\lambda_{\text{max}}(W)} \alpha_{\text{DkS}} \tilde{w}(\tilde{S}_{\text{OPT}}) \quad (\because (8))
\]
\[
= \frac{1}{|S| - 1} \frac{\lambda_{\text{min}}(W)}{\lambda_{\text{max}}(W)} \alpha_{\text{DkS}} \text{OPT}.
\]

Therefore, we obtain
\[
Z \geq \left( \frac{1}{k-1} \frac{\lambda_{\text{min}}(W)}{\lambda_{\text{max}}(W)} \alpha_{\text{DkS}} \right) \text{OPT}.
\]

**F.4 Proof of Theorem 2**

Proof. Updating \( A^{-1}_x \) can be done in \( O(n^2) \) time, and computing the empirical best super-arm can be done in \( O(n) \) time. Moreover, confidence maximization CEM can be approximately solved in polynomial-time, since quadratic maximization QP is solved in polynomial-time as long as we employ polynomial-time algorithm as the DkS-Oracle. Let \( \text{poly}(n)_{\text{DkS}} \) be the computation time of DkS-Oracle. Then, we can guarantee that \( \text{SAQM} \) runs in \( O(\max\{n^2, \text{poly}(n)_{\text{DkS}}\}) \) time. Most existing approximation algorithms for the DkS have efficient computation time. For example, if we employ the algorithm by Feige, Peleg, and Kortsarz [13] as the DkS-Oracle that runs in \( O(n^\omega) \) time in Algorithm 1, the running time of \( \text{SAQM} \) becomes \( O(n^2) \), where the exponent \( \omega \leq 2.373 \) is equal to that of the computation time of matrix multiplication (e.g., see [35]). If we employ the algorithm by Asahiro et al. [3] that runs in \( O(n^2) \), the running time of \( \text{SAQM} \) also becomes \( O(n^2) \).

**F.5 Proof of Theorem 3**

Before stating the proof of Theorem 3, we give the two technical lemmas.

**Lemma 7.** For any round \( t \), the condition number of \( A_{x_t} \) is bound by
\[
\frac{\lambda_{\text{max}}(A_{x_t})}{\lambda_{\text{min}}(A_{x_t})} = O(k).
\]
Proof. For $\lambda_{\text{max}}(A_{\chi_t})$, we have

$$\lambda_{\text{max}}(A_{\chi_t}) = \max_{||y||_2=1} y^\top A_{\chi_t}^{-1} y = \max_{||y||_2=1} y^\top \sum_{t'=1}^t x_{t'}^\top x_{t'} y = \max_{||y||_2=1} \sum_{t'=1}^t (x_{t'}^\top y)^2 \leq kt.$$ 

Next, we give a lower bound of $\lambda_{\text{min}}(A_{\chi_t})$. Recall that the sequence $\mathbf{x}_t = (\chi_{M_1}, \ldots, \chi_{M_t})$ represents for the sequence of $t$-set selections $\mathbf{M}_t = (M_1, M_2, \ldots, M_t) \in \mathcal{M}^t$ and $T_M(t)$ is the number of times that super-arm $M$ is selected before $t + 1$-th round. In any super-arm selection strategy that samples $M_t$ for any $t \in [T]$ such that $\min_{M \in \mathcal{M}} T_M(t)/t \geq r$ for some constant $r > 0$, we have $\lambda_{\text{min}}(A_{\chi_t}) \geq r \lambda_{\text{min}}(\sum_{M \in \mathcal{M}} \chi_M \chi_M^\top) / t$.

From the above discussion, we have $\frac{\lambda_{\text{max}}(A_{\chi_t})}{\lambda_{\text{min}}(A_{\chi_t})} = O(k)$.

Next, for any $t > n$, let us define random event $\mathcal{E}_t'$ as

$$\left\{ \forall M \in \mathcal{M}, |\theta(M) - \hat{\theta}(M)| \leq C_t \|\chi_M\|_{A_{\chi_t}^{-1}} \right\}.$$ 

We note that random event $\mathcal{E}_t'$ characterizes the event that the confidence bounds of all super-arm $M \in \mathcal{M}$ are valid at round $t$. Next lemma indicates that, if the confidence bounds are valid, then SAQM always outputs $\varepsilon$-optimal super-arm $\hat{M}^*$ when it stops.

**Lemma 8.** Given any $t > n$, assume that $\mathcal{E}_t'$ occurs. Then, if SAQM (Algorithm 2) terminates at round $t$, we have $\theta(M^*) - \theta(\hat{M}^*) \leq \varepsilon$.

**Proof of Lemma 8.** If $\hat{M}^* = M^*$, we have the desired result. Then, we shall assume $\hat{M}^* \neq M^*$. We have the following inequalities:

$$\theta(\hat{M}^*) \geq \hat{\theta}(\hat{M}^*_t) - C_t \|\chi_{\hat{M}^*_t}\|_{A_{\chi_t}^{-1}} \quad (\therefore \text{event } \mathcal{E}_t')$$

$$\geq \max_{M \in \mathcal{M} \setminus \{\hat{M}^*_t\}} \hat{\theta}(M) + \frac{1}{\alpha_t} Z_t - \varepsilon \quad (\therefore \text{stopping condition})$$

$$\geq \max_{M \in \mathcal{M} \setminus \{\hat{M}^*_t\}} \hat{\theta}(M) + \max_{M \in \mathcal{M}} C_t \|\chi_M\|_{A_{\chi_t}^{-1}} \geq \varepsilon \quad (\therefore Z_t \geq \alpha_t \max_{M \in \mathcal{M}} C_t \|\chi_M\|_{A_{\chi_t}^{-1}})$$

$$\geq \hat{\theta}(M^*) + C_t \|\chi_{M^*}\|_{A_{\chi_t}^{-1}} - \varepsilon$$

$$\geq \theta(M^*) - \varepsilon. \quad (\therefore \text{event } \mathcal{E}_t')$$

We are now ready to prove Theorem 3.

**Proof of Theorem 3.** We define event $\mathcal{E}'$ as $\bigcap_{t=1}^{\infty} \mathcal{E}_t'$. We can see that the probability that event $\mathcal{E}'$ occurs is at least $1 - \delta$ from Proposition 1. In the rest of the proof, we shall assume that this event holds. By Lemma 8 and the assumption on $\mathcal{E}'$, we see that the output $\hat{M}^*$ is $\varepsilon$-optimal super-arm. Next, we focus on bounding the sample complexity.

A sufficient condition for stopping is that for $M^*$ and for $t > n$,

$$\hat{\theta}(M^*) - C_t \|\chi_{M^*}\|_{A_{\chi_t}^{-1}} \geq \max_{M \in \mathcal{M} \setminus \{M^*\}} \hat{\theta}(M) + \frac{1}{\alpha_t} Z_t - \varepsilon. \quad (10)$$

From the definition of $A_{\chi_t}^{-1}$, we have $A_p = \frac{A_{\chi_t}}{t}$. Using $\|\chi_{M^*}\|_{A_{\chi_t}^{-1}} \leq \max_{M \in \mathcal{M}} \|\chi_M\|_{A_{\chi_t}^{-1}}$ and $Z_t \leq \max_{M \in \mathcal{M}} \|\chi_M\|_{A_{\chi_t}^{-1}}$, a sufficient condition for (10) is equivalent to:

$$\hat{\Delta}(M^*, \hat{M}) \geq \left(1 + \frac{1}{\alpha_t}\right) C_t \sqrt{\frac{\rho(p)}{t}} - \varepsilon, \quad (11)$$

20
where $\overline{M} = \text{argmax}_{M \in M} \Delta_t(M^*, M)$. On the other hand, we have

\[
\|\chi_{\mathcal{M}} - \chi_\pi\|_{A_{x_t}} \leq 2 \max_{M \in M} \|\chi_M\|_{A_{x_t}} \leq 2 \frac{\rho(p)}{t}.
\]

Therefore, from Proposition 1 with $x = \chi_{\mathcal{M}} - \chi_M$, with at least probability $1 - \delta$, we have

\[
\Delta_t(M^*, \overline{M}) \geq \Delta(M^*, \overline{M}) - C_t \|\chi_{\mathcal{M}} - \chi_\pi\|_{A_{x_t}} \geq \Delta(M^*, \overline{M}) - 2C_t \frac{\rho(p)}{t}.
\]

Combining (11) and (12), we see that a sufficient condition for stopping becomes the following inequality.

\[
\Delta_{\min} - 2C_t \frac{\rho(p)}{t} \geq \left(1 + \frac{1}{\alpha_t}\right) C_t \frac{\rho(p)}{t} - \varepsilon.
\]

Therefore, we have that a sufficient condition to stop is $t \geq \left(3 + \frac{1}{\alpha_t}\right)^2 C_t^2 H_\varepsilon$, where $H_\varepsilon = \frac{\rho(p)}{\Delta_{\min} + \tau_r}$. Let $\tau > n$ be the stopping time of the algorithm. From the above discussion, we see that $\tau \leq \left(3 + \frac{1}{\alpha_t}\right)^2 C_t^2 H_\varepsilon$.

Recalling that $C_{\tau} = c \sqrt{\log(c\tau^2K/\delta)}$, we have that

\[
\tau \leq (3 + 1/\alpha_t)^2 C_t^2 H_\varepsilon = (3 + 1/\alpha_t)^2 c^2 \log(c\tau^2K/\delta)H_\varepsilon.
\]

Let $\tau'$ be a parameter that satisfies

\[
\tau = (3 + 1/\alpha_t)^2 c^2 \log(c\tau^2K/\delta)H_\varepsilon.
\]

Then, it is obvious that $\tau' \leq \tau$ holds. For $N$ defined as $N = (3 + 1/\alpha_t)^2 c^2 \log(cK/\delta)H_\varepsilon$, we have

\[
\tau' \leq \tau = (3 + 1/\alpha_t)^2 c^2 \log(\tau')H_\varepsilon + N \leq (3 + 1/\alpha_t)^2 c^2 \sqrt{\tau'}H_\varepsilon + N.
\]

By solving this inequality with $c = 2\sqrt{2}\sigma$, we obtain

\[
\sqrt{\tau'} \leq 4 (3 + 1/\alpha_t)^2 \sigma^2 H_\varepsilon + \sqrt{16 (3 + 1/\alpha_t)^4 \sigma^4 H_\varepsilon^2 + N}
\]

\[
\leq 2 \sqrt{16 (3 + 1/\alpha_t)^4 \sigma^4 H_\varepsilon^2 + N}.
\]

Let $L = 2\sqrt{16 (3 + 1/\alpha_t)^4 \sigma^4 H_\varepsilon^2 + N}$, which is equal to the RHS of the inequality. We see that $\log L = O \left( \log \left( \frac{\sigma}{\alpha_t}H_\varepsilon \left( \left( \frac{\sigma}{\alpha_t}^2 H_\varepsilon + \log \left( \frac{K}{\delta} \right) \right) \right) \right) \right)$. Then, using this upper bound of $\tau'$ in (13), we have

\[
\tau \leq 8 \left(3 + \frac{1}{\alpha_t}\right)^2 \sigma^2 H_\varepsilon \log \left( \frac{cK}{\delta} \right) + C(H_\varepsilon, \delta),
\]

where

\[
C(H_\varepsilon, \delta) = 16 \left(3 + \frac{1}{\alpha_t}\right)^2 \sigma^2 H_\varepsilon \log(L)
\]

\[
= O \left( \sigma^2 H_\varepsilon \log \left( \frac{\sigma}{\alpha_t} H_\varepsilon \left( \frac{\sigma^2}{\alpha_t^2} H_\varepsilon + \log \left( \frac{K}{\delta} \right) \right) \right) \right).
\]

We see that $1/\alpha_t = O \left( k n^{1/8} \right)$ from Theorem 1 and Lemma 7, if we use the best approximation algorithm for the DKS as the DKS-Oracle $[5]$. Recalling that $\sigma = kR$ and $\log(K/\delta) \leq k \log(n/\delta)$, we obtain

\[
\tau = O \left( k^2 R^2 H_\varepsilon \left( n^{\frac{1}{5}} k^{\frac{3}{2}} \log \left( \frac{K}{\delta} \right) \right) + \log \left( n^{\frac{1}{4}} k^{\frac{3}{2}} R H_\varepsilon \left( n^{\frac{1}{5}} k^{\frac{3}{2}} R^2 H_\varepsilon + \log \left( \frac{n}{\delta} \right) \right) \right) \right).
\]