# **Pure Exploration of Combinatorial Bandits**

## Anonymous Author(s)

Affiliation Address email

#### Abstract

The abstract paragraph should be indented 1/2 inch (3 picas) on both left and right-hand margins. Use 10 point type, with a vertical spacing of 11 points. The word **Abstract** must be centered, bold, and in point size 12. Two line spaces precede the abstract. The abstract must be limited to one paragraph.

#### 1 Introduction

The pure exploration problem is about designing strategies that make the best use of the limited budget.

#### Motivation.

#### Contributions.

Therefore, our results provide a complete characterization (within logarithmic factors) of the sample complexity for a large class of combinatorial problems, including MULTI and MATROID problem.

Our lower bound result also resolves the conjecture of Kalyanakrishnan et al. [2] on the lower bound sample complexity for the MULTI problem.

#### 1.1 Related Work

#### Notations.

# 2 Pure Exploration of Combinatorial Bandits

**ExpCMAB:** problem formulation. Suppose that there are n arms and the arms are numbered  $1,2,\ldots,n$ . Each arm  $e\in[n]$  is associated with a reward distribution  $\varphi_e$  and define  $w(e)=\mathbb{E}_{X\sim\varphi_e}[X]$  be the expected reward. Let  $\boldsymbol{w}=\left(w(1),\ldots,w(n)\right)^T$  denote the vector of expected rewards.

Let  $\mathcal{M}\subseteq 2^{[n]}$  be the family of all feasible solutions to a combinatorial problem. A learner wants to find the optimal solution of  $\mathcal{M}$  which maximizes the expected reward  $M_*=\arg\max_{M\in\mathcal{M}}w(M)$  by playing the following game. At the beginning of the game, the reward distributions  $\{\varphi_e\}_{e\in[n]}$  are unknown to the learner. Then, the game is played for multiple rounds; on each round t, the learner pulls an arm  $p_t\in[n]$  and observes a reward sampled from the associated reward distribution  $\varphi_{p_t}$ . The game continues until certain stopping condition is satisfied. After the game finishes, the learner need to output a solution  $\mathrm{Out}\in\mathcal{M}$ .

We consider two different stopping conditions of the game, which are known as *fixed confidence* setting and *fixed budget* setting. In the fixed confidence setting, the learner can stop the game at any point and her goal is to achieve a fixed confidence about the optimality of the returned set while uses a small number of pulls. Specifically, given a confidence parameter  $\delta$ , the learner need to guarantee

that  $\Pr[\mathsf{Out} = M_*] \geq 1 - \delta$ . The performance is evaluated by the number of pulls used by the learner. In the fixed budget setting, the game stops after a fixed number rounds. The learner tries to minimize the probability of error  $\Pr[\mathsf{Out} \neq M_*]$  within these rounds. In this case, the learner's performance is measured by the probability of error.

**Examples of combinatorial problems.** The formulation of the ExpCMAB problem covers many online learning tasks. We consider the following problems as examples.

• MULTI.

- MATROID.
- MATCH.
- PATH.

We assume that all reward distributions have R-sub-Gaussian tails. Formally, for all  $t \in \mathbb{R}$ , we assume that  $\mathbb{E}_{X \sim \varphi_e} \left[ \exp(tX - tw(e)) \right] \leq \exp(R^2 t^2/2)$ . It is well known that all distributions that are supported on [0, R] satisfy this property [].

# 3 Algorithm and Main Result

In this section, we present CGapExp, a learning algorithm for the ExpCMAB problem in the fixed confidence setting, and analyze its sample complexity. The CGapExp algorithm can be extended to the fixed budget and PAC learning settings. We will discuss these extensions in Section 5.

**Oracle.** We allow the CGapExp algorithm to access a *maximization oracle*. A maximization oracle takes a weight vector  $v \in \mathbb{R}^n$  as input and computes an optimal solution with respect to the weight vector v. Formally, we call a function Oracle:  $\mathbb{R}^n \to \mathcal{M}$  a maximization oracle if, for all  $v \in \mathbb{R}^n$ , we have  $\operatorname{Oracle}(v) \in \arg\max_{M \in \mathcal{M}} v(M)$ . It is clear that a very broad class of combinatorial problems admit such maximization oracles. Besides the access to the oracle, CGapExp does not need any additional knowledge of the combinatorial problem  $\mathcal{M}$ .

**Algorithm.** The CGapExp algorithm maintains empirical mean  $\bar{w}_t(e)$  and confidence radius rad<sub>t</sub>(e) for each arm  $e \in [n]$  and each round t. The construction of confidence radius ensures that |w(e)| $|\bar{w}_t(e)| \leq \operatorname{rad}_t(e)$  holds with high probability for each arm  $e \in [n]$  and each round t > 0. CGapExp begins with an initialization phase in which each arm is pulled once. Then, at round  $t \geq n$ , CGapExp uses the following procedure to choose an arm to play. First, CGapExp calls the oracle which computes the solution  $M_t = \text{Oracle}(\bar{w}_t)$ . The solution  $M_t$  is the "best" solution with respect to the empirical means  $\bar{w}_t$ . Then, CGapExp explores possible refinements of  $M_t$ . In particular, CGapExp uses the confidence radius to compute an adjusted expectation vector  $\tilde{\boldsymbol{w}}_t$  in the following way: for each arm  $e \in M_t$ ,  $\tilde{w}_t(e)$  equals to the lower confidence bound  $\tilde{w}_t(e) = \bar{w}_t(e) - \mathrm{rad}_t(e)$ ; and for each arm  $e \notin M_t$ ,  $\tilde{w}_t(e)$  equals to the upper confidence bound  $\tilde{w}_t(e) = \bar{w}_t(e) + \mathrm{rad}_t(e)$ . Intuitively, the adjusted expectation vector  $\tilde{\boldsymbol{w}}_t$  penalizes arms belonging to the current solution  $M_t$  and encourages exploring arms out of  $M_t$ . CGapExp then calls the oracle using the adjusted expectation vector  $\tilde{\boldsymbol{w}}_t$  as input to compute a refined solution  $M_t = \text{Oracle}(\tilde{\boldsymbol{w}}_t)$ . If  $\tilde{w}_t(M_t) = \tilde{w}_t(M_t)$  then CGapExp stops and returns  $Out = M_t$ . Otherwise, CGapExp pulls the arm belonging to the symmetric difference  $(M_t \setminus M_t) \cup (M_t \setminus M_t)$  between  $M_t$  and  $M_t$  with the largest confidence radius in the end of round t. The pseudo-code of CGapExp is shown in Algorithm 1.

### 3.1 Analysis

Now we prove a problem-dependent sample complexity bound of the CGapExp algorithm. Our sample complexity bound depends on several combinatorial properties of  $\mathcal{M}$ . Therefore, to state our result, we first introduce notions to capture these properties.

**Gap.** We begin with defining a hardness complexity measure of the ExpCMAB problem. For each arm  $e \in [n]$ , we define gap  $\Delta_e$  as

$$\Delta_e = \begin{cases} w(M_*) - \max_{M \in \mathcal{M}: e \in M} w(M) & \text{if } e \notin M_*, \\ w(M_*) - \max_{M \in \mathcal{M}: e \notin M} w(M) & \text{if } e \in M_*, \end{cases}$$
(1)

## Algorithm 1 CGapExp: Combinatorial Gap Exploration

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109 **Require:** Confidence parameter:  $\delta \in (0,1)$ ; Maximization oracle: Oracle(·):  $\mathbb{R}^n \to \mathcal{M}$ . 110 **Initialize:** Play each arm  $e \in [n]$  once. Initialize empirical means  $\bar{w}_n$  and set  $T_n(e) \leftarrow 1$  for 111 112 1: **for**  $t = n, n + 1, \dots$  **do** 113  $M_t \leftarrow \text{Oracle}(\bar{\boldsymbol{w}}_t)$ 2: 114 for  $e \in [n]$  do 3: if  $e \in M_t$  then 115 4: 116 5:  $\tilde{w}_t(e) \leftarrow \bar{w}_t(e) - \mathrm{rad}_t(e)$ 6: 117  $\tilde{w}_t(e) \leftarrow \bar{w}_t(e) + \mathrm{rad}_t(e)$ 7: 118 8: end if 119 9: end for 120 10:  $M_t \leftarrow \text{Oracle}(\tilde{\boldsymbol{w}}_t)$ 121 if  $\tilde{w}_t(\tilde{M}_t) = \tilde{w}_t(M_t)$  then 11: 122 Out  $\leftarrow M_t$ 12: 123 return Out 13: 124 14: end if 125 15:  $p_t \leftarrow \arg\max_{e \in (\tilde{M}_t \setminus M_t) \cup (M_t \setminus \tilde{M}_t)} \operatorname{rad}_t(e)$ 126 16: Pull arm  $p_t$  and observe the reward 127 17: Update empirical means  $\bar{\boldsymbol{w}}_{t+1}$  using the observed reward 128 Update number of pulls:  $T_{t+1}(p_t) \leftarrow T_t(p_t) + 1$  and  $T_{t+1}(e) \leftarrow T_t(e)$  for all  $e \neq p_t$ 18: 129 19: **end for** 

where we use the convention that the maximum value of an empty set is  $-\infty$ . We also define the hardness **H** as the sum of inverse squared gaps

$$\mathbf{H} = \sum_{e \in [n]} \Delta_e^{-2}.$$
 (2)

From Eq. (1), we see that, for each arm  $e \notin M_*$ ,  $\Delta_e$  represents the gap between the optimal set  $M_*$  and the best set that includes arm e; and, for each arm  $e \in M_*$ ,  $\Delta_e$  is the sub-optimality of the best set that does not include arm e. We notice that this definition resembles the previous definition of gaps for the MULTI problem [2, 1].

**Exchange class and the width of**  $\mathcal{M}$ . The analysis of our algorithm depends on certain exchange properties of combinatorial structures. To capture these properties, we introduce notions of *exchange set* and *exchange class* as tools for our analysis. We present their definitions in the following.

We begin with the definition of exchange set. We define an exchange set b as an ordered pair of disjoint sets  $b=(b_+,b_-)$  where  $b_+\cap b_-=\emptyset$ . Then, we define operator  $\oplus$  such that, for any set M and any exchange set  $b=(b_+,b_-)$ , we have  $M\oplus b\triangleq M\backslash b_-\cup b_+$ . Similarly, we also define operator  $\oplus$  such that  $M\oplus b\triangleq M\backslash b_+\cup b_-$ .

We call a family of exchange sets  $\mathcal{B}$  an exchange class for  $\mathcal{M}$  if  $\mathcal{B}$  satisfies the following property. Let M and M' be two elements of  $\mathcal{M}$ . Then, for any  $e \in (M \backslash M')$ , there exists an exchange set  $(b_+, b_-) \in \mathcal{B}$  which satisfies  $e \in b_-, b_+ \subseteq M' \backslash M, b_- \subseteq M \backslash M', (M \oplus b) \in \mathcal{M}$  and  $(M' \ominus b) \in \mathcal{M}$ . We define the width of exchange class  $\mathcal{B}$  to be the size of largest exchange set as follows

width(
$$\mathcal{B}$$
) =  $\max_{(b_+, b_-) \in \mathcal{B}} |b_+| + |b_-|$ . (3)

Intuitively, for any feasible sets M and M', there exists an exchange set  $(b_+, b_-) \in \mathcal{B}$  belonging to the exchange class  $\mathcal{B}$  which can be seen as an "operation" that transforms M one step towards M': this operation generates a new feasible set  $M \oplus b$  by removing elements (including e) from M and adding elements which belongs to M'. One can chain these operations together: for any  $M \neq M'$ , there exists a sequence of exchange sets  $b_1, \ldots, b_k$  of  $\mathcal{B}$  such that  $M' = M \oplus b_1 \oplus \ldots \oplus b_k$ .

We notice that an exchange class for  $\mathcal{M}$  can be "redundant". It may contains some unnecessary exchange set b, such that  $M \oplus b \not\in \mathcal{M}$  for any  $M \in \mathcal{M}$ . These redundant exchange sets do not

(a) An element of 
$$\mathcal{B}_{\text{MAICH}}$$
. (b) An element of  $\mathcal{B}_{\text{MAICH}}$ .

Figure 1: Examples of exchange sets belonging to the exchange classes  $\mathcal{B}_{\text{MULTI}}$ ,  $\mathcal{B}_{\text{MATROID}}$ ,  $\mathcal{B}_{\text{MATCH}}$  and  $\mathcal{B}_{\text{PATH}}$ : green-solid elements constitute the set  $b_+$ , red-dotted elements constitute the set  $b_-$  and the example exchange set is  $b = (b_+, b_-)$ . (In Figure 1b, we consider spanning tree as a specific instance for the MATROID problem.)

affect our analysis. But allowing them would simplify the construction and description of exchange classes for certain combinatorial problems.

Finally, let  $\operatorname{Exchange}(\mathcal{M})$  denote the collection of all possible exchange classes for  $\mathcal{M}$ . We define the width of a combinatorial problem  $\mathcal{M}$  as the width of the thinnest exchange class

$$\operatorname{width}(\mathcal{M}) = \min_{\mathcal{B} \in \operatorname{Exchange}(\mathcal{M})} \operatorname{width}(\mathcal{B}).$$

For many problems, the exchange classes with small widths corresponding to natural combinatorial structures. To see this, we construct the exchange classes for our running examples. Our constructions are summarized in Fact 1.

**Fact 1.** There exist exchange classes  $\mathcal{B}_{\text{MULTI}}$ ,  $\mathcal{B}_{\text{MATROID}}$ ,  $\mathcal{B}_{\text{MATCH}}$  and  $\mathcal{B}_{\text{PATH}}$  for  $\mathcal{M}_{\text{MULTI}}$ ,  $\mathcal{M}_{\text{MATROID}}$ ,  $\mathcal{M}_{\text{MATCH}}$  and  $\mathcal{M}_{\text{PATH}}$ , respectively. These exchange classes can be constructed as follows

1.  $\mathcal{B}_{\text{MULTI}} = \{(\{i\}, \{j\}) \mid \forall i \in [n], j \in [n]\}.$ 

- 2.  $\mathcal{B}_{MATROID} = \{(\{i\}, \{j\}) \mid \forall i \in [n], j \in [n]\}.$
- 3.  $\mathcal{B}_{MATCH} = \{ (C_+, C_-) \mid C_+ \cup C_- \text{ is a cycle of } G \}.$
- 4.  $\mathcal{B}_{PATH} = \{(P_1, P_2) \mid P_1, P_2 \text{ are two disjoint paths of } G \text{ with same endpoints} \}.$

In addition, we have  $\operatorname{width}(\mathcal{B}_{\text{Multi}}) = 2$ ,  $\operatorname{width}(\mathcal{B}_{\text{MATROID}}) = 2$ ,  $\operatorname{width}(\mathcal{B}_{\text{MATROID}}) = |V|$  and  $\operatorname{width}(\mathcal{B}_{\text{PATH}}) = |V|$ . This means that  $\operatorname{width}(\mathcal{M}_{\text{Multi}}) \leq 2$ ,  $\operatorname{width}(\mathcal{M}_{\text{MATROID}}) \leq 2$ ,  $\operatorname{width}(\mathcal{M}_{\text{MATROID}}) \leq |V|$  and  $\operatorname{width}(\mathcal{M}_{\text{PATH}}) \leq |V|$ .

We illustrate these exchanges classes in Figure 1. The construction for MULTI problem is straightforward. For MATROID problem, we leverage the basis exchange property of matroids (see Lemma 13 in the supplementary material). And for MATCH and PATH problems, we use standard graph-theoretical properties of matchings and paths. A detailed proof of Fact 1 is deferred to the supplementary material.

**Main result.** Our main result is a problem-dependent sample complexity bound of the CGapExp algorithm. In particular, we show that CGapExp returns the optimal set with high probability and uses at most  $\tilde{O}(\operatorname{width}(\mathcal{M})^2\mathbf{H})$  samples.

**Theorem 1.** Given any  $\delta \in (0,1)$ , any  $\mathcal{M} \subseteq 2^{[n]}$  and any  $\mathbf{w} \in \mathbb{R}^n$ . Assume that the reward distribution  $\varphi_e$  for each arm  $e \in [n]$  is R-sub-Gaussian with mean w(e). Set  $\mathrm{rad}_t(e) = R\sqrt{\frac{2\log\left(\frac{4nt^2}{\delta}\right)}{T_e(t)}}$  for all t > 0 and  $e \in [n]$ . Then, with probability at least  $1 - \delta$ , the CGapExp algorithm (Algorithm 1) returns the optimal set  $\mathrm{Out} = M_*$  and

$$T \le O\left(R^2 \operatorname{width}(\mathcal{M})^2 \mathbf{H} \log \left(R^2 \operatorname{width}(\mathcal{M})^2 \mathbf{H} \cdot n/\delta\right)\right),\tag{4}$$

where T denotes the number of samples used by Algorithm 1 and  $\mathbf{H}$  is defined in Eq. (2).

**Remarks.** For the MULTI problem, we see that Fact 1 shows that width(MULTI) = O(1). Therefore, the sample complexity bound of CGapExp is  $O(\mathbf{H} \log(n\mathbf{H}/\delta))$  for this problem. This

matches the previous problem-dependent bounds for the MULTI problem [2, 1]. For the MATROID problem, we know that width(MATROID) = O(1) and hence the sample complexity is also  $O(\mathbf{H}\log(n\mathbf{H}/\delta))$ . For MATCH and PATH problem, we see that the sample complexity is bounded by  $\tilde{O}(|V|^2\mathbf{H})$ .

### 4 Lower Bound

In this section, we present a problem-dependent lower bound on the sample complexity of the ExpCMAB problem. To state our results, we first define the notion of  $\delta$ -correct algorithm as follows. For any  $\delta \in (0,1)$ , we call an algorithm  $\mathbb A$  a  $\delta$ -correct algorithm if, for any expected reward  $\boldsymbol w \in \mathbb R^n$ , the probability of error of  $\mathbb A$  is at most  $\delta$ , i.e.  $\Pr[M_* \neq \operatorname{Out}] \leq \delta$ , where  $\operatorname{Out}$  is the output of algorithm  $\mathbb A$ .

We show that, for any family of feasible solutions  $\mathcal{M}$  and any expected rewards  $\boldsymbol{w}$ , any  $\delta$ -correct algorithm  $\mathbb{A}$  must use at least  $\Omega(\mathbf{H}\log(1/\delta))$  samples in expectation.

**Theorem 2.** Fix any  $\mathcal{M} \subseteq 2^{[n]}$  and any vector  $\mathbf{w} \in \mathbb{R}^n$ . Suppose that, for each arm  $e \in [n]$ , the reward distribution  $\varphi_e$  is given by  $\varphi_e = \mathcal{N}(w(e), 1)$ , where  $\mathcal{N}(\mu, \sigma^2)$  denotes a Gaussian distribution with mean  $\mu$  and variance  $\sigma^2$ . Then, for any  $\delta \in (0, e^{-16}/4)$  and any  $\delta$ -correct algorithm  $\mathbb{A}$ , we have

$$\mathbb{E}[T] \ge \frac{1}{16} \mathbf{H} \log \left( \frac{1}{4\delta} \right), \tag{5}$$

where T denote the number of total samples used by algorithm  $\mathbb{A}$  and  $\mathbf{H}$  is defined in Eq. (2).

Theorem 2 resolves the conjecture of Kalyanakrishnan et al. [2] that the lower bound of sample complexity of MULTI problem is  $\Omega(\mathbf{H}\log(1/\delta))$ . In addition, our upper bound Theorem 1 shows that, for MULTI and MATROID, the sample complexity of CGapExp is  $O(\mathbf{H}\log(n\mathbf{H}/\delta))$ . Hence, we see that the CGapExp algorithm achieves the optimal sample complexity within logarithmic factors for these two problems.

On the other hand, for general combinatorial problems with non-constant widths, we see that there is a gap of  $\tilde{\Theta}(\operatorname{width}(\mathcal{M})^2)$  between the upper bound Eq. (4) and the lower bound Eq. (5). Ignoring the logarithmic factors, this gap only depends on the underlying combinatorial structure of  $\mathcal{M}$ . This suggests that the sample complexity of CGapExp has an optimal dependency on the hardness  $\mathbf{H}$  up to logarithmic factors for general combinatorial problems. Furthermore, we conjecture that the sample complexity lower bound might intrinsically depend on the size of exchange sets which is bounded by width( $\mathcal{M}$ ). We provide evidence on this conjecture which lower bounds the sample complexity of exploration on exchange sets in the supplementary material.

## 5 Extensions

CGapExp is a general and flexible learning algorithm for the ExpCMAB problem. In this section, we present two extensions to CGapExp that allow it to work in the fixed budget setting and PAC learning setting.

## 5.1 Fixed Budget Setting

We can extend the CGapExp algorithm to the fixed budget setting using two simple modifications: (1) requiring CGapExp to terminate after T rounds; and (2) using a different construction of confidence intervals. The first modification ensures that CGapExp uses at most T samples, which meets the requirement of the fixed budget setting. And the second modification bounds the probability that the confidence intervals are valid for all arms in T rounds. The following theorem shows that the probability of error of the modified CGapExp is bounded by  $O\left(Tn\exp\left(\frac{-T}{\operatorname{width}(\mathcal{M})^2\mathbf{H}}\right)\right)$ .

**Theorem 3.** Use the same notations as in Theorem 1. Given T > n and parameter  $\alpha > 0$ , set the confidence radius  $\mathrm{rad}_t(e) = R\sqrt{\frac{\alpha}{T_e(t)}}$  for all arms  $e \in [n]$  and all t > 0. Run CGapExp algorithm

for at most T rounds. Then, for  $0 \le \alpha \le \frac{1}{9}(T-n)\left(R^2\operatorname{width}(\mathcal{M})^2\mathbf{H}\right)^{-1}$ , we have  $\Pr\left[\operatorname{Out} \ne M_*\right] \le 2Tn\exp\left(-2\alpha\right). \tag{6}$ 

The right-hand side of Eq. (6) equals to  $O\left(Tn\exp\left(\frac{-T}{\operatorname{width}(\mathcal{M})^2\mathbf{H}}\right)\right)$  when parameter  $\alpha=O(T\mathbf{H}^{-1}\operatorname{width}(\mathcal{M})^{-2})$ . For MULTI problem, we see that this matches the guarantees of the previous fixed budget algorithm due to Gabillon et al. [1].

## 5.2 PAC Learning

Now we consider a setting where the learner is only required to report an approximately optimal set of arms. More specifically, we consider the notion of  $(\epsilon, \delta)$ -PAC algorithm. Formally, an algorithm  $\mathbb{A}$  is called an  $(\epsilon, \delta)$ -PAC algorithm if its output Out satisfies  $\Pr\left[w(M_*) - w(\mathsf{Out}) > \epsilon\right] \leq \delta$ .

We show that a simple modification on the CGapExp algorithm gives an  $(\epsilon, \delta)$ -PAC algorithm, with guarantees similar to Theorem 1. In fact, the only modification needed is to change the stopping condition from  $\tilde{w}_t(\tilde{M}_t) \leq \tilde{w}_t(M_t)$  to  $w(\tilde{M}_t) - w(M_t) \leq \epsilon$  on line 15 of Algorithm 1. We let CGapExpPAC denote the modified algorithm. In the following theorem, we show that CGapExpPAC is indeed an  $(\epsilon, \delta)$ -PAC algorithm and has sample complexity similar to CGapExp.

**Theorem 4.** Use the same notations as in Theorem 1. Fix  $\delta \in (0,1)$  and  $\epsilon \geq 0$ . Then, with probability at least  $1-\delta$ , the output Out of CGapExpPAC satisfies  $w(M_*)-w(Out) \leq \epsilon$ . In addition, the number of samples T used by the algorithm satisfies

$$T \le O\left(R^2 \sum_{e \in [n]} \min\left\{\frac{\operatorname{width}(\mathcal{M})^2}{\Delta_e^2}, \frac{K^2}{\epsilon^2}\right\} \log\left(\frac{R^2 n}{\delta} \sum_{e \in [n]} \min\left\{\frac{\operatorname{width}(\mathcal{M})^2}{\Delta_e^2}, \frac{K^2}{\epsilon^2}\right\}\right)\right), (7)$$

where  $K = \max_{M \in \mathcal{M}} |M|$  is the size of the largest feasible solution.

We see that the sample complexity of CGapExpPAC decreases when  $\epsilon$  increases. And if  $\epsilon=0$ , the sample complexity Eq. (7) of CGapExpPAC equals to that of CGapExp.

There are several PAC algorithms for the MULTI problem in the literature with different guarantees [2, 3, 1]. Zhou et al. [3] proposed an  $(\epsilon, \delta)$ -PAC algorithm for the MULTI problem with a problem-independent sample complexity bound of  $O(\frac{K^2n}{\epsilon^2} + \frac{Kn\log(1/\delta)}{\epsilon^2})$ . If we ignore logarithmic factors, then the sample complexity bound of CGapExpPAC for the MULTI problem is better than theirs  $\tilde{O}(\sum_{e \in [n]} \min\{\Delta_e^{-2}, K^2\epsilon^{-2}\}) \leq \tilde{O}(nK^2\epsilon^{-2})$ . On the other hand, the algorithms of Kalyanakrishnan et al. [2] and Gabillon et al. [1] guarantee to find K arms such that each of them is better than the K-th optimal arm within a factor of  $\epsilon$  with probability  $1-\delta$ . Unless  $\epsilon=0$ , their guarantee is different from ours which concerns the optimality of the sum of K arms.

<sup>&</sup>lt;sup>1</sup>We notice that Zhou et al. [3] allow an  $(\epsilon', \delta)$ -PAC algorithm to produce an output with *average* sub-optimality of  $\epsilon'$ . This is equivalent to our definition of  $(\epsilon, \delta)$ -PAC algorithm with  $\epsilon = K\epsilon'$ .

# References

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- [2] Shivaram Kalyanakrishnan, Ambuj Tewari, Peter Auer, and Peter Stone. Pac subset selection in stochastic multi-armed bandits. In *ICML*, pages 655–662, 2012.
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# **A** Proof of Main Result

In this section, we prove our main result: Theorem 1.

**Notations.** We need some additional notations for our analysis. For any set  $a \subseteq [n]$ , let  $\chi_a \in \{0,1\}^n$  denote the incidence vector of set  $a \subseteq [n]$ , i.e.  $\chi_a(e) = 1$  if and only if  $e \in a$ . For an exchange set  $b = (b_+, b_-)$ , we define  $\chi_b \triangleq \chi_{b_+} - \chi_{b_-}$  as the incidence vector of b. We notice that  $\chi_b \in \{-1, 0, 1\}^n$ .

For each round t, we define vector  $\mathbf{rad}_t = (\mathrm{rad}_t(1), \ldots, \mathrm{rad}_t(n))^T$  and recall that  $\bar{\boldsymbol{w}}_t \in \mathbb{R}^n$  is the empirical mean rewards of arms up to round t.

Let  $u \in \mathbb{R}^n$  and  $v \in \mathbb{R}^n$  be two vectors. Let  $\langle u, v \rangle$  denote the inner product of u and v. We define  $u \circ v \triangleq \big(u(1) \cdot v(1), \dots, u(n) \cdot v(n)\big)^T$  as the element-wise product of u and v. For any  $s \in \mathbb{R}$ , we also define  $u^s \triangleq \big(u(1)^s, \dots, u(n)^s)^T$  as the element-wise exponentiation of u. Let  $|u| = \big(|u(1)|, \dots, |u(n)|\big)^T$  denote the element-wise absolute value of u.

## A.1 Preparatory Lemmas

**Lemma 1.** Let  $M_1 \subseteq [n]$  be a set. Let  $b = (b_+, b_-)$  be an exchange set such that  $b_- \subseteq M_1$  and  $b_+ \cap M_1 = \emptyset$ . Define  $M_2 = M_1 \oplus b$ . Then, we have

$$\chi_{M_1} + \chi_b = \chi_{M_2}.$$

*Proof.* Recall that  $M_2 = M_1 \setminus b_- \oplus b_+$  and  $b_+ \cap b_- = \emptyset$ . Therefore we see that  $M_2 \setminus M_1 = b_+$  and  $M_1 \setminus M_2 = b_-$ . Then, we decompose  $\chi_{M_1}$  as  $\chi_{M_1} = \chi_{M_1 \setminus M_2} + \chi_{M_1 \cap M_2}$ . Hence, we have

$$egin{aligned} m{\chi}_{M_1} + m{\chi}_b &= m{\chi}_{M_1 \setminus M_2} + m{\chi}_{M_1 \cap M_2} + m{\chi}_{b_+} - m{\chi}_{b_-} \ &= m{\chi}_{M_1 \cap M_2} + m{\chi}_{M_2 \setminus M_1} \ &= m{\chi}_{M_2}. \end{aligned}$$

**Lemma 2.** Let  $\mathcal{M} \subseteq 2^{[n]}$  and  $\mathcal{B}$  be an exchange class for  $\mathcal{M}$ . Then, for any two different elements M, M' of  $\mathcal{M}$  and any  $e \in (M \setminus M') \cup (M' \setminus M)$ , there exists an exchange set  $b = (b_+, b_-) \in \mathcal{B}$  such that  $e \in (b_+ \cup b_-)$ ,  $b_- \subseteq (M \setminus M')$ ,  $b_+ \subseteq (M' \setminus M)$ ,  $(M \oplus b) \in \mathcal{M}$  and  $(M' \oplus b) \in \mathcal{M}$ . Moreover, if  $M' = M_*$ , then we have  $\langle \boldsymbol{w}, \boldsymbol{\chi}_b \rangle \geq \Delta_e > 0$ , where  $\Delta_e$  is the gap defined in Eq. (1).

*Proof.* We decompose our proof into two cases.

Case (1):  $e \in M \backslash M'$ .

By the definition of exchange class, we know that there exists  $b = (b_+, b_-) \in \mathcal{B}$  which satisfies that  $e \in b_-, b_- \subseteq (M \setminus M'), b_+ \subseteq (M' \setminus M), (M \oplus b) \in \mathcal{M}$  and  $(M' \ominus b) \in \mathcal{M}$ .

Next, if  $M'=M_*$ , we see that  $e\not\in M_*$ . Let us consider the set  $M_1=\arg\max_{M':M'\in\mathcal{M}\wedge e\in M'}w(M')$ . Also define  $M_0=M_*\ominus b$ . We have already proved that  $M_0\in\mathcal{M}$ . Combining with the fact that  $e\in M_0$ , we see that  $w(M_0)\leq w(M_1)$ . Therefore, we obtain that  $w(M_*)-w(M_0)\geq w(M_*)-w(M_1)=\Delta_e$ . Notice that the left-hand side of the former inequality can be rewritten using Lemma 1 as follows

$$w(M_*) - w(M_0) = \langle \boldsymbol{w}, \boldsymbol{\chi}_{M_*} \rangle - \langle \boldsymbol{w}, \boldsymbol{\chi}_{M_0} \rangle = \langle \boldsymbol{w}, \boldsymbol{\chi}_{M_*} - \boldsymbol{\chi}_{M_0} \rangle = \langle \boldsymbol{w}, \boldsymbol{\chi}_b \rangle.$$

Therefore, we obtain  $\langle \boldsymbol{w}, \boldsymbol{\chi}_b \rangle \geq \Delta_e$ .

Case (2):  $e \in M' \setminus M$ .

Using the definition of exchange class, we see that there exists  $c = (c_+, c_-) \in \mathcal{B}$  such that  $e \in c_-$ ,  $c_- \subseteq (M' \setminus M), c_+ \subseteq (M \setminus M'), (M' \oplus c) \in \mathcal{M}$  and  $(M \ominus c) \in \mathcal{M}$ .

We construct  $b=(b_+,b_-)$  by setting  $b_+=c_-$  and  $b_-=c_+$ . Notice that, by the construction of b, we have  $M\oplus b=M\oplus c$  and  $M'\oplus b=M'\oplus c$ . Therefore, it is clear that b satisfies the requirement of the lemma.

Now, suppose that  $M'=M_*$ . In this case, we have  $e\in M_*$ . Consider the set  $M_3=\arg\max_{M':M'\in\mathcal{M}\wedge e\not\in M'}w(M')$ . We see that  $w(M_*)-w(M_3)=\Delta_e$ . Define  $M_2=M_*\ominus b$  and notice that  $M_2\in\mathcal{M}$ . Combining with the fact that  $e\not\in M_2$ , we obtain that  $w(M_2)\leq w(M_3)$ . Hence, we have  $w(M_*)-w(M_2)\geq w(M_*)-w(M_3)=\Delta_e$ . Similar to Case (1), applying Lemma 1 again, we have

$$\langle \boldsymbol{w}, \boldsymbol{\chi}_b \rangle = w(M_*) - w(M_2) \ge \Delta_e.$$

**Lemma 3.** Let M and M' be two sets. Then, we have

$$\max_{e \in (M \setminus M') \cup (M' \setminus M)} \operatorname{rad}_t(e) = \left\| \operatorname{\mathbf{rad}}_t \circ \left| \chi_{M'} - \chi_M \right| \right\|_{\infty}.$$

*Proof.* Notice that  $\chi_{M'} - \chi_M = \chi_{M' \setminus M} - \chi_{M \setminus M'}$ . In addition, since  $(M' \setminus M) \cap (M \setminus M') = \emptyset$ , we have  $\chi_{M' \setminus M} \circ \chi_{M \setminus M'} = \mathbf{0}_n$ . Also notice that  $\chi_{M' \setminus M} - \chi_{M \setminus M'} \in \{-1, 0, 1\}^n$ . Therefore, we have

$$\begin{aligned} |\chi_{M'\setminus M} - \chi_{M\setminus M'}| &= (\chi_{M'\setminus M} - \chi_{M\setminus M'})^2 \\ &= \chi_{M'\setminus M}^2 + \chi_{M\setminus M'}^2 + 2\chi_{M'\setminus M} \circ \chi_{M\setminus M'} \\ &= \chi_{M'\setminus M} + \chi_{M\setminus M'} \\ &= \chi_{(M'\setminus M)\cup (M\setminus M')}, \end{aligned}$$

where the third equation follows from the fact that  $\chi_{M\setminus M'} \in \{0,1\}^n$  and  $\chi_{M'\setminus M} \in \{0,1\}^n$ . The lemma follows immediately from the fact that  $\operatorname{rad}_t(e) \geq 0$  and  $\chi_{(M\setminus M')\cup (M'\setminus M)} \in \{0,1\}^n$ .

**Lemma 4.** Let  $a, b, c \in \mathbb{R}^n$  be three vectors. Then, we have  $\langle a, b \circ c \rangle = \langle a \circ b, c \rangle$ .

*Proof.* We have

$$\langle \boldsymbol{a}, \boldsymbol{b} \circ \boldsymbol{c} \rangle = \sum_{i=1}^{n} a(i) \big( b(i) c(i) \big) = \sum_{i=1}^{n} \big( a(i) b(i) \big) c(i) = \langle \boldsymbol{a} \circ \boldsymbol{b}, \boldsymbol{c} \rangle.$$

**Lemma 5.** Let  $M_t$  and  $\tilde{w}_t$  be defined in Algorithm 1. Let  $M' \in \mathcal{M}$  be a feasible set. We have

$$ilde{w}_t(M') - ilde{w}_t(M_t) = \left\langle ilde{m{w}}_t, m{\chi}_{M'} - m{\chi}_{M_t} 
ight
angle = \left\langle ar{m{w}}_t, m{\chi}_{M'} - m{\chi}_{M_t} 
ight
angle + \left\langle \mathbf{rad}_t, |m{\chi}_{M'} - m{\chi}_{M_t}| 
ight
angle.$$

*Proof.* We begin with proving the first part. It is easy to verify that  $\tilde{w}_t = \bar{w}_t + \mathbf{rad}_t \circ (\mathbf{1}_n - 2\chi_{M_t})$ . Then, we have

$$\langle \tilde{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}} \rangle = \langle \bar{\boldsymbol{w}}_{t} + \operatorname{\mathbf{rad}}_{t} \circ (1 - 2\boldsymbol{\chi}_{M_{t}}), \ \boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}} \rangle$$

$$= \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}} \rangle + \langle \operatorname{\mathbf{rad}}_{t}, (\mathbf{1}_{n} - 2\boldsymbol{\chi}_{M_{t}}) \circ (\boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}}) \rangle$$

$$= \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}} \rangle + \langle \operatorname{\mathbf{rad}}_{t}, \boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}} - 2\boldsymbol{\chi}_{M_{t}} \circ \boldsymbol{\chi}_{M'} + 2\boldsymbol{\chi}_{M_{t}}^{2} \rangle$$

$$= \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}} \rangle + \langle \operatorname{\mathbf{rad}}_{t}, \boldsymbol{\chi}_{M'}^{2} - \boldsymbol{\chi}_{M_{t}}^{2} - 2\boldsymbol{\chi}_{M_{t}} \circ \boldsymbol{\chi}_{M'} + 2\boldsymbol{\chi}_{M_{t}}^{2} \rangle$$

$$= \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}} \rangle + \langle \operatorname{\mathbf{rad}}_{t}, (\boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}})^{2} \rangle$$

$$= \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}} \rangle + \langle \operatorname{\mathbf{rad}}_{t}, |\boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}} | \rangle,$$

$$(10)$$

where Eq. (8) follows from Lemma 4; Eq. (9) holds since  $\chi_{M'} \in \{0,1\}^n$  and  $\chi_{M_t} \in \{0,1\}^n$  and therefore  $\chi_{M'} = \chi_{M'}^2$  and  $\chi_{M_t} = \chi_{M_t}^2$ ; and Eq. (10) follows since  $\chi_{M'} - \chi_{M_t} \in \{-1,0,1\}^n$ .

## A.2 Confidence Intervals

 For all t > 0, we define random event  $\xi_t$  as follows

$$\xi_t = \left\{ \forall i \in [n], \quad |w(i) - \bar{w}_t(i)| \le \operatorname{rad}_t(i) \right\}. \tag{11}$$

We notice that random event  $\xi_t$  characterizes the event that the confidence bounds of all arms are valid at round t.

If the confidence bounds are valid, we can generalize Eq. (11) to inner products as follows.

**Lemma 6.** Given any t > 0, assume that event  $\xi_t$  as defined in Eq. (11) occurs. Then, for any vector  $a \in \mathbb{R}^n$ , we have

$$\left| \left\langle oldsymbol{w}, oldsymbol{a} 
ight
angle - \left\langle ar{oldsymbol{w}}_t, oldsymbol{a} 
ight
angle \left| \leq \left\langle \operatorname{\mathbf{rad}}_t, \left| oldsymbol{a} 
ight| 
ight
angle.$$

*Proof.* Suppose that  $\xi$  occurs. Then, we have

$$\left| \langle \boldsymbol{w}, \boldsymbol{a} \rangle - \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{a} \rangle \right| = \left| \langle \boldsymbol{w} - \bar{\boldsymbol{w}}_{t}, \boldsymbol{a} \rangle \right|$$

$$= \left| \sum_{i=1}^{n} \left( w(i) - \bar{w}_{t}(i) \right) a(i) \right|$$

$$\leq \sum_{i=1}^{n} \left| w(i) - \bar{w}_{t}(i) \right| |a(i)|$$

$$\leq \sum_{i=1}^{n} \operatorname{rad}_{t}(i) \cdot |a(i)|$$

$$= \langle \operatorname{rad}_{t}, |\boldsymbol{a}| \rangle,$$
(12)

where Eq. (12) follows the definition of event  $\xi_t$  in Eq. (11) and the assumption that it occurs.  $\Box$ 

Next, we construct the high probability confidence intervals for the fixed confidence setting.

**Lemma 7.** Suppose that the reward distribution  $\varphi_e$  is a R-sub-Gaussian distribution for all  $e \in [n]$ . And if, for all t > 0 and all  $e \in [n]$ , the confidence radius  $rad_t(e)$  is given by

$$\operatorname{rad}_{t}(e) = R\sqrt{\frac{2\log\left(\frac{4nt^{2}}{\delta}\right)}{T_{e}(t)}},$$

where  $T_e(t)$  is the number of samples of arm e up to round t. Then, we have

$$\Pr\left[\bigcap_{t=1}^{\infty} \xi_t\right] \ge 1 - \delta.$$

*Proof.* For any t>0 and  $e\in[n]$ , notice  $\varphi_e$  is a R-sub-Gaussian distribution with mean w(e) and  $w_t(e)$  is the empirical mean of  $\varphi_e$  for  $T_e(t)$  samples. Using Hoeffding's inequality (see Lemma 14 in Section D), we obtain

$$\Pr\left|\left|\bar{w}_t(e) - w(e)\right| \ge R\sqrt{\frac{2\log\left(\frac{4nt^2}{\delta}\right)}{T_e(t)}}\right| \le \frac{\delta}{2nt^2}.$$

By union bound over all  $e \in [n]$ , we see that  $\Pr[\xi_t] \ge 1 - \frac{\delta}{2t^2}$ . Using a union bound again over all t > 0, we have

$$\Pr\left[\bigcap_{t=1}^{\infty} \xi_t\right] \ge 1 - \sum_{t=1}^{\infty} \Pr[\neg \xi_t]$$

$$\ge 1 - \sum_{t=1}^{\infty} \frac{\delta}{2t^2}$$

$$= 1 - \frac{\pi^2}{12} \delta \ge 1 - \delta.$$

#### A.3 Main Lemmas

**Lemma 8.** Given any t > 0, assume that event  $\xi_t$  (defined in Eq. (11)) occurs. Then, if Algorithm 1 terminates at round t, we have  $M_t = M_*$ .

*Proof.* Suppose that  $M_t \neq M_*$ . By definition, we have  $w(M_*) > w(M_t)$ . Rewriting the former inequality, we obtain that  $\langle w, \chi_{M_*} \rangle > \langle w, \chi_{M_t} \rangle$ .

Applying Lemma 2 by setting  $M=M_t$  and  $M'=M_*$ , we see that there exists  $b=(b_+,b_-)\in\mathcal{B}$  such that  $(M_t\oplus b)\in\mathcal{M}$ .

Now define  $M'_t = M_t \oplus b$ . Recall that  $\tilde{M}_t = \arg\max_{M \in \mathcal{M}} \tilde{w}_t(M)$  and therefore  $\tilde{w}_t(\tilde{M}_t) \geq \tilde{w}_t(M'_t)$ . Hence, we have

$$\tilde{w}_{t}(\tilde{M}_{t}) - \tilde{w}_{t}(M_{t}) \geq \tilde{w}_{t}(M_{t}') - \tilde{w}_{t}(M_{t}) 
= \left\langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{M_{t}'} - \boldsymbol{\chi}_{M_{t}} \right\rangle + \left\langle \mathbf{rad}_{t}, |\boldsymbol{\chi}_{M'} - \boldsymbol{\chi}_{M_{t}}| \right\rangle$$
(13)

$$\geq \left\langle \boldsymbol{w}, \boldsymbol{\chi}_{M_t'} - \boldsymbol{\chi}_{M_t} \right\rangle \tag{14}$$

$$= w(M_t') - w(M_t) > 0, (15)$$

where Eq. (13) follows from Lemma 5; and Eq. (14) follows the assumption that event  $\xi_t$  occurs and Lemma 6;

Therefore Eq. (15) shows that  $\tilde{w}_t(\tilde{M}_t) > \tilde{w}_t(M_t)$ . However, this contradicts to the stopping condition of CGapExp:  $\tilde{w}_t(\tilde{M}_t) \leq \tilde{w}_t(M_t)$  and the assumption that the algorithm terminates on round t.

**Lemma 9.** Given any t > 0 and suppose that event  $\xi_t$  (defined in Eq. (11)) occurs. For any  $e \in [n]$ , if  $\operatorname{rad}_t(e) < \frac{\Delta_e}{3 \operatorname{width}(\mathcal{M})}$ , then, arm e will not be pulled on round t, i.e.  $p_t \neq e$ .

*Proof.* Fix an exchange class  $\mathcal{B} \in \arg\min_{\mathcal{B}' \in \operatorname{Exchange}(\mathcal{M})} \operatorname{width}(\mathcal{B}')$ . Suppose, in the contrary, that  $p_t = e$ . By Lemma 2, there exists an exchange set  $c = (c_+, c_-) \in \mathcal{B}$  such that  $e \in (c_+ \cup c_-)$ ,  $c_- \subseteq (M_t \setminus \tilde{M}_t)$ ,  $c_+ \subseteq (\tilde{M}_t \setminus M_t)$ ,  $(M_t \oplus c) \in \mathcal{M}$  and  $(\tilde{M}_t \oplus c) \in \mathcal{M}$ .

Now, we decompose our proof into two cases.

**Case (1):**  $(e \in M_* \land e \in c_+) \lor (e \not\in M_* \land e \in c_-)$ .

Define  $M'_t = \tilde{M}_t \ominus c$  and recall that  $M'_t \in \mathcal{M}$  due to the definition of exchange class.

First, we claim that  $M'_t \neq M_*$ . Suppose that  $e \in M_*$  and  $e \in c_+$ . Then, we see that  $e \notin M'_t$  and hence  $M'_t \neq M_*$ . On the other hand, if  $e \notin M_*$  and  $e \in c_-$ , then  $e \in M'_t$  which also means that  $M'_t \neq M_*$ . Therefore we have  $M'_t \neq M_*$  in either cases.

Next, we apply Lemma 2 by setting  $M=M'_t$  and  $M'=M_*$ . We see that there exists an exchange set  $b \in \mathcal{B}$  such that,  $e \in (b_+ \cup b_-)$ ,  $(M'_t \oplus b) \in \mathcal{M}$  and  $\langle \boldsymbol{w}, \boldsymbol{\chi}_b \rangle \geq \Delta_e > 0$ .

Now, we define vectors  $d=\chi_{\tilde{M}_t}-\chi_{M_t}$ ,  $d_1=\chi_{M'_t}-\chi_{M_t}$  and  $d_2=\chi_{M'_t\oplus b}-\chi_{M_t}$ . By the definition of  $M'_t$  and Lemma 2, we see that  $d_1=d-\chi_c$  and  $d_2=d_1+\chi_b=d-\chi_c+\chi_b$ .

Then, we claim that  $\|\mathbf{rad}_t \circ (\mathbf{d} - \chi_c)\|_{\infty} < \frac{\Delta_e}{3 \operatorname{width}(\mathcal{B})}$ . Since  $c_- \subseteq M_t$  and  $c_+ \cap M_t = \emptyset$ , using standard set theoretical manipulations, we can show that  $M_t \setminus \tilde{M}_t = (M_t \setminus M_t') \cup c_-$ . Similarly, one can show that  $\tilde{M}_t \setminus M_t = (M_t' \setminus M_t) \cup c_+$ . This means that  $((M_t \setminus M_t') \cup (M_t' \setminus M_t)) \subseteq ((M_t \setminus \tilde{M}_t) \cup (\tilde{M}_t \setminus M_t))$ . Then, applying Lemma 3, we obtain

$$\begin{aligned} \|\mathbf{rad}_{t} \circ (\boldsymbol{d} - \boldsymbol{\chi}_{c})\|_{\infty} &= \left\|\mathbf{rad}_{t} \circ (\boldsymbol{\chi}_{M'_{t}} - \boldsymbol{\chi}_{M_{t}})\right\|_{\infty} \\ &= \max_{i \in (M_{t} \setminus M'_{t}) \cup (M'_{t} \setminus M_{t})} \mathrm{rad}_{t}(i) \\ &\leq \max_{i \in (M_{t} \setminus \tilde{M}_{t}) \cup (\tilde{M}_{t} \setminus M_{t})} \mathrm{rad}_{t}(i) \end{aligned}$$

$$= \operatorname{rad}_{t}(e) < \frac{\Delta_{e}}{3\operatorname{width}(\mathcal{B})}.$$
 (16)

We claim that  $\|\mathbf{rad}_t \circ \boldsymbol{\chi}_c\|_{\infty} < \frac{\Delta_e}{3 \operatorname{width}(\mathcal{B})}$ . Recall that, by the definition of c, we have  $c_+ \subseteq (\tilde{M}_t \backslash M_t)$  and  $c_- \subseteq (M_t \backslash \tilde{M}_t)$ . Hence  $c_+ \cup c_- \subseteq (\tilde{M}_t \backslash M_t) \cup (M_t \backslash \tilde{M}_t)$ . Since  $\boldsymbol{\chi}_c \in [-1,1]^n$ , we see that

$$\|\mathbf{rad}_{t} \circ |\boldsymbol{\chi}_{c}|\|_{\infty} = \max_{i \in c_{+} \cup c_{-}} \operatorname{rad}_{t}(i)$$

$$\leq \max_{i \in (\tilde{M}_{t} \setminus M_{t}) \cup (M_{t} \setminus \tilde{M}_{t})} \operatorname{rad}_{t}(i)$$

$$= \operatorname{rad}_{t}(e) < \frac{\Delta_{e}}{3 \operatorname{width}(\mathcal{B})}.$$
(17)

Next, we claim that  $d \circ \chi_c = |\chi_c|$ . Recall that  $\chi_c = \chi_{c_+} - \chi_{c_-}$  and  $d = \chi_{\tilde{M}_t} - \chi_{M_t} = \chi_{\tilde{M}_t \setminus M_t} - \chi_{M_t \setminus \tilde{M}_t}$ . We also notice that  $c_+ \subseteq (\tilde{M}_t \setminus M_t)$  and  $c_- \subseteq (M_t \setminus \tilde{M}_t)$ . This implies that  $c_+ \cap (M_t \setminus \tilde{M}_t) = \emptyset$  and  $c_- \cap (\tilde{M}_t \setminus M_t) = \emptyset$ . Therefore, we have

$$egin{aligned} oldsymbol{d} \circ oldsymbol{\chi}_c &= (oldsymbol{\chi}_{ ilde{M}_t} - oldsymbol{\chi}_{M_t \setminus ilde{M}_t}) \circ (oldsymbol{\chi}_{c_+} - oldsymbol{\chi}_{c_-}) \ &= oldsymbol{\chi}_{ ilde{M}_t \setminus ilde{M}_t} \circ oldsymbol{\chi}_{c_+} + oldsymbol{\chi}_{M_t \setminus ilde{M}_t} \circ oldsymbol{\chi}_{c_-} - oldsymbol{\chi}_{ ilde{M}_t \setminus ilde{M}_t} \circ oldsymbol{\chi}_{c_-} \\ &= oldsymbol{\chi}_{ ilde{M}_t \setminus ilde{M}_t} \circ oldsymbol{\chi}_{c_+} + oldsymbol{\chi}_{M_t \setminus ilde{M}_t} \circ oldsymbol{\chi}_{c_-} \\ &= oldsymbol{\chi}_{c_+} + oldsymbol{\chi}_{c_-} = |oldsymbol{\chi}_c|. \end{aligned}$$

where the last equality holds since  $c_+ \cap c_- = \emptyset$ .

Now, we bound quantity  $\langle \mathbf{rad}_t, |d_2| \rangle - \langle \mathbf{rad}_t, |d| \rangle$  as follows

$$\langle \mathbf{rad}_{t}, | \mathbf{d}_{2} | \rangle - \langle \mathbf{rad}_{t}, | \mathbf{d} | \rangle = \langle \mathbf{rad}_{t}, | \mathbf{d}_{2} | - | \mathbf{d} | \rangle = \langle \mathbf{rad}_{t}, \mathbf{d}_{2}^{2} - \mathbf{d}^{2} \rangle$$

$$= \langle \mathbf{rad}_{t}, (\mathbf{d} - \boldsymbol{\chi}_{c} + \boldsymbol{\chi}_{b})^{2} - \mathbf{d}^{2} \rangle$$

$$= \langle \mathbf{rad}_{t}, \boldsymbol{\chi}_{b}^{2} + \boldsymbol{\chi}_{c}^{2} - 2\boldsymbol{\chi}_{b} \circ \boldsymbol{\chi}_{c} - 2\mathbf{d} \circ \boldsymbol{\chi}_{c} + 2\mathbf{d} \circ \boldsymbol{\chi}_{b} \rangle$$

$$= \langle \mathbf{rad}_{t}, \boldsymbol{\chi}_{b}^{2} - \boldsymbol{\chi}_{c}^{2} + 2\boldsymbol{\chi}_{b} \circ (\mathbf{d} - \boldsymbol{\chi}_{c}) \rangle$$

$$= \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - 2 \langle \mathbf{rad}_{t}, \boldsymbol{\chi}_{b} \circ (\mathbf{d} - \boldsymbol{\chi}_{c}) \rangle$$

$$= \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - 2 \langle \mathbf{rad}_{t} \circ (\mathbf{d} - \boldsymbol{\chi}_{c}), \boldsymbol{\chi}_{b} \rangle$$

$$\geq \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - 2 \| \mathbf{rad}_{t} \circ (\mathbf{d} - \boldsymbol{\chi}_{c}) \|_{\infty} \| \boldsymbol{\chi}_{b} \|_{1}$$

$$> \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - \frac{2\Delta_{e}}{3 \operatorname{width}(\mathcal{B})} \| \boldsymbol{\chi}_{b} \|_{1}$$

$$\geq \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - \frac{2\Delta_{e}}{3},$$

$$\geq \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - \frac{2\Delta_{e}}{3},$$

$$\geq \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - \frac{2\Delta_{e}}{3},$$

$$\geq \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - \frac{2\Delta_{e}}{3},$$

$$\geq \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - \frac{2\Delta_{e}}{3},$$

$$\geq \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{b} | \rangle - \langle \mathbf{rad}_{t}, | \boldsymbol{\chi}_{c} | \rangle - \frac{2\Delta_{e}}{3},$$

where Eq. (18) holds since  $d \in \{-1,0,1\}^n$  and  $d_2 \in \{-1,0,1\}^n$ ; Eq. (19) follows from the claim that  $d \circ \chi_c = |\chi_c| = \chi_c^2$ ; Eq. (20) and Eq. (21) follow from Lemma 4 and Hölder's inequality; Eq. (22) follows from Eq. (16); and Eq. (23) holds since  $b \in \mathcal{B}$  and  $\|\chi_b\|_1 = |b_+| + |b_-| \leq \operatorname{width}(\mathcal{B})$ .

Applying Lemma 5 by setting  $M' = M'_t \oplus b$  and using the fact that  $\tilde{w}_t(\tilde{M}_t) \geq \tilde{w}_t(M'_t \oplus b)$ , we have

$$\begin{split} \langle \bar{\boldsymbol{w}}_t, \boldsymbol{d} \rangle + \langle \mathbf{rad}_t, |\boldsymbol{d}| \rangle &= \left\langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_{\tilde{M}_t} - \boldsymbol{\chi}_{M_t} \right\rangle + \left\langle \mathbf{rad}_t, |\boldsymbol{\chi}_{\tilde{M}_t} - \boldsymbol{\chi}_{M_t}| \right\rangle \\ &= \tilde{w}_t(\tilde{M}_t) - \tilde{w}_t(M_t) \\ &\geq \tilde{w}_t(M_t' \oplus b) - \tilde{w}_t(M_t) \\ &= \left\langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_{M_t' \oplus b} - \boldsymbol{\chi}_{M_t} \right\rangle + \left\langle \mathbf{rad}_t, |\boldsymbol{\chi}_{M_t' \oplus b} - \boldsymbol{\chi}_{M_t}| \right\rangle \\ &= \langle \bar{\boldsymbol{w}}_t, \boldsymbol{d}_2 \rangle + \langle \mathbf{rad}_t, |\boldsymbol{d}_2| \rangle \\ &= \langle \bar{\boldsymbol{w}}_t, \boldsymbol{d} \rangle - \langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_c \rangle + \langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_b \rangle + \langle \mathbf{rad}_t, |\boldsymbol{d}_2| \rangle, \end{split}$$

where the last equality follows from the fact that  $d_2 = d - \chi_c + \chi_b$ . Rearranging the above inequality, we obtain

$$\langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{c} \rangle \geq \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{b} \rangle + \langle \mathbf{rad}_{t}, |\boldsymbol{d}_{2}| \rangle - \langle \mathbf{rad}_{t}, |\boldsymbol{d}| \rangle$$

$$\geq \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{b} \rangle + \langle \mathbf{rad}_{t}, |\boldsymbol{\chi}_{b}| \rangle - \langle \mathbf{rad}_{t}, |\boldsymbol{\chi}_{c}| \rangle - \frac{2\Delta_{e}}{3}$$
(24)

$$>\langle \boldsymbol{w}, \boldsymbol{\chi}_b \rangle - \langle \mathbf{rad}_t, \boldsymbol{\chi}_c \rangle - \frac{2\Delta_e}{3}$$
 (25)

$$>\langle w, \chi_b \rangle - \frac{\Delta_e}{3} - \frac{2\Delta_e}{3}$$
 (26)

$$= \langle \boldsymbol{w}, \boldsymbol{\chi}_b \rangle - \Delta_e \ge 0, \tag{27}$$

where Eq. (24) uses Eq. (23); Eq. (25) follows from the assumption that event  $\xi_t$  occurs and Lemma 6; and Eq. (25) holds since Eq. (17).

We have shown that  $\langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_c \rangle > 0$ . Now we can bound  $\bar{w}_t(M_t')$  as follows

$$\bar{w}_t(M_t') = \left\langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_{M_t'} \right\rangle = \left\langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_{M_t} + \boldsymbol{\chi}_c \right\rangle = \left\langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_{M_t} \right\rangle + \left\langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_c \right\rangle > \left\langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_{M_t} \right\rangle = w_t(M_t).$$

However, the definition of  $M_t$  ensures that  $M_t = \arg \max_{M \in \mathcal{M}} \bar{w}_t(M)$ , i.e.  $\bar{w}_t(M_t) \geq \bar{w}_t(M_t')$ . Contradiction.

**Case (2):**  $(e \in M_* \land e \in c_-) \lor (e \not\in M_* \land e \in c_+)$ .

 First, we claim that  $\tilde{M}_t \neq M_*$ . Suppose that  $e \in M_*$  and  $e \in c_-$ . Then, we see that  $e \notin \tilde{M}_t$ , which implies that  $\tilde{M}_t \neq M_*$ . If  $e \notin M_*$  and  $e \in c_+$ , then  $e \in \tilde{M}_t$ , which also implies that  $\tilde{M}_t \neq M_*$ . Therefore we have  $\tilde{M}_t \neq M_*$  in either cases.

Hence, by Lemma 2, there exists an exchange set  $b=(b_+,b_-)\in\mathcal{B}$  such that  $e\in(b_+\cup b_-),b_-\subseteq(\tilde{M}_t\backslash M_*),b_+\subseteq(M_*\backslash \tilde{M}_t)$  and  $(\tilde{M}_t\oplus b)\in\mathcal{M}$ . Lemma 2 also indicates that  $\langle \boldsymbol{w},\boldsymbol{\chi}_b\rangle\geq\Delta_e>0$ .

Next, we define vectors  $d=\chi_{\tilde{M}_t}-\chi_{M_t}$  and  $d_1=\chi_{\tilde{M}_t\oplus b}-\chi_{M_t}$ . Notice that Lemma 2 gives that  $d_1=d+b$ .

Then, we apply Lemma 3 by setting  $M=M_t$  and  $M'=\tilde{M}_t$ . This shows that

$$\|\mathbf{rad}_t \circ \mathbf{d}\|_{\infty} \le \max_{i:(\tilde{M}_t \setminus M_t) \cup (M_t \setminus \tilde{M}_t)} \mathrm{rad}_t(i) = \mathrm{rad}_t(e) < \frac{\Delta_e}{3}.$$
 (28)

Now, we bound quantity  $\langle \bar{w}_t, d_1 \rangle + \langle \mathbf{rad}_t, |d_1| \rangle - \langle \bar{w}_t, d \rangle - \langle \mathbf{rad}_t, |d| \rangle$  as follows

$$\langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{d}_{1} \rangle + \langle \operatorname{rad}_{t}, |\boldsymbol{d}_{1}| \rangle - \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{d} \rangle - \langle \operatorname{rad}_{t}, |\boldsymbol{d}| \rangle = \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{b} \rangle + \langle \operatorname{rad}_{t}, |\boldsymbol{d}_{1}| - |\boldsymbol{d}| \rangle$$

$$= \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{b} \rangle + \langle \operatorname{rad}_{t}, d_{1}^{2} - d^{2} \rangle \qquad (29)$$

$$= \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{b} \rangle + \langle \operatorname{rad}_{t}, 2\boldsymbol{d} \circ \boldsymbol{\chi}_{b} + \boldsymbol{\chi}_{b}^{2} \rangle \qquad (30)$$

$$= \langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{b} \rangle + \langle \operatorname{rad}_{t}, \boldsymbol{\chi}_{b}^{2} \rangle + 2 \langle \operatorname{rad}_{t} \circ \boldsymbol{d}, \boldsymbol{\chi}_{b} \rangle$$

$$\geq \langle \boldsymbol{w}, \boldsymbol{\chi}_{b} \rangle - 2 \langle \operatorname{rad}_{t} \circ \boldsymbol{d}, \boldsymbol{\chi}_{b} \rangle \qquad (31)$$

$$\geq \langle \boldsymbol{w}, \boldsymbol{\chi}_{b} \rangle - 2 \| \operatorname{rad}_{t} \circ \boldsymbol{d} \|_{\infty} \| \boldsymbol{\chi}_{b} \|_{1} \qquad (32)$$

$$> \langle \boldsymbol{w}, \boldsymbol{\chi}_{b} \rangle - \frac{2\Delta_{e}}{3} \qquad (33)$$

$$> 0, \qquad (34)$$

where Eq. (29) follows from the fact that  $d_1 \in \{-1,0,1\}^n$  and  $d \in \{-1,0,1\}^n$ ; Eq. (30) holds since  $d_1 = d + \chi_b$ ; Eq. (31) follows from the assumption that  $\xi_t$  occurs and Lemma 6; Eq. (32) follows from Lemma 4 and Hölder's inequality; and Eq. (33) is due to Eq. (28).

Therefore, we have proved that  $\langle \bar{\boldsymbol{w}}_t, \boldsymbol{d} \rangle + \langle \mathbf{rad}_t, |\boldsymbol{d}| \rangle < \langle \bar{\boldsymbol{w}}_t, \boldsymbol{d}_1 \rangle + \langle \mathbf{rad}_t, |\boldsymbol{d}_1| \rangle$ . However, Lemma 5 shows that

$$egin{aligned} \langle ar{m{w}}_t, m{d} 
angle + \langle \mathbf{rad}_t, |m{d}| 
angle &= \left\langle ar{m{w}}_t, m{\chi}_{ ilde{M}_t} - m{\chi}_{M_t} 
ight
angle + \left\langle \mathbf{rad}_t, |m{\chi}_{ ilde{M}_t} - m{\chi}_{M_t}| 
ight
angle \\ &= ilde{w}_t( ilde{M}_t) - ilde{w}_t(M_t) \end{aligned}$$

$$\geq \tilde{w}_t(\tilde{M}_t \oplus b) - \tilde{w}_t(M_t)$$

$$= \langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_{\tilde{M}_t \oplus b} - \boldsymbol{\chi}_{M_t} \rangle + \langle \mathbf{rad}_t, |\boldsymbol{\chi}_{\tilde{M}_t \oplus b} - \boldsymbol{\chi}_{M_t}| \rangle$$

$$= \langle \bar{\boldsymbol{w}}_t, \boldsymbol{d}_1 \rangle + \langle \mathbf{rad}_t, |\boldsymbol{d}_1| \rangle.$$

This is a contradiction and therefore  $p_t \neq e$ .

#### A.4 Proof of Theorem 1

Theorem 1 is now a straightforward corollary of Lemma 8 and Lemma 9. For the readers' convenience, we first restate Theorem 1 in the following.

**Theorem 1.** Given any  $\delta \in (0,1)$ , any  $\mathcal{M} \subseteq 2^{[n]}$  and any  $\mathbf{w} \in \mathbb{R}^n$ . Assume that the reward distribution  $\varphi_e$  for each arm  $e \in [n]$  is R-sub-Gaussian with mean w(e). Set  $\mathrm{rad}_t(e) = R\sqrt{\frac{2\log\left(\frac{4nt^2}{\delta}\right)}{T_e(t)}}$  for all t > 0 and  $e \in [n]$ . Then, with probability at least  $1 - \delta$ , the CGapExp algorithm (Algorithm 1) returns the optimal set  $\mathrm{Out} = M_*$  and

$$T \le O\left(R^2 \operatorname{width}(\mathcal{M})^2 \mathbf{H} \log\left(R^2 \operatorname{width}(\mathcal{M})^2 \mathbf{H} \cdot n/\delta\right)\right),$$
 (4)

where T denotes the number of samples used by Algorithm 1 and  $\mathbf{H}$  is defined in Eq. (2).

*Proof.* Lemma 7 indicates that the event  $\xi \triangleq \bigcap_{t=1}^{\infty} \xi_t$  occurs with probability at least  $1 - \delta$ . In the rest of the proof, we shall assume that this event holds.

By Lemma 8 and the assumption on  $\xi$ , we see that  $\mathsf{Out} = M_*$ . Next, we focus on bounding the total number T of samples.

Fix any arm  $e \in [n]$ . Let  $T_e$  denote the total number of pull of arm  $e \in [n]$ . Let  $t_e$  be the last round which arm e is pulled, i.e.  $p_{t_e} = e$ . It is easy to see that  $T_e(t_e) = T_e - 1$ . By Lemma 9, we see that  $\operatorname{rad}_{t_e}(e) \geq \frac{\Delta_e}{3 \operatorname{width}(\mathcal{M})}$ . By plugging the definition of  $\operatorname{rad}_{t_e}$ , we have

$$\frac{\Delta_e}{3 \operatorname{width}(\mathcal{M})} \le R \sqrt{\frac{2 \log (4nt_e^2/\delta)}{T_e - 1}} \le R \sqrt{\frac{2 \log (4nT^2/\delta)}{T_e - 1}}.$$
(35)

Solving Eq. (35) for  $T_e$ , we obtain

$$T_e \le \frac{18 \operatorname{width}(\mathcal{M})^2 R^2}{\Delta_e^2} \log(4nT^2/\delta) + 1.$$
(36)

Notice that  $T = \sum_{i \in [n]} T_i$ . Hence the theorem follows by summing up Eq. (36) for all  $e \in [n]$  and solving for T.

## **B** Proof of Lower Bound

**Theorem 2.** Fix any  $\mathcal{M} \subseteq 2^{[n]}$  and any vector  $\mathbf{w} \in \mathbb{R}^n$ . Suppose that, for each arm  $e \in [n]$ , the reward distribution  $\varphi_e$  is given by  $\varphi_e = \mathcal{N}(w(e), 1)$ , where  $\mathcal{N}(\mu, \sigma^2)$  denotes a Gaussian distribution with mean  $\mu$  and variance  $\sigma^2$ . Then, for any  $\delta \in (0, e^{-16}/4)$  and any  $\delta$ -correct algorithm  $\mathbb{A}$ , we have

$$\mathbb{E}[T] \ge \frac{1}{16} \mathbf{H} \log \left( \frac{1}{4\delta} \right), \tag{5}$$

where T denote the number of total samples used by algorithm  $\mathbb{A}$  and  $\mathbf{H}$  is defined in Eq. (2).

*Proof.* Fix  $\delta > 0$ ,  $\boldsymbol{w} = (w(1), \dots, w(n))^T$  and a  $\delta$ -correct algorithm  $\mathbb{A}$ . For each  $e \in [n]$ , assume that the reward distribution is given by  $\varphi_e = \mathcal{N}(w(e), 1)$ . For any  $e \in [n]$ , let  $T_e$  denote the number of trials of arm e used by algorithm  $\mathbb{A}$ . In the rest of the proof, we will show that for any  $e \in [n]$ , the number of trials of arm e is lower-bounded by

$$\mathbb{E}[T_e] \ge \frac{1}{16\Delta_e^2} \log(1/4\delta). \tag{37}$$

Notice that the theorem follows immediately by summing up Eq. (37) for all  $e \in [n]$ .

Fix an arm  $e \in [n]$ . We now focus on proving Eq. (37). Consider two hypothesis  $H_0$  and  $H_1$ . Under hypothesis  $H_0$ , all reward distributions are same with our assumption before

$$H_0: \varphi_l = \mathcal{N}(w(l), 1)$$
 for all  $l \in [n]$ .

Under hypothesis  $H_1$ , we change the means of reward distributions such that

$$H_1: \varphi_e = \begin{cases} \mathcal{N}(w(e) - 2\Delta_e, 1) & \text{if } e \in M_* \\ \mathcal{N}(w(e) + 2\Delta_e, 1) & \text{if } e \notin M_* \end{cases} \quad \text{and } \varphi_l = \mathcal{N}(w(l), 1) \quad \text{for all } l \neq e.$$

For  $l \in \{0, 1\}$ , we use  $\mathbb{E}_l$  and  $\Pr_l$  to denote the expectation and probability, respectively, under the hypothesis  $H_l$ .

Define  $M_e$  be the "next-to-optimal" set as follows

$$M_e = \begin{cases} \arg\max_{M \in \mathcal{M}: e \in M} w(M) & \text{if } e \notin M_*, \\ \arg\max_{M \in \mathcal{M}: e \notin M} w(M) & \text{if } e \in M_*. \end{cases}$$

By definition of  $\Delta_e$  in Eq. (1), we know that  $w(M_*) - w(M_e) = \Delta_e$ 

Let  $w_0$  and  $w_1$  be expected reward vectors under  $H_0$  and  $H_1$  respectively. Notice that  $w_0(M_*) - w_0(M_e) = \Delta_e > 0$ . On the other hand, we have

$$w_1(M_*) - w_1(M_e) = w(M_*) - w(M_e) - 2\Delta_e$$
  
=  $-\Delta_e < 0$ .

This means that under  $H_1$ , the set  $M_*$  is not the optimal set.

Define  $\theta = 4\delta$ . Define

$$t_e^* = \frac{1}{16\Delta_e^2} \log\left(\frac{1}{\theta}\right). \tag{38}$$

Recall that  $T_e$  denotes the total number of samples of arm e. Define the event  $\mathcal{A} = \{T_e \leq 4t_e^*\}$ .

First, we show that  $Pr_0[A] \ge 3/4$ . This can be proved by Markov inequality as follows.

$$\Pr_0[T_e > 4t_e^*] \le \frac{\mathbb{E}_0[T_e]}{4t_e^*}$$

$$= \frac{t_e^*}{4t^*} = \frac{1}{4}.$$

Let  $X_1, \ldots, X_{T_e}$  denote the sequence of reward outcomes of arm e. For all t > 0, we define  $K_t = \sum_{i \in [t]} X_i$  as the sum of outcomes of arm e up to round t. Next, we define the event

$$C = \left\{ \max_{1 \le t \le 4t_e^*} |K_t - t \cdot w(e)| < \sqrt{t_e^* \log(1/\theta)} \right\}.$$

We now show that  $\Pr_0[\mathcal{C}] \ge 3/4$ . First, notice that  $\{K_t - t \cdot w(e)\}_{t=1,...}$  is a martingale under  $H_0$ . Then, by Kolmogorov's inequality, we have

$$\Pr_{0} \left[ \max_{1 \le t \le 4t_{e}^{*}} |K_{t} - t \cdot w(e)| \ge \sqrt{t_{e}^{*} \log(1/\theta)} \right] \le \frac{\mathbb{E}_{0}[(K_{4t_{e}^{*}} - 4w(e)t_{e}^{*})^{2}]}{t_{e}^{*} \log(1/\theta)} \\
= \frac{4t_{e}^{*}}{t_{e}^{*} \log(1/\theta)} \\
< \frac{1}{4},$$

where the second inequality follows from the fact that the variance of  $\varphi_e$  equals to 1 and therefore  $\mathbb{E}_0[(K_{4t_e^*}-4w(e)t_e^*)^2]=4t_e^*$ ; the last inequality follows since  $\theta < e^{-16}$ .

Then, we define the event  $\mathcal{B}$  as the event that the algorithm eventually returns  $M_*$ , i.e.

$$\mathcal{B} = \{ \mathsf{Out} = M_* \}.$$

Since the probability of error of the algorithm is smaller than  $\delta < 1/4$ , we have  $\Pr_0[\mathcal{B}] \geq 3/4$ . Define  $\mathcal{S}$  be  $\mathcal{S} = \mathcal{A} \cap \mathcal{B} \cap \mathcal{C}$ . Then, by union bound, we have  $\Pr_0[\mathcal{S}] \geq 1/4$ .

Now, we show that if  $\mathbb{E}_0[T_e] \leq t_e^*$ , then  $\Pr_1[\mathcal{B}] \geq \delta$ . Let W be the history of the sampling process until the algorithm stops (including the sequence of arms chosen at each time and the sequence of observed outcomes). Define the likelihood function  $L_l$  as

$$L_l(w) = p_l(W = w),$$

where  $p_l$  is the probability density function under hypothesis  $H_l$ . Let K be the shorthand of  $K_{T_e}$ .

Assume that the event S occurred. We will bound the likelihood ratio  $L_1(W)/L_0(W)$  under this assumption. To do this, we divide our analysis into two different cases.

Case (1):  $e \notin M_*$ . In this case, the reward distribution of arm e under  $H_1$  is a Gaussian distribution with mean  $w(e) + 2\Delta_e$  and variance 1. Recall that the probability density function of a Gaussian distribution with mean  $\mu$  and variance  $\sigma^2$  is given by  $\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$ . Hence, we have

$$\frac{L_1(W)}{L_0(W)} = \prod_{i=1}^{T_e} \exp\left(\frac{-(X_i - w(e) - 2\Delta_e)^2 + (X_i - w(e))^2}{2}\right) 
= \prod_{i=1}^{T_e} \exp\left(\Delta_e(2X_i - 2w(e)) - 2\Delta_e^2\right) 
= \exp\left(\Delta_e(2K - 2w(e)T_e) - 2\Delta_e^2T_e\right) 
= \exp\left(\Delta_e(2K - 2w(e)T_e)\right) \exp(-2\Delta_e^2T_e).$$
(39)

Next, we bound each individual term on the right-hand side of Eq. (39). We begin with bounding the second term of Eq. (39)

$$\exp(-2\Delta_e^2 T_e) \ge \exp(-8\Delta_e^2 t_e^*) \tag{40}$$

$$= \exp\left(-\frac{8}{16}\log(1/\theta)\right) \tag{41}$$

$$=\theta^{1/2},\tag{42}$$

where Eq. (40) follows from the assumption that event S occurred, which implies that event A occurred and therefore  $T_e \leq 4t_e^*$ ; Eq. (41) follows from the definition of  $t_e^*$ .

Then, we bound the first term on the right-hand side of Eq. (39) as follows

$$\exp\left(\Delta_e(2K - 2w(e)T_e)\right) \ge \exp\left(-2\Delta_e\sqrt{t_e^*\log(1/\theta)}\right) \tag{43}$$

$$= \exp\left(-\frac{2}{4}\log(1/\theta)\right) \tag{44}$$

$$=\theta^{1/2},\tag{45}$$

where Eq. (43) follows from the assumption that event  $\mathcal{S}$  occurred, which implies that event  $\mathcal{C}$  and therefore  $|2K - 2w(e)T_e| \leq \sqrt{t_e^* \log(1/\theta)}$ ; Eq. (44) follows from the definition of  $t_e^*$ .

Combining Eq. (42) and Eq. (45), we can bound  $L_1(W)/L_0(W)$  for this case as follows

$$\frac{L_1(W)}{L_0(W)} \ge \theta. \tag{46}$$

(End of Case (1).)

Case (2):  $e \in M_*$ . In this case, we know that the mean reward of arm e under  $H_1$  is  $w(e) - 2\Delta$ . Therefore, the likelihood ratio  $L_1(W)/L_0(W)$  is given by

$$\frac{L_1(W)}{L_0(W)} = \prod_{i=1}^{T_e} \exp\left(\frac{-(X_i - w(e) + 2\Delta_e)^2 + (X_i - w(e))^2}{2}\right)$$

$$= \prod_{i=1}^{T_e} \exp\left(\Delta_e(2w(e) - 2X_i) - 2\Delta_e^2\right)$$

$$= \exp\left(\Delta_e(2w(e)T_e - 2K)\right) \exp(-2\Delta_e^2 T_e). \tag{47}$$

Notice that the right-hand side of Eq. (47) differs from Eq. (39) only in its first term. Now, we bound the first term as follows

$$\exp\left(\Delta_e(2w(e)T_e - 2K)\right) \ge \exp\left(-2\Delta_e\sqrt{t_e^*\log(1/\theta)}\right) \tag{48}$$

$$= \exp\left(-\frac{2}{4}\log(1/\theta)\right) \tag{49}$$

$$=\theta^{1/2},\tag{50}$$

where the inequalities hold due to reasons similar to Case (1): Eq. (48) follows from the assumption that event  $\mathcal{S}$  occurred, which implies that event  $\mathcal{C}$  and therefore  $|2K-2w(e)T_e| \leq \sqrt{t_e^* \log(1/\theta)}$ ; Eq. (49) follows from the definition of  $t_e^*$ .

Combining Eq. (42) and Eq. (45), we can obtain the same bound of  $L_1(W)/L_0(W)$  as in Eq. (46), i.e.  $L_1(W)/L_0(W) \ge \theta$ .

(End of Case (2).)

At this point, we have proved that, if the event S occurred, then the bound of likelihood ratio Eq. (46) holds, i.e.  $\frac{L_1(W)}{L_0(W)} \ge \theta$ . Hence, we have

$$\frac{L_1(W)}{L_0(W)} \ge \theta$$

$$= 4\delta.$$
(51)

Define  $1_S$  as the indicator variable of event S, i.e.  $1_S = 1$  if and only if S occurs and otherwise  $1_S = 0$ . Then, we have

$$\frac{L_1(W)}{L_0(W)} 1_S \ge 4\delta 1_S$$

holds regardless the occurrence of event S. Therefore, we can obtain

$$\begin{aligned} \Pr_{1}[\mathcal{B}] &\geq \Pr_{1}[\mathcal{S}] = \mathbb{E}_{1}[1_{S}] \\ &= \mathbb{E}_{0} \left[ \frac{L_{1}(W)}{L_{0}(W)} 1_{S} \right] \\ &\geq 4\delta \mathbb{E}_{0}[1_{S}] \\ &= 4\delta \Pr_{0}[\mathcal{S}] > \delta. \end{aligned}$$

Now we have proved that, if  $\mathbb{E}_0[T_e] \leq t_e^*$ , then  $\Pr_1[\mathcal{B}] > \delta$ . This means that, if  $\mathbb{E}_0[T_e] \leq t_e^*$ , algorithm  $\mathbb{A}$  will choose  $M_*$  as the output with probability at least  $\delta$ , under hypothesis  $H_1$ . However, under  $H_1$ , we have shown that  $M_*$  is not the optimal set since  $w_1(M_e) > w_1(M_*)$ . Therefore, algorithm  $\mathbb{A}$  has a probability of error at least  $\delta$  under  $H_1$ . This contradicts to the assumption that algorithm  $\mathbb{A}$  is a  $\delta$ -correct algorithm. Hence, we must have  $\mathbb{E}_0[T_e] > t_e^* = \frac{1}{16\Delta_e^2}\log(1/4\delta)$ .  $\square$ 

# **B.1** Exchange set size dependent lower bound

We show that, for any arm  $e \in [n]$ , there exists an exchange set b which contains e such that a  $\delta$ -correct algorithm must spend  $\tilde{\Omega}\Big(\big(|b_+|+|b_-|\big)^2/\Delta_e^2\Big)$  samples on the arms belonging to b. This result is formalized in the following theorem.

**Theorem 5.** Fix any  $\mathcal{M} \subseteq 2^{[n]}$  and any vector  $\mathbf{w} \in \mathbb{R}^n$ . Suppose that, for each arm  $e \in [n]$ , the reward distribution  $\varphi_e$  is given by  $\varphi_e = \mathcal{N}(w(e), 1)$ , where  $\mathcal{N}(\mu, \sigma^2)$  denotes a Gaussian distribution with mean  $\mu$  and variance  $\sigma^2$ . Fix any  $\delta \in (0, e^{-16}/4)$  and any  $\delta$ -correct algorithm  $\mathbb{A}$ .

Then, for any  $e \in [n]$ , there exists an exchange set  $b = (b_+, b_-)$ , such that  $e \in b_+ \cup b_-$  and

$$\mathbb{E}\left[\sum_{i \in b_{+} \cup b_{-}} T_{i}\right] \geq \frac{(|b_{+}| + |b_{-}|)^{2}}{32\Delta_{e}^{2}} \log(1/4\delta),$$

where  $T_i$  is the number of samples of arm i.

*Proof.* Fix  $\delta > 0$ ,  $w \in \mathbb{R}^n$ , diff-set  $b = (b_+, b_-)$  and a  $\delta$ -correct algorithm  $\mathbb{A}$ . Assume that  $\varphi_e(e) = \mathcal{N}(w(e), 1)$  for all  $e \in [n]$ .

We define three hypotheses  $H_0$ ,  $H_1$  and  $H_2$ . Under hypothesis  $H_0$ , the reward distribution

$$H_0: \varphi_l = \mathcal{N}(w(l), 1)$$
 for all  $l \in [n]$ .

Under hypothesis  $H_1$ , the mean reward of each arm is given by

$$H_1: \varphi_e = \begin{cases} \mathcal{N}\left(w(e) + 2\frac{w(b)}{|b_-|}, 1\right) & \text{if } e \in b_-, \\ \mathcal{N}(w(e), 1) & \text{if } e \notin b_-. \end{cases}$$

And under hypothesis  $H_2$ , the mean reward of each arm is given by

$$H_2: \varphi_e = \begin{cases} \mathcal{N}\left(w(e) - 2\frac{w(b)}{|b_-|}, 1\right) & \text{if } e \in b_+, \\ \mathcal{N}(w(e), 1) & \text{if } e \notin b_+. \end{cases}$$

Since  $b \in \mathcal{B}_{\text{opt}}$ , it is clear that  $\neg b \prec M_*$ . Hence we define  $M = M_* \ominus b$ . Let  $w_0, w_1$  and  $w_2$  be the expected reward vectors under  $H_0, H_1$  and  $H_2$  respectively. It is easy to check that  $w_1(M_*) - w_1(M) = -w(b) < 0$  and  $w_2(M_*) - w_2(M) = -w(b) < 0$ . This means that under  $H_1$  or  $H_2$ ,  $M_*$  is not the optimal set. Further, for  $l \in \{0,1,2\}$ , we use  $\mathbb{E}_l$  and  $\Pr_l$  to denote the expectation and probability, respectively, under the hypothesis  $H_l$ . In addition, let W be the history of the sampling process until algorithm  $\mathbb{A}$  stops. Define the likelihood function  $L_l$  as

$$L_l(w) = p_l(W = w),$$

where  $p_l$  is the probability density function under  $H_l$ .

Define  $\theta = 4\delta$ . Let  $T_{b_-}$  and  $T_{b_+}$  denote the number of trials of arms belonging to  $b_-$  and  $b_+$ , respectively. In the rest of the proof, we will bound  $\mathbb{E}_0[T_{b_-}]$  and  $\mathbb{E}_0[T_{b_+}]$  individually.

Part (1): Lower bound of  $\mathbb{E}_0[T_{b_-}]$ . In this part, we will show that  $\mathbb{E}_0[T_{b_-}] \geq t_{b_-}^*$ , where we define  $t_{b_-}^* = \frac{|b_-|^2}{16m(b)^2}\log(1/\theta)$ .

Consider the complete sequence of sampling process by algorithm  $\mathbb{A}$ . Formally, let  $W=\{(\tilde{I}_1,\tilde{X}_1),\ldots,(\tilde{I}_T,\tilde{X}_T)\}$  be the sequence of all trials by algorithm  $\mathbb{A}$ , where  $\tilde{I}_i$  denotes the arm played in i-th trial and  $\tilde{X}_i$  be the reward outcome of i-th trial. Then, consider the subsequence  $W_1$  of W which consists all the trials of arms in  $b_-$ . Specifically, we write  $W=\{(I_1,X_1),\ldots,(I_{T_b_-},X_{T_b_-})\}$  such that  $W_1$  is a subsequence of W and  $I_i\in b_-$  for all i.

Next, we define several random events in a way similar to the proof of Theorem 2. Define event  $A_1 = \{T_{b_-} \leq 4t_{b_-}^*\}$ . Define event

$$C_1 = \left\{ \max_{1 \le t \le 4t_{b-}^*} \left| \sum_{i=1}^t X_i - \sum_{i=1}^t w(I_i) \right| < \sqrt{t_{b-}^* \log(1/\theta)} \right\}.$$

Define event

$$\mathcal{B} = \{ \mathsf{Out} = M_* \}. \tag{52}$$

Define event  $S_1 = A_1 \cap B \cap C_1$ . Then, we bound the probability of events  $A_1$ , B,  $C_1$  and  $S_1$  under  $H_0$  using methods similar to Theorem 2. First, we show that  $\Pr_0[A_1] \geq 3/4$ . This can be proved by Markov inequality as follows.

$$\Pr_0[T_{b_-} > 4t_{b_-}^*] \le \frac{\mathbb{E}_0[T_{b_-}]}{4t_{b_-}^*}$$

$$=\frac{t_{b_{-}}^{*}}{4t_{b}^{*}}=\frac{1}{4}.$$

Next, we show that  $\Pr_0[\mathcal{C}_1] \geq 3/4$ . Notice that the sequence  $\left\{\sum_{i=1}^t X_i - \sum_{i=1}^t p_{I_i}\right\}_{t \in [4t_{b_-}^*]}$  is a martingale. Hence, by Kolmogorov's inequality, we have

$$\Pr_{0} \left[ \max_{1 \le t \le 4t_{b_{-}}^{*}} \left| \sum_{i=1}^{t} X_{i} - \sum_{i=1}^{t} w(I_{i}) \right| \ge \sqrt{t_{e}^{*} \log(1/\theta)} \right] \le \frac{\mathbb{E}_{0} \left[ \left( \sum_{i=1}^{4t_{b_{-}}^{*}} X_{i} - \sum_{i=1}^{4t_{b_{-}}^{*}} w(I_{i}) \right)^{2} \right]}{t_{e}^{*} \log(1/\theta)}$$

$$= \frac{4t_{b_{-}}^{*}}{t_{b_{-}}^{*} \log(1/\theta)}$$

$$< \frac{1}{4},$$

where the second inequality follows from the fact that all reward distributions have unit variance and hence  $\mathbb{E}_0\left[\left(\sum_{i=1}^{4t_{b-}^*}X_i-\sum_{i=1}^{4t_{b-}^*}p_{I_i}\right)^2\right]=4t_{b-}^*$ ; the last inequality follows since  $\theta< e^{-16}$ .

Last, since algorithm  $\mathbb{A}$  is a  $\delta$ -correct algorithm with  $\delta < 1/4$ . Therefore, it is easy to see that  $\Pr_0[\mathcal{B}] \geq 3/4$ . And by union bound, we have

$$\Pr_0[\mathcal{S}_1] \ge 1/4.$$

Now, we show that if  $\mathbb{E}_0[T_{b_-}] \leq t_{b_-}^*$ , then  $\Pr_1[\mathcal{B}] \geq \delta$ . Assume that the event  $\mathcal{S}_1$  occurred. We bound the likelihood ratio  $L_1(W)/L_0(W)$  under this assumption as follows

$$\frac{L_{1}(W)}{L_{0}(W)} = \prod_{i=1}^{T_{b_{-}}} \exp\left(\frac{-\left(X_{i} - w(I_{i}) - \frac{2w(b)}{|b_{-}|}\right)^{2} + (X_{i} - w(I_{i})^{2})}{2}\right)$$

$$= \prod_{i=1}^{T_{b_{-}}} \exp\left(\frac{w(b)}{|b_{-}|} (2X_{i} - 2w(I_{i})) - \frac{2w(b)^{2}}{|b_{-}|^{2}}\right)$$

$$= \exp\left(\frac{w(b)}{|b_{-}|} \left(\sum_{i=1}^{T_{b_{-}}} 2X_{i} - 2w(I_{i})\right) - \frac{2w(b)^{2}}{|b_{-}|^{2}} T_{b_{-}}\right)$$

$$= \exp\left(\frac{w(b)}{|b_{-}|} \left(\sum_{i=1}^{T_{b_{-}}} 2X_{i} - 2w(I_{i})\right)\right) \exp\left(-\frac{2w(b)^{2}}{|b_{-}|^{2}} T_{b_{-}}\right). \tag{53}$$

Then, we bound each term on the right-hand side of Eq. (53). First, we bound the second term of Eq. (53).

$$\exp\left(-\frac{2w(b)^2}{|b_-|^2}T_{b_-}\right) \ge \exp\left(-\frac{2w(b)^2}{|b_-|^2}4t_b^*\right)$$
(54)

$$= \exp\left(-\frac{8}{16}\log(1/\theta)\right) \tag{55}$$

$$=\theta^{1/2},\tag{56}$$

where Eq. (54) follows from the assumption that events  $S_1$  and  $A_1$  occurred and therefore  $T_{b_-} \le 4t_b^*$ ; Eq. (55) follows from the definition of  $t_b^*$ . Next, we bound the first term of Eq. (53) as follows

$$\exp\left(\frac{w(b)}{|b_{-}|} \left(\sum_{i=1}^{T_{b_{-}}} 2X_{i} - 2w(I_{i})\right)\right) \ge \exp\left(-\frac{2w(b)}{|b_{-}|} \sqrt{t_{b}^{*} \log(1/\theta)}\right)$$
(57)

$$= \exp\left(-\frac{2}{4}\log(1/\theta)\right) \tag{58}$$

$$=\theta^{1/2},\tag{59}$$

where Eq. (57) follows since event  $S_1$  and  $C_1$  occurred and therefore  $|2K - 2p_eT_e| \le \sqrt{t_e^* \log(1/\theta)}$ ; Eq. (58) follows from the definition of  $t_h^*$ .

Hence, if event  $S_1$  occurred, we can bound the likelihood ratio as follows

$$\frac{L_1(W)}{L_0(W)} \ge \theta = 4\delta. \tag{60}$$

Let  $1_{S_1}$  denote the indicator variable of event  $S_1$ . Then, we have  $\frac{L_1(W)}{L_0(W)}1_{S_1} \geq 4\delta 1_{S_1}$ . Therefore, we can bound  $\Pr_1[\mathcal{B}]$  as follows

$$\Pr_{1}[\mathcal{B}] \ge \Pr_{1}[\mathcal{S}_{1}] = \mathbb{E}_{1}[1_{S_{1}}]$$

$$= \mathbb{E}_{0} \left[ \frac{L_{1}(W)}{L_{0}(W)} 1_{S_{1}} \right]$$

$$\ge 4\delta \mathbb{E}_{0}[1_{S_{1}}]$$

$$= 4\delta \Pr_{0}[\mathcal{S}_{1}] > \delta. \tag{61}$$

This means that, if  $\mathbb{E}_0[T_{b_-}] \leq t_{b_-}^*$ , then, under  $H_1$ , the probability of algorithm  $\mathbb{A}$  returning  $M_*$  as output is at least  $\delta$ . But  $M_*$  is not the optimal set under  $H_1$ . Hence this contradicts to the assumption that  $\mathbb{A}$  is a  $\delta$ -correct algorithm. Hence we have proved that

$$\mathbb{E}_0[T_{b_-}] \ge t_{b_-}^* = \frac{|b_-|^2}{16w(b)^2} \log(1/4\delta). \tag{62}$$

(End of Part (1).)

Part (2): Lower bound of  $\mathbb{E}_0[T_{b_+}]$ . In this part, we will show that  $\mathbb{E}_0[T_{b_+}] \geq t_{b_+}^*$ , where we define  $t_{b_+}^* = \frac{|b_+|^2}{16w(b)^2}\log(1/\theta)$ . The arguments used in this part are similar to that of Part (1). Hence, we will omit the redundant parts and highlight the differences.

Recall that we have defined that W to be the history of all trials by algorithm  $\mathbb{A}$ . We define W be the subsequence of  $\tilde{S}$  which contains the trials of arms belonging to  $b_+$ . We write  $S_2 = \{(J_1, Y_1), \ldots, (J_{T_{b_+}}, Y_{T_{b_+}})\}$ , where  $J_i$  is i-th played arm in sequence  $S_2$  and  $Y_i$  is the associated reward outcome.

We define the random events  $A_2$  and  $C_2$  similar to Part (1). Specifically, we define

$$\mathcal{A}_2 = \{T_{b_+} \leq 4t_{b_+}^*\} \quad \text{and} \quad \mathcal{C}_2 = \left\{ \max_{1 \leq t \leq 4t_{b_+}^*} \left| \sum_{i=1}^t Y_i - \sum_{i=1}^t w(J_i) \right| < \sqrt{t_{b_+}^* \log(1/\theta)} \right\}.$$

Using the similar arguments, we can show that  $\Pr_0[A_2] \ge 3/4$  and  $\Pr_0[C_2] \ge 3/4$ . Define event  $S_2 = A_2 \cap B \cap C_2$ , where B is defined in Eq. (52). By union bound, we see that

$$\Pr_0[\mathcal{S}_2] \ge 1/4.$$

Then, we show that if  $\mathbb{E}_0[T_{b_+}] \leq t_{b_+}^*$ , then  $\Pr_2[\mathcal{B}] \geq \delta$ . We bound likelihood ratio  $L_2(W)/L_0(W)$  under the assumption that  $\mathcal{S}_2$  occurred as follows

$$\frac{L_2(W)}{L_0(W)} = \prod_{i=1}^{T_{b_+}} \exp\left(\frac{-\left(Y_i - w(J_i)\right) + \frac{2w(b)}{|b_-|}\right)^2 + (Y_i - w(J_i))^2}{2}\right)$$

$$= \prod_{i=1}^{T_{b_+}} \exp\left(\frac{w(b)}{|b_+|}(2w(J_i) - 2Y_i) - \frac{2w(b)^2}{|b_+|^2}\right)$$

$$= \exp\left(\frac{w(b)}{|b_{+}|} \left(\sum_{i=1}^{T_{b_{+}}} 2w(J_{i}) - 2Y_{i}\right) - \frac{2w(b)^{2}}{|b_{+}|^{2}} T_{b_{+}}\right)$$

$$= \exp\left(\frac{w(b)}{|b_{+}|} \left(\sum_{i=1}^{T_{b_{+}}} 2w(J_{i}) - 2Y_{i}\right)\right) \exp\left(-\frac{2w(b)^{2}}{|b_{+}|^{2}} T_{b_{+}}\right)$$

$$\geq \theta$$

$$= 4\delta.$$
(63)

where Eq. (63) can be obtained using same method as in Part (1) as well as the assumption that  $S_2$  occurred.

Next, similar to the derivation in Eq. (61), we see that

$$\Pr_2[\mathcal{B}] \ge \Pr_2[\mathcal{S}_2] = \mathbb{E}_2[1_{S_2}] = \mathbb{E}_0\left[\frac{L_2(W)}{L_0(W)}1_{S_2}\right] \ge 4\delta\mathbb{E}_0[1_{S_2}] > \delta,$$

where  $1_{S_2}$  is the indicator variable of event  $S_2$ . Therefore, we see that if  $\mathbb{E}_0[T_{b_+}] \leq t_{b_+}^*$ , then, under  $H_2$ , the probability of algorithm  $\mathbb{A}$  returning  $M_*$  as output is at least  $\delta$ , which is not the optimal set under  $H_2$ . This contradicts to the assumption that algorithm  $\mathbb{A}$  is a  $\delta$ -correct algorithm. In sum, we have proved that

$$\mathbb{E}_0[T_{b_+}] \ge t_{b_+}^* = \frac{|b_+|^2}{16w(b)^2} \log(1/4\delta). \tag{64}$$

(End of Part (2))

Finally, we combine the results from both parts, i.e. Eq. (62) and Eq. (64). We obtain

$$\mathbb{E}_0[T_b] = \mathbb{E}_0[T_{b_-}] + \mathbb{E}_0[T_{b_+}]$$

$$\geq \frac{|b_+|^2 + |b_-|^2}{16w(b)^2} \log(1/4\delta)$$

$$\geq \frac{|b|^2}{32w(b)^2} \log(1/4\delta).$$

# C Proof of Extension Results

#### C.1 Fixed Budget Setting

In this part, we analyze the probability of error of the modified CGapExp algorithm in the fixed budget setting and prove Theorem 3. First, we prove a lemma which characterizes the confidence intervals constructed in Theorem 3.

**Lemma 10.** Fix parameter  $\alpha > 0$  and the number of rounds T > 0. Assume that the reward distribution  $\varphi_e$  is a R-sub-Gaussian distribution for all  $e \in [n]$ . Let the confidence radius  $\mathrm{rad}_t(e)$  of arm  $e \in [n]$  and round t > 0 be  $\mathrm{rad}_t(e) = R\sqrt{\frac{\alpha}{T_e(t)}}$ . Then, we have

$$\Pr\left[\bigcap_{t=1}^{T} \xi_t\right] \ge 1 - 2nT \exp\left(-2\alpha\right).$$

*Proof.* For any t > 0 and  $e \in [n]$ , using Hoeffding's inequality, we have

$$\Pr\left[\left|\bar{w}_t(e) - w(e)\right| \ge \operatorname{rad}_t(e)\right] \le 2\exp(-2\alpha).$$

By a union bound over all arms  $e \in [n]$ , we see that  $\Pr[\xi_t] \ge 1 - 2n \exp(-2\alpha)$ . The lemma follows immediately by using union bound again over all round  $t \in [T]$ .

Then, Theorem 3 can be obtained from the key lemmas (Lemma 8 and Lemma 9) and Lemma 10.

**Theorem 3.** Use the same notations as in Theorem 1. Given T > n and parameter  $\alpha > 0$ , set the confidence radius  $\mathrm{rad}_t(e) = R\sqrt{\frac{\alpha}{T_e(t)}}$  for all arms  $e \in [n]$  and all t > 0. Run CGapExp algorithm

for at most T rounds. Then, for  $0 \le \alpha \le \frac{1}{9}(T-n)\left(R^2 \operatorname{width}(\mathcal{M})^2 \mathbf{H}\right)^{-1}$ , we have

$$\Pr\left[\mathsf{Out} \neq M_*\right] \le 2Tn\exp\left(-2\alpha\right). \tag{6}$$

*Proof.* Define random event  $\xi = \bigcap_{t=1}^T \xi_t$ . By Lemma 10, we see that  $\Pr[\xi] \ge 1 - 2nT \exp(-2\alpha)$ . In the rest of the proof, we assume that  $\xi$  happens.

Let  $T^*$  denote the round that the algorithm stops. We claim that the algorithm  $T^* < T$ . If the claim is true, then the algorithm stops since it meets the stopping condition on round  $T^*$ . Hence  $\tilde{M}_{T^*} = M_{T^*}$  and  $\text{Out} = M_{T^*}$ . By assumption on  $\xi$  and Lemma 8, we know that  $M_{T^*} = M_*$ . Therefore the theorem follows immediately from this claim and the bound of  $\Pr[\xi]$ .

Next, we show that this claim is true. Let  $t_e$  be the last round that arm e is pulled. Hence  $T_e(t_e) = T_e - 1$ . By Lemma 9, we see that  $\operatorname{rad}_{t_e}(e) \geq \frac{\Delta}{3 \operatorname{width}(\mathcal{B})}$ . Now plugging in the definition of  $\operatorname{rad}_{t_e}(e)$ , we have

$$\begin{split} \frac{\Delta}{3 \operatorname{width}(\mathcal{B})} &\leq \operatorname{rad}_{t_e}(e) \\ &= R \sqrt{\frac{\alpha}{T_e(t_e)}} = R \sqrt{\frac{\alpha}{T_e - 1}}. \end{split}$$

Hence we have

$$T_e \le \frac{9R^2 \operatorname{width}(\mathcal{B})^2}{\Delta_e^2} \cdot \alpha + 1.$$
 (65)

By summing up Eq. (65) for all  $e \in [n]$ , we have

$$T^* = \sum_{e \in [n]} T_e \le \alpha \cdot 9R^2 \operatorname{width}(\mathcal{B})^2 \left( \sum_{e \in [n]} \Delta_e^{-2} \right) + n < T,$$

where we have used the assumption that  $\alpha < \frac{1}{9}(T-n) \cdot \left(R^2 \operatorname{width}(\mathcal{B})^2 \left(\sum_{e \in [n]} \Delta_e^{-2}\right)\right)^{-1}$ .

## C.2 PAC Learning

First, we prove a  $(\epsilon, \delta)$ -PAC counterpart of Lemma 8.

**Lemma 11.** If CGapExpPAC stops on round t and suppose that event  $\xi_t$  occurs. Then, we have  $w(M_*) - w(\mathsf{Out}) \leq \epsilon$ .

*Proof.* By definition, we know that  $\text{Out} = M_t$ . Notice that the stopping condition of CGapExpPAC ensures that  $\tilde{w}_t(\tilde{M}_t) - \tilde{w}_t(M_t) \leq \epsilon$ . Therefore, we have

$$\epsilon \ge \tilde{w}_t(\tilde{M}_t) - \tilde{w}_t(M_t) \ge \tilde{w}_t(M_*) - \tilde{w}_t(M_t)$$
(66)

$$= \langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_{M_*} - \boldsymbol{\chi}_{M_t} \rangle + \langle \mathbf{rad}_t, |\boldsymbol{\chi}_{M_*} - \boldsymbol{\chi}_{M_t}| \rangle \tag{67}$$

$$\geq \langle \boldsymbol{w}, \boldsymbol{\chi}_{M_*} - \boldsymbol{\chi}_{M_t} \rangle$$

$$= w(M_*) - w(M_t),$$
(68)

where Eq. (66) follows from the definition of  $\tilde{M}_t \triangleq \arg \max_{M \in \mathcal{M}} \tilde{w}_t(M)$ ; Eq. (67) follows from Lemma 5; Eq. (68) follows from the assumption that  $\xi_t$  occurs and Lemma 6.

The next lemma generalizes Lemma 9. It shows that, with high probability, each arm  $e \in [n]$  will not be played on round t if  $\operatorname{rad}_t(e) \leq \max\left\{\frac{\Delta_e}{3\operatorname{width}(\mathcal{M})}, \frac{\epsilon}{2K}\right\}$ .

**Lemma 12.** Let  $K = \max_{M \in \mathcal{M}} |M|$ . For any arm  $e \in [n]$  and any round t > n after initialization, if  $\operatorname{rad}_t(e) \leq \max\left\{\frac{\Delta_e}{3\operatorname{width}(\mathcal{M})}, \frac{\epsilon}{2K}\right\}$ , then arm e will not be played on round t, i.e.  $p_t \neq e$ .

*Proof.* If  $\operatorname{rad}_t(e) \leq \frac{\Delta_e}{3\operatorname{width}(\mathcal{M})}$ , then we can apply Lemma 9 which immediately gives that  $p_t \neq e$ . Hence, we only need to prove the case that  $\frac{\Delta_e}{3\operatorname{width}(\mathcal{M})} \leq \operatorname{rad}_t(e) \leq \frac{\epsilon}{2K}$ .

Now suppose that  $p_t = e$ . By the choice of  $p_t$ , we know that for each  $i \in (M_t \setminus \tilde{M}_t) \cup (\tilde{M}_t \setminus M_t)$ , we have  $\operatorname{rad}_t(i) \leq \operatorname{rad}_t(e) \leq \frac{\epsilon}{2K}$ . By summing up this inequality for all  $i \in (M_t \setminus \tilde{M}_t) \cup (\tilde{M}_t \setminus M_t)$ , we have

$$\epsilon \ge \sum_{i \in (M_t \setminus \tilde{M}_t) \cup (\tilde{M}_t \setminus M_t)} \operatorname{rad}_t(i)$$
(69)

$$= \left\langle \mathbf{rad}_{t}, \left| \chi_{M_{t}} - \chi_{\tilde{M}_{t}} \right| \right\rangle, \tag{70}$$

where Eq. (69) follows from the fact that  $|(M_t \setminus \tilde{M}_t) \cup (\tilde{M}_t \setminus M_t)| \leq |M_t| + |\tilde{M}_t| \leq 2K$ ; and Eq. (70) uses the fact that  $\chi_{(M_t \setminus \tilde{M}_t) \cup (\tilde{M}_t \setminus M_t)} = |\chi_{M_t} - \chi_{\tilde{M}_t}|$ .

Then, we have

$$\tilde{w}_t(\tilde{M}_t) - \tilde{w}_t(M_t) = \langle \bar{\boldsymbol{w}}_t, \boldsymbol{\chi}_{\tilde{M}_t} - \boldsymbol{\chi}_{M_t} \rangle + \langle \mathbf{rad}_t, |\boldsymbol{\chi}_{\tilde{M}_t} - \boldsymbol{\chi}_{M_t}| \rangle$$
(71)

$$\leq \left\langle \bar{\boldsymbol{w}}_{t}, \boldsymbol{\chi}_{\tilde{M}_{t}} - \boldsymbol{\chi}_{M_{t}} \right\rangle + \epsilon \tag{72}$$

$$= \bar{w}_t(\tilde{M}_t) - \bar{w}_t(M_t) + \epsilon$$

$$\leq \epsilon, \tag{73}$$

where Eq. (71) follows from Lemma 5; Eq. (72) uses Eq. (70); and Eq. (73) follows from  $\bar{w}_t(M_t) \ge \bar{w}_t(\tilde{M}_t)$ .

Therefore, we see that  $\tilde{w}_t(\tilde{M}_t) - \tilde{w}_t(M_t) \leq \epsilon$ . By the stopping condition of CGapExpPAC, the algorithm must terminate on round t. This contradicts to the assumption that  $p_t = e$ .

Using Lemma 12 and Lemma 11, we are ready to prove Theorem 4.

**Theorem 4.** Use the same notations as in Theorem 1. Fix  $\delta \in (0,1)$  and  $\epsilon \geq 0$ . Then, with probability at least  $1-\delta$ , the output Out of CGapExpPAC satisfies  $w(M_*)-w(\text{Out}) \leq \epsilon$ . In addition, the number of samples T used by the algorithm satisfies

$$T \le O\left(R^2 \sum_{e \in [n]} \min\left\{\frac{\operatorname{width}(\mathcal{M})^2}{\Delta_e^2}, \frac{K^2}{\epsilon^2}\right\} \log\left(\frac{R^2 n}{\delta} \sum_{e \in [n]} \min\left\{\frac{\operatorname{width}(\mathcal{M})^2}{\Delta_e^2}, \frac{K^2}{\epsilon^2}\right\}\right)\right), (7)$$

where  $K = \max_{M \in \mathcal{M}} |M|$  is the size of the largest feasible solution.

*Proof.* Similar to the proof of Theorem 1, we appeal to Lemma 7, which shows that the event  $\xi \triangleq \bigcap_{t=1}^{\infty} \xi_t$  occurs with probability at least  $1 - \delta$ . And we shall assume that  $\xi$  occurs in the rest of the proof.

By the assumption of  $\xi$  and Lemma 11, we know that  $Out = M_*$ . Therefore, we only remain to bound the number of samples T.

Consider an arbitrary arm  $e \in [n]$ . Let  $T_e$  denote the total number of pull of arm  $e \in [n]$ . Let  $t_e$  be the last round which arm e is pulled, i.e.  $p_{t_e} = e$ . Hence  $T_e(t_e) = T_e - 1$ . By Lemma 12, we see that  $\operatorname{rad}_{t_e}(e) \ge \min\{\frac{\Delta_e}{3\operatorname{width}(B)}, \frac{\epsilon}{2K}\}$ . Then, by the construction of  $\operatorname{rad}_{t_e}(e)$ , we have

$$\min\left\{\frac{\Delta_e}{3\operatorname{width}(\mathcal{B})}, \frac{\epsilon}{2K}\right\} \le R\sqrt{\frac{2\log\left(4nt_e^2/\delta\right)}{T_e - 1}} \le R\sqrt{\frac{2\log\left(4nT^2/\delta\right)}{T_e - 1}}.$$
(74)

Solving Eq. (74) for  $T_e$ , we obtain

$$T_e \le R^2 \min\left\{\frac{18 \operatorname{width}(\mathcal{B})^2}{\Delta_e^2}, \frac{16K^2}{\epsilon^2}\right\} \log(4nT^2/\delta) + 1.$$
 (75)

Notice that  $T = \sum_{i \in [n]} T_i$ . Hence the theorem follows by summing up Eq. (75) for all  $e \in [n]$  and solving for T.

## **D** Technical Lemmas

Lemma 13 (Basis exchange property). AA

**Lemma 14** (Hoeffding's inequality). Let  $X_1, \ldots, X_n$  be n independent R-sub-Gaussian random variables. Let  $\bar{X} = \frac{1}{n} \sum X_i$  be the average of these random variables. Then, we have

$$\Pr\left[\left|\bar{X} - \mathbb{E}[\bar{X}]\right| \geq t\right] \leq 2\exp\left(-\frac{2nt^2}{R^2}\right).$$

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