Nearly Instance Optimal Sample Complexity Bounds for Top-k Arm Selection

Lijie Chen  Jian Li  Mingda Qiao
Institute for Interdisciplinary Information Sciences (IIIS), Tsinghua University

Abstract

In the Best-k-Arm problem, we are given $n$ stochastic bandit arms, each associated with an unknown reward distribution. We are required to identify the $k$ arms with the largest means by taking as few samples as possible. In this paper, we make progress towards a complete characterization of the instance-wise sample complexity bounds for the Best-k-Arm problem. On the lower bound side, we obtain a novel complexity term to measure the sample complexity that every Best-k-Arm instance requires. This is derived by an interesting and nontrivial reduction from the Best-1-Arm problem. We also provide an elimination-based algorithm that matches the instance-wise lower bound within doubly-logarithmic factors. The sample complexity of our algorithm strictly dominates the state-of-the-art for Best-k-Arm (modulo constant factors).

1 INTRODUCTION

The stochastic multi-armed bandit is a classical and well-studied model for characterizing the exploration-exploitation tradeoff in various decision-making problems in stochastic settings. The most well-known objective in the multi-armed bandit model is to maximize the cumulative gain (or equivalently, to minimize the cumulative regret) that the agent achieves. Another line of research, called the pure exploration multi-armed bandit problem, which is motivated by a variety of practical applications including medical trials [Rob85, AB10], communication network [AB10], and crowdsourcing [ZCL14, CLTL15], has also attracted significant attention recently. In the pure exploration problem, the agent draws samples from the arms adaptively (the exploration phase), and finally commits to one of the feasible solutions specified by the problem. In a sense, the exploitation phase in the pure exploration problem simply consists of exploiting the solution to which the agent commits indefinitely. Therefore, the agent’s objective is to identify the optimal (or near-optimal) feasible solution with high probability.

In this paper, we focus on the problem of identifying the top-$k$ arms (i.e., the $k$ arms with the largest means) in a stochastic multi-armed bandit model. The problem is known as the Best-k-Arm problem, and has been extensively studied in the past decade [KS10, GGL12, GGLB11, KTAS12, BWV12, KK13, ZCL14, KCG15, SJR16]. We formally define the Best-k-Arm problem as follows.

Definition 1.1 (Best-k-Arm). An instance of Best-k-Arm is a set of stochastic arms $\mathcal{I} = \{A_1, A_2, \ldots, A_n\}$. Each arm has a 1-sub-Gaussian reward distribution with an unknown mean in $[0, 1/2]$.

At each step, algorithm $\mathcal{A}$ chooses an arm and observes an i.i.d. sample from its reward distribution. The goal of $\mathcal{A}$ is to identify the $k$ arms with the largest means in $\mathcal{I}$ using as few samples as possible. Let $\mu[i]$ denote the $i$-th largest mean in an instance of Best-k-Arm. We assume that $\mu[k] > \mu[k+1]$ in order to ensure the uniqueness of the solution.

Note that in our upper bound, we assume that all reward distributions are 1-sub-Gaussian$^1$, which is a standard assumption in multi-armed bandit literature. In our lower bound (Theorem 1.1), however, we assume that all reward distributions are sub-Gaussian.

---

$^1$ A distribution $\mathcal{D}$ is $\sigma$-sub-Gaussian, if it holds that $\mathbf{E}_{X \sim \mathcal{D}}[\exp(tX - t\mathbf{E}_{X \sim \mathcal{D}}[X])] \leq \exp(\sigma^2 t^2/2)$ for all $t \in \mathbb{R}$. 

assume that all reward distributions are Gaussian with unit variance\(^2\).

When we only want to identify the single best arm, we get the following Best-1-Arm problem, which is a well-studied special case of Best-\(k\)-Arm. The problem plays an important role in our lower bound for Best-\(k\)-Arm.

**Definition 1.2 (Best-1-Arm).** The Best-1-Arm problem is a special case of Best-\(k\)-Arm where \(k = 1\).

Generally, we focus on algorithms that solve Best-\(k\)-Arm with probability at least \(1 - \delta\).

**Definition 1.3 (δ-correct Algorithms).** \(A\) is a \(δ\)-correct algorithm for Best-\(k\)-Arm if and only if \(A\) returns the correct answer with probability at least \(1 - \delta\) on every Best-\(k\)-Arm instance \(I\).

**1.1 Our Results**

Before stating our results on the Best-\(k\)-Arm problem, we first define a few useful notations that characterize the hardness of Best-\(k\)-Arm instances.

**1.1.1 Notations**

**Means and gaps.** Let \(\mu_A\) denote the mean of arm \(A\). \(\mu[i]\) denotes the \(i\)-th largest mean among all arms in a specific instance. We define the gap of arm \(A\) as

\[
\Delta_A = \begin{cases} 
\mu_A - \mu[k+1], & \mu_A \geq \mu[k], \\
\mu[k] - \mu_A, & \mu_A \leq \mu[k+1].
\end{cases}
\]

Note that the gap of an arm is the minimum value by which its mean needs to change in order to alter the top \(k\) arms. We let \(\Delta[i]\) denote the gap of the \(i\)-th largest arm.

**Arm groups.** Let \(\varepsilon_r\) denote \(2^{-r}\). For an instance \(I\) of Best-\(k\)-Arm and positive integer \(r\), we define the arm groups as

\[
G_{r}^{\text{large}} = \{A \in I : \mu_A \geq \mu[k], \Delta_A \in (\varepsilon_{r+1}, \varepsilon_r]\}, \quad \text{and}
\]

\[
G_{r}^{\text{small}} = \{A \in I : \mu_A \leq \mu[k+1], \Delta_A \in (\varepsilon_{r+1}, \varepsilon_r]\}.
\]

In other words, \(G_{r}^{\text{large}}\) and \(G_{r}^{\text{small}}\) contain the arms with gaps in \((\varepsilon_{r+1}, \varepsilon_r] \) among and outside the best \(k\) arms, respectively.

Note that since we assume that the mean of each arm is in \([0, 1/2]\), the gap of every arm is at most 1/2. Therefore by definition each arm is contained in one of the arm groups.

We also use the following shorthand notations:

\[
G_{\geq r}^{\text{large}} = \bigcup_{i=r}^{\infty} G_{i}^{\text{large}} \quad \text{and} \quad G_{\geq r}^{\text{small}} = \bigcup_{i=r}^{\infty} G_{i}^{\text{small}}.
\]

**1.1.2 Lower Bound**

In order to state our instance-wise lower bound precisely, we need to elaborate what is an instance. By Definition 1.1, a given instance is a set of arms, meaning the particular input order of the arms should not matter. Note that there indeed exists algorithms that take advantage of the input order and may perform better for some “lucky” input orders than the others\(^3\). In order to prove a tighter lower bound, we need to consider all possible input orders and take the average. From technical perspective, we use the following definition of an instance.

\(^2\)For arbitrary distributions, one may be able to distinguish two distributions with very close means using very few samples. It is impossible to establish a nontrivial lower bound in such generality.

\(^3\)For example, a sorting algorithm can first check if the input sequence \(a_1, \ldots, a_n\) is in increasing order in \(O(n)\) time, and then run an \(O(n \log n)\) time algorithm. This algorithm is particularly fast for a particular input order.
**Definition 1.4** (Instance). An instance is considered as a random permutation of a sequence of arms. Consequently, the sample complexity of an algorithm on an instance should be considered as the average of the number of samples over all permutations.

In fact, the random permutation is crucial to establishing instance-wise lower bounds for Best-$k$-Arm (i.e., the minimum number of samples that every $\delta$-correct algorithm for Best-$k$-Arm needs to take on an instance). Without the random permutation, the algorithm might use fewer samples on some "lucky" permutations than on others, and it is impossible to prove a tight instance-wise lower bound as ours. The use of random permutation to define instance-wise lower bounds is also used in computational geometry [ABC09] and the Best-1-Arm problem [CL15 CL16b].

We say that an instance of Best-$k$-Arm is Gaussian, if all reward distributions are normal distributions with unit variance.

**Theorem 1.1.** There exists a constant $\delta_0 > 0$, such that for any $\delta < \delta_0$, every $\delta$-correct algorithm for Best-$k$-Arm takes

$$\Omega \left( H \ln \delta^{-1} + H^{\text{large}} + H^{\text{small}} \right)$$

samples in expectation on every Gaussian instance. Here $H = \sum_{i=1}^{n} \Delta_{[i]}^{-2}$,

$$H^{\text{large}} = \sum_{i=1}^{\infty} \left| G_i^{\text{large}} \right| \cdot \max_{j \geq 1} \varepsilon_j^{-2} \ln \left| G_j^{\text{small}} \right|,$$

and

$$H^{\text{small}} = \sum_{i=1}^{\infty} \left| G_i^{\text{small}} \right| \cdot \max_{j \leq i} \varepsilon_j^{-2} \ln \left| G_j^{\text{large}} \right|.$$  

We notice that Simchowitz et al. [SJR16], independently of our work, derived instance-wise lower bounds for Best-$k$-Arm similar to Theorem 1.1 using a somewhat different method.

### 1.1.3 Upper Bound

**Theorem 1.2.** For all $\delta > 0$, there is a $\delta$-correct algorithm for Best-$k$-Arm that takes

$$O \left( H \ln \delta^{-1} + \tilde{H} + \tilde{H}^{\text{large}} + \tilde{H}^{\text{small}} \right)$$

samples in expectation on every instance. Here

$$\tilde{H} = \sum_{i=1}^{n} \Delta_{[i]}^{-2} \ln \Delta_{[i]}^{-1},$$

$$\tilde{H}^{\text{large}} = \sum_{i=1}^{\infty} \left| G_i^{\text{large}} \right| \sum_{j=1}^{i} \varepsilon_j^{-2} \ln \left| G_j^{\text{small}} \right|,$$

and

$$\tilde{H}^{\text{small}} = \sum_{i=1}^{\infty} \left| G_i^{\text{small}} \right| \sum_{j=1}^{i} \varepsilon_j^{-2} \ln \left| G_j^{\text{large}} \right|.$$  

The following theorem relates the $\tilde{H}^{\text{large}}$ and $\tilde{H}^{\text{small}}$ terms to $H^{\text{large}}$ and $H^{\text{small}}$ in the lower bound.

**Theorem 1.3.** For every Best-$k$-Arm instance, the following statements hold:

1. $\tilde{H}^{\text{large}} + \tilde{H}^{\text{small}} = O \left( \left( H^{\text{large}} + H^{\text{small}} \right) \ln \ln n \right).$

2. $\tilde{H}^{\text{large}} + \tilde{H}^{\text{small}} = O \left( H \ln k \right).$
Table 1: Upper Bounds of Best-k-Arm

| Source   | Sample Complexity                                      |
|----------|--------------------------------------------------------|
| GGL12    | $O(H \ln \delta^{-1} + H \ln H)$                      |
| KTAS12   | $O(H \ln \delta^{-1} + H \ln H)$                      |
| CLK+14   | $O(H \ln \delta^{-1} + H \ln H)$                      |
| CGL16    | $O(H \ln \delta^{-1} + \bar{H} + H \ln k)$            |
| This paper | $O(H \ln \delta^{-1} + \bar{H} + \bar{H}\text{large} + \bar{H}\text{small})$ |

Combining Theorems 1.1, 1.2 and 1.3(1), our algorithm is instance-wise optimal within doubly-logarithmic factors (i.e., $\ln \ln n, \ln \ln \Delta^{-1}[i]$). In other words, the sample complexity of our algorithm on every single instance nearly matches the minimum number of samples that every $\delta$-correct algorithm has to take on that instance.

Theorem 1.2 and Theorem 1.3(2) also imply that our algorithm strictly dominates the state-of-the-art algorithm for Best-k-Arm obtained in [CGL16], which achieves a sample complexity of

$$\begin{align*}
O \left( \sum_{i=1}^{n} \Delta^{-2}[i] \left( \ln \delta^{-1} + \ln k + \ln \ln \Delta^{-1}[i] \right) \right) \\
= O \left( H \ln \delta^{-1} + H \ln k + \bar{H} \right).
\end{align*}$$

In particular, we give a specific example in Appendix A in which the sample complexity achieved by Theorem 1.2 is significantly better than that obtained in [CGL16]. See Table 1 for more previous upper bounds on the sample complexity of Best-k-Arm.

1.2 Related Work

**Best-1-Arm.** In the Best-1-Arm problem, the algorithm is required to identify the arm with the largest mean. As a special case of Best-k-Arm, the problem has a history dating back to 1954 [Bec54]. The problem continues to attract significant attention over the past decade [AB10, EDMM06, MT04, JMNB14, KKS13, CL15, CL16a, GK16, CLO16].

**Combinatorial pure exploration.** The combinatorial pure exploration problem, which further generalizes the cardinality constraint in Best-k-Arm (i.e., to choose exactly $k$ arms) to combinatorial constraints (e.g., matroid constraints), was also studied [CLK+14, CGL16, GLG+16].

**PAC learning.** In the PAC learning setting, the algorithm is required to find an approximate solution to the pure exploration problem. The sample complexity of Best-1-Arm and Best-k-Arm in PAC setting has been extensively studied. A tight (worst case) bound of $\Theta(n\varepsilon^{-2} \ln \delta^{-1})$ was obtained for the PAC version of the Best-1-Arm problem in [EDMM02, EDMM06, MT04]. The worst case sample complexity of Best-k-Arm in the PAC setting has also been well-studied [KS10, KTAS12, ZCL14, CLTL15].

2 PRELIMINARIES

**Kullback-Leibler divergence.** Let $KL(P, Q)$ denote the Kullback-Leibler divergence from distribution $Q$ to $P$. The following well-known fact (e.g., a special case of [Duc07]) states the Kullback-Leibler divergence between two normal distributions with unit variance.
Fact 2.1. Let $N(\mu, \sigma^2)$ denote the normal distribution with mean $\mu$ and variance $\sigma^2$. It holds that
\[
\text{KL}(N(\mu_1, 1), N(\mu_2, 1)) = \frac{(\mu_1 - \mu_2)^2}{2}.
\]

**Binary relative entropy.** Let
\[
d(x, y) = x \ln(x/y) + (1 - x) \ln((1 - x)/(1 - y))
\]
be the binary relative entropy function. The monotonicity of $d(\cdot, \cdot)$ is useful to our following analysis.

Fact 2.2. For $0 \leq y \leq y_0 \leq x_0 \leq x \leq 1$, $d(x, y) \geq d(x_0, y_0)$.

**Probability and expectation.** $\Pr_{A, \mathcal{I}}$ and $E_{A, \mathcal{I}}$ denote the probability and expectation when algorithm $A$ runs on instance $\mathcal{I}$. These notations are useful since we frequently consider the execution of different algorithms on various instances in our proof of the lower bound.

**Change of Distribution.** The following “Change of Distribution” lemma, developed in [KCC15], is a useful tool to quantify the behavior of an algorithm when the instance is modified.

**Lemma 2.1** (Change of Distribution). Suppose algorithm $A$ runs on $n$ arms. $\mathcal{I} = (A_1, A_2, \ldots, A_n)$ and $\mathcal{I}' = (A_1', A_2', \ldots, A_n')$ are two sequences of arms. $\tau_i$ denotes the number of samples taken on $A_i$. For any event $\mathcal{E}$ in $\mathcal{F}_\sigma$, where $\sigma$ is an almost-surely finite stopping time with respect to the filtration $\{\mathcal{F}_t\}_{t \geq 0}$, it holds that
\[
\sum_{i=1}^{n} E_{A, \mathcal{I}}(\tau_i) \text{KL}(A_i, A_i') \geq d \left( \Pr_{A, \mathcal{I}}[\mathcal{E}], \Pr_{A, \mathcal{I}'}[\mathcal{E}] \right).
\]

3 LOWER BOUND

Throughout our proof of the lower bound, we assume that the reward distributions of all arms are Gaussian distributions with unit variance. Moreover, we assume that the number of arms is sufficiently large. This assumption is used only once in the proof of Lemma 3.3. Note that when there is only a constant number of arms, our lower bound $\Omega(H_{\text{large}} + H_{\text{small}})$ is implied by the $\Omega(H \ln \delta^{-1})$ term.

3.1 Instance Embedding

The following simple lemma is useful in lower bounding the expected number of samples taken from an arm in the top-$k$ set, by restricting to a Best-1-Arm instance embedded in the original Best-$k$-Arm instance. We postpone its proof to Appendix C.

**Lemma 3.1** (Instance Embedding). Let $\mathcal{I}$ be a Best-$k$-Arm instance. Let $A$ be an arm among the top $k$ arms, and $\mathcal{I}^{\text{emb}}$ be a Best-1-Arm instance consisting of $A$ and a subset of arms in $\mathcal{I}$ outside the top $k$ arms. If some algorithm $\mathcal{A}$ solves $\mathcal{I}$ with probability $1 - \delta$ while taking less than $N$ samples on $A$ in expectation, there exists another algorithm $\mathcal{A}^{\text{emb}}$ that solves $\mathcal{I}^{\text{emb}}$ with probability $1 - \delta$ while taking less than $N$ samples on $A$ in expectation.

3.2 Proof of Theorem [1.1]

We show a lower bound on the number of samples required by each arm separately, and then the lower bound stated in Theorem 1.1 follows from a direct summation. Formally, we have the following lemma.

**Lemma 3.2.** Let $\mathcal{I}$ be an instance of Best-$k$-Arm. There exist universal constants $\delta$ and $c$ such that for all $1 \leq j \leq i$, any $\delta$-correct algorithm for Best-$k$-Arm takes at least $c \delta^{-2} \ln(\ln G_{\geq j})$ samples on every arm $A \in G_{\text{large}}^i$. The same holds if we swap $G_{\text{large}}$ and $G_{\text{small}}$.

Before proving Lemma 3.2, we show that Theorem 1.1 follows from Lemma 3.2 directly.
Proof of Theorem 3.1. Since the $\Omega(H \ln \delta^{-1})$ lower bound has been established in Theorem 2 of [CLK+14], it remains to show that the sample complexity is lower bounded by both $\Omega(H_{\text{large}})$ and $\Omega(H_{\text{small}})$. Let $\mathcal{A}$ be a $\delta$-correct algorithm for Best-$k$-Arm. According to Lemma 3.2, $\mathcal{A}$ draws at least $c \cdot \max_{j \leq i} \varepsilon_j^{-2} \ln |G_{g_j}|$ samples from each arm in $G_i^{\text{large}}$. Therefore $\mathcal{A}$ draws at least

$$\sum_{i=1}^{\infty} c_{i}^{\text{large}} \cdot c \cdot \max_{j \leq i} \varepsilon_j^{-2} \ln |G_{g_j}| = \Omega(H_{\text{large}})$$

samples in total from the arms in $G^{\text{large}}$. The $\Omega(H_{\text{small}})$ lower bound is analogous. \qed

3.3 Reduction to Best-1-Arm

In order to prove Lemma 3.2, we construct a Best-1-Arm instance consisting of one arm in $G_i^{\text{large}}$ and all arms in $G_i^{\text{small}}$. By Instance Embedding (Lemma 3.1), to lower bound the number of samples taken on each arm in $G_i^{\text{large}}$, it suffices to prove that every algorithm for Best-1-Arm takes sufficiently many samples on the best arm. Formally, we would like to show the following key technical lemma.

Lemma 3.3. Let $\mathcal{I}$ be an instance of Best-1-Arm consisting of one arm with mean $\mu$ and $n$ arms with means on $[\mu - \Delta, \mu]$. There exist universal constants $\delta$ and $c$ (independent of $n$ and $\Delta$) such that for any algorithm $\mathcal{A}$ that correctly solves $\mathcal{I}$ with probability $1 - \delta$, the expected number of samples drawn from the optimal arm is at least $c \Delta^{-2} \ln n$.

The proof of Lemma 3.3 is somewhat technical and we present it in the next subsection. Now we prove Lemma 3.2 from Lemma 3.3 by reducing a Best-1-Arm instance to an instance of Best-$k$-Arm using the Instance Embedding technique. Intuitively, if an algorithm $\mathcal{A}$ solves Best-$k$-Arm without taking sufficient number of samples from a specific arm, we may extract an instance of Best-1-Arm and derive a contradiction to Lemma 3.3.

Proof of Lemma 3.2. Let $\delta_0$ and $c_0$ be the constants in Lemma 3.3. We claim that Lemma 3.2 holds for constants $\delta = \delta_0$ and $c = c_0/4$.

Suppose for a contradiction that when $\delta$-correct algorithm $\mathcal{A}$ runs on Best-$k$-Arm instance $\mathcal{I}$, the number of samples drawn from arm $A \in G_i^{\text{large}}$ is less than $c \varepsilon_j^{-2} \ln |G_{g_j}|$ for some $j \leq i$.

We construct a Best-1-Arm instance $\mathcal{I}^{\text{new}}$ consisting of $A$ and all arms in $G_i^{\text{small}}$. By Instance Embedding (Lemma 3.1), there exists algorithm $\mathcal{A}^{\text{new}}$ that solves $\mathcal{I}^{\text{new}}$ with probability $1 - \delta$, while the number of samples drawn from arm $A$ is upper bounded by $c \varepsilon_j^{-2} \ln |G_{g_j}|$ in expectation.

However, Lemma 3.3 implies that $\mathcal{A}^{\text{new}}$ must take more than

$$c_0 \Delta^{-2} \ln n \geq 4c(\varepsilon_i + \varepsilon_j)^{-2} \ln |G_{g_j}| \geq c \varepsilon_j^{-2} \ln |G_{g_j}|$$

samples on the optimal arm, which leads to a contradiction. The case that $G^{\text{large}}$ and $G^{\text{small}}$ are swapped is analogous. \qed

3.4 Reduction to Symmetric Best-1-Arm

In order to prove Lemma 3.4, we first study a special case that the instance consists of one optimal arm and several sub-optimal arms with equal means (we call it a Symmetric Best-1-Arm instance). For the symmetric Best-1-Arm instances, we have the following lower bound on the best arm.

Lemma 3.4. Let $\mathcal{I}$ be an instance of Best-1-Arm with one arm with mean $\mu$ and $n$ arms with mean $\mu - \Delta$. There exist universal constants $\delta$ and $c$ (independent of $n$ and $\Delta$) such that for any algorithm $\mathcal{A}$ that correctly solves $\mathcal{I}$ with probability $1 - \delta$, the expected number of samples drawn from the optimal arm is at least $c \Delta^{-2} \ln n$. 

Proof of Lemma 3.3. We claim that the lemma holds for constants \( \delta = 0.5 \) and \( c = 1 \).

Recall that \( \mathcal{N}(\mu, \sigma^2) \) denotes the normal distribution with mean \( \mu \) and variance \( \sigma^2 \). Let \( \mathcal{I} \) be the instance consisting of arm \( A^* \) with mean \( \mu \) and \( n \) arms with mean \( \mu - \Delta \), and \( \mathcal{I}^{\text{new}} \) be the instance obtained from \( \mathcal{I} \) by replacing the reward distribution of \( A^* \) with \( \mathcal{N}(\mu - \Delta, 1) \). \( \tau \) denotes the number of samples drawn from \( A^* \).

Let \( \mathcal{E} \) be the event that \( \hat{A} \) identifies arm \( A^* \) as the best arm. Recall that \( \Pr_{\hat{A}, \mathcal{I}} \) and \( \Pr_{\hat{A}, \mathcal{I}} \) denote the probability and expectation when algorithm \( \hat{A} \) runs on instance \( \mathcal{I} \) respectively. Since \( \hat{A} \) solves \( \mathcal{I} \) correctly with probability at least \( 1 - \delta \), we have \( \Pr_{\hat{A}, \mathcal{I}}(\mathcal{E}) \geq 1 - \delta \). On the other hand, \( \mathcal{I}^{\text{new}} \) consists of \( n + 1 \) completely identical arms. By Definition 1.4, \( \hat{A} \) takes a random permutation of \( \mathcal{I}^{\text{new}} \) as its input. Therefore the probability that \( \hat{A} \) returns each arm is the same, and it follows that \( \Pr_{\hat{A}, \mathcal{I}^{\text{new}}}(\mathcal{E}) \leq 1/(n + 1) \).

By Change of Distribution (Lemma 2.1), we have

\[
\frac{1}{2} \Pr_{\hat{A}, \mathcal{I}}[\tau] \Delta^2 = \Pr_{\hat{A}, \mathcal{I}}[\tau] \cdot \KL(\mathcal{N}(\mu, 1), \mathcal{N}(\mu - \Delta, 1))
\geq d \left( \Pr_{\hat{A}, \mathcal{I}}[\mathcal{E}], \Pr_{\hat{A}, \mathcal{I}^{\text{new}}}[\mathcal{E}] \right)
\geq d(1 - \delta, 1/(n + 1))
\geq (1 - \delta) \ln n.
\]

Therefore we conclude that

\[
\Pr_{\hat{A}, \mathcal{I}}[\tau] \geq 2(1 - \delta) \Delta^{-2} \ln n \geq c \Delta^{-2} \ln n.
\]

Given Lemma 3.4, Lemma 3.3 may appear to be quite intuitive, as the symmetric instance \( \mathcal{I}^{\text{sym}} \) seems to be the worst case. However, a rigorous proof of Lemma 3.3 is still quite nontrivial and is in fact the most technical part of the lower bound proof. The proof consists of several steps which transform a general instance \( \mathcal{I} \) of Best-1-Arm to a symmetric instance \( \mathcal{I}^{\text{sym}} \).

Suppose that some algorithm \( \hat{A} \) violates Lemma 3.3 on a Best-1-Arm instance \( \mathcal{I} \). We divide the interval \([\mu - \Delta, \mu]\) into \( n^{0.9} \) short segments, then at least one segment contains \( n^{0.1} \) arms. We construct a smaller and denser instance \( \mathcal{I}^{\text{dense}} \) consisting of the optimal arm and \( n^{0.1} \) arms from the same segment. By Instance Embedding, there exists algorithm \( \hat{A}^{\text{new}} \) that solves \( \mathcal{I}^{\text{dense}} \) while taking few samples on the optimal arm. Note that the reduction crucially relies on the fact that since our lower bound is logarithmic in \( n \), the bound merely shrinks by a constant factor after the number of arms decreases to \( n^{0.1} \).

Finally, we transform \( \mathcal{I}^{\text{dense}} \) into a symmetric Best-1-Arm instance \( \mathcal{I}^{\text{sym}} \) consisting of the optimal arm in \( \mathcal{I}^{\text{dense}} \) along with \( n^{0.1} \) copies of one of the sub-optimal arms. We also define an algorithm \( \hat{A}^{\text{sym}} \) that solves \( \mathcal{I}^{\text{sym}} \) with few samples drawn from the optimal arm, thus contradicting Lemma 3.3. The full proof of Lemma 3.3 is postponed to Appendix C.

4 UPPER BOUND

4.1 Building Blocks

We start by introducing three subroutines that are useful for building our algorithm for Best-k-Arm.

PAC algorithm for Best-k-Arm. PAC-Best-k is a PAC algorithm for Best-k-Arm adapted from the PAC-SamplePrune algorithm in [CGL10]. PAC-Best-k is guaranteed to partition the given arm set into two sets \( S_{\text{large}} \) and \( S_{\text{small}} \), such that \( S_{\text{large}} \) approximates the best \( k \) arms with high probability.

Lemma 4.1. PAC-Best-k(\( \mathcal{S}, k, \varepsilon, \delta \)) takes

\[
O \left( |\mathcal{S}| \varepsilon^{-2} \left[ \ln \delta^{-1} + \ln \min(k, |\mathcal{S}| - k) \right] \right)
\]
samples and returns a partition \((S_{\text{large}}, S_{\text{small}})\) of \(S\) with \(|S_{\text{large}}| = k\) and \(|S_{\text{small}}| = |S| - k\). Let \(\mu_{[k]}\) and \(\mu_{[k+1]}\) denote the \(k\)-th and the \((k+1)\)-th largest means in \(S\). With probability \(1 - \delta\), it holds that
\[
\mu_A \geq \mu_{[k]} - \varepsilon \quad \text{for all } A \in S_{\text{large}},
\]
\[
\mu_A \leq \mu_{[k+1]} + \varepsilon \quad \text{for all } A \in S_{\text{small}}.
\]

Lemma \(4.1\) is proved in Appendix D. We say that a specific call to PAC-Best-\(k\) returns correctly if both (1) and (2) hold.

**PAC algorithms for Best-1-Arm.** EstMean-Large and EstMean-Small approximate the largest and the smallest mean among several arms respectively. Both algorithms can be easily implemented by calling PAC-Best-\(k\) with \(k = 1\), and then sampling the best arm identified by PAC-Best-\(k\).

**Lemma 4.2.** Both EstMean-Large\((S, \varepsilon, \delta)\) and EstMean-Small\((S, \varepsilon, \delta)\) take \(O(|S|\varepsilon^{-2}\ln \delta^{-1})\) samples and output a real number. Each of the following inequalities holds with probability \(1 - \delta\):
\[
\left|\text{EstMean-Large}(S, \varepsilon, \delta) - \max_{A \in S} \mu_A\right| \leq \varepsilon
\]
\[
\left|\text{EstMean-Small}(S, \varepsilon, \delta) - \min_{A \in S} \mu_A\right| \leq \varepsilon
\]

Lemma \(4.2\) is proved in Appendix D. We say that a specific call to EstMean-Large (or EstMean-Small) returns correctly if inequality (3) (or (1)) holds.

**Elimination procedures.** Finally, Elim-Large and Elim-Small are two elimination procedures. Roughly speaking, Elim-Large guarantees that after the elimination, the fraction of arms with means above the larger threshold \(\theta_{\text{large}}\) is bounded by a constant. Meanwhile, a fixed arm with mean below the smaller threshold \(\theta_{\text{small}}\) are unlikely to be eliminated. Analogously, Elim-Small removes arms with means below \(\theta_{\text{small}}\), and preserves arms above \(\theta_{\text{large}}\). The properties of Elim-Large and Elim-Small are formally stated below.

**Lemma 4.3.** Both Elim-Large\((S, \theta_{\text{small}}, \theta_{\text{large}}, \delta)\) and Elim-Small\((S, \theta_{\text{small}}, \theta_{\text{large}}, \delta)\) take \(O(|S|\varepsilon^{-2}\ln \delta^{-1})\) samples and return a set \(T \subseteq S\). For Elim-Large and a fixed arm \(A^* \in S\) with \(\mu_{A^*} \leq \theta_{\text{small}}\), it holds with probability \(1 - \delta\) that \(A^* \in T\) and
\[
|\{A \in T : \mu_A \geq \theta_{\text{large}}\}| \leq |T|/10.
\]
Similarly, for Elim-Small and fixed \(A^* \in S\) with \(\mu_{A^*} \geq \theta_{\text{large}}\), it holds with probability \(1 - \delta\) that \(A^* \in T\) and
\[
|\{A \in T : \mu_A \leq \theta_{\text{small}}\}| \leq |T|/10.
\]

Lemma \(4.3\) is proved in Appendix D. We say that a call to Elim-Large (or Elim-Small) returns correctly if inequality (4) (or (1)) holds.

**4.2 Algorithm**

Our algorithm for Best-\(k\)-Arm, Bilateral-Elimination, is formally described below. Bilateral-Elimination takes a parameter \(k\), an instance \(I\) of Best-\(k\)-Arm and a confidence level \(\delta\) as input, and returns the best \(k\) arms in \(I\).

Throughout the algorithm, Bilateral-Elimination maintains two sets of arms \(S_r\) and \(T_r\) for each round \(r\). \(S_r\) contains the arms that are still under consideration at the beginning of round \(r\), while \(T_r\) denotes the set of arms that have been included in the answer. We say that an arm is removed (or eliminated) at round \(r\), if it is in \(S_r \setminus S_{r+1}\). Note that we may remove an arm either because its mean is so small that it cannot be among the best \(k\) arms, or its mean is large enough so that we decide to include it in the answer. This justifies the name of our algorithm, Bilateral-Elimination.

In each round \(r\), Bilateral-Elimination performs the following four steps.
Therefore during the elimination process, it is crucial that such misclassified arms are not mistakenly eliminated. The following observation, due to a simple union bound, lower bounds the probability of each good event.

**Algorithm 1: Bilateral-Elimination**

**Input:** Parameter $k$, instance $I$, and confidence $\delta$.
**Output:** The best $k$ arms in $I$.

1. $S_1 \leftarrow I$; $T_1 \leftarrow 0$;
2. for $r = 1$ to $\infty$ do
3.  $k_{r,\text{large}} \leftarrow k - |T_r|$; $k_{r,\text{small}} \leftarrow |S_r| - k_{r,\text{large}}$;
4.  if $k_{r,\text{large}} = 0$ then return $T_r$;
5.  if $k_{r,\text{small}} = 0$ then return $T_r \cup S_r$;
6.  $\delta_r \leftarrow \delta/(20r^2)$;
7.  $(S_{r,\text{large}}, S_{r,\text{small}}) \leftarrow \text{PAC-Best-k}(S_r, k_{r,\text{large}}, \varepsilon_r/8, \delta_r)$;
8.  $\theta_{r,\text{large}} \leftarrow \text{EstMean-Large}(S_{r,\text{large}}, \varepsilon_r/8, \delta_r)$;
9.  $\theta_{r,\text{small}} \leftarrow \text{EstMean-Small}(S_{r,\text{large}}, \varepsilon_r/8, \delta_r)$;
10. $\delta_r' \leftarrow \delta / \min(k_{r,\text{large}}, k_{r,\text{small}})$;
11. $S_{r+1} \leftarrow \text{Elim-Large}(S_{r,\text{large}}, \theta_{r,\text{large}} + \varepsilon_r/8, \theta_{r,\text{large}} + \varepsilon_r/4, \delta_r') \cup \text{Elim-Small}(S_{r,\text{small}}, \theta_{r,\text{small}} - \varepsilon_r/4, \theta_{r,\text{small}} - \varepsilon_r/8, \delta_r')$;
12. $T_{r+1} \leftarrow T_r \cup (S_{r,\text{large}} \setminus S_{r+1})$;

**Step 1: Initialization.** Bilateral-Elimination first calculates $k_{r,\text{large}}$ and $k_{r,\text{small}}$, which indicate that it needs to identify the $k_{r,\text{large}}$ largest arms (or equivalently, the $k_{r,\text{small}}$ smallest arms) in $S_r$. In the base case that either $k_{r,\text{large}} = 0$ or $k_{r,\text{small}} = 0$, it directly returns the answer.

**Step 2: Find a PAC solution.** Then Bilateral-Elimination calls PAC-Best-k to partition $S_r$ into $S_{r,\text{large}}$ and $S_{r,\text{small}}$ with size $k_{r,\text{large}}$ and $k_{r,\text{small}}$ respectively, such that $S_{r,\text{large}}$ denotes an approximation of the best $k_{r,\text{large}}$ arms in $S_r$.

**Step 3: Estimate Thresholds.** After that, Bilateral-Elimination calls EstMean-Large and EstMean-Small to compute two thresholds $\theta_{r,\text{large}}$ and $\theta_{r,\text{small}}$. $\theta_{r,\text{large}}$ is an estimation of the largest mean in $S_{r,\text{small}}$, which is approximately the mean of the $(k_{r,\text{large}} + 1)$-th largest arm in $S_r$. Analogously, $\theta_{r,\text{small}}$ approximates the $k_{r,\text{large}}$-th largest mean in $S_r$.

It might seem weird at first glance that $\theta_{r,\text{large}}$ and $\theta_{r,\text{small}}$ approximates the $(k_{r,\text{large}} + 1)$-th mean and the $k_{r,\text{large}}$-th mean respectively, implying that $\theta_{r,\text{large}}$ is expected to be smaller than $\theta_{r,\text{small}}$. In fact, the superscript “large” in $\theta_{r,\text{large}}$ indicates that it is the threshold used for eliminating arms in $S_{r,\text{large}}$.

**Step 4: Elimination.** Finally, Bilateral-Elimination calls Elim-Large and Elim-Small to eliminate the arms in $S_{r,\text{large}}$ that are significantly larger than $\theta_{r,\text{large}}$, and the arms in $S_{r,\text{small}}$ that are much smaller than $\theta_{r,\text{small}}$. The arms removed from $S_{r,\text{large}}$ are included into the answer.

**Caveats.** Note that our algorithm uses a different confidence level, $\delta_r'$, in Step 4. Intuitively, at most $\min(k_{r,\text{large}}, k_{r,\text{small}})$ arms among the best $k_{r,\text{large}}$ arms in $S_r$ are misclassified as “small arms” by PAC-Best-k. Therefore during the elimination process, it is crucial that such misclassified arms are not mistakenly eliminated. As a result, we need a union bound on these arms, which contributes to the min($k_{r,\text{large}}, k_{r,\text{small}}$) factor in our confidence level.

**4.3 Observations**

We start our analysis of Bilateral-Elimination with a few simple yet useful observations.

**Good events.** We define $\mathcal{E}_r^{\text{good}}$ as the event that in round $r$, all the five calls to PAC-Best-k, EstMean, and Elim return correctly. These events are crucial to our following analysis, as they guarantee that the partition $(S_{r,\text{large}}, S_{r,\text{small}})$ and thresholds $\theta_{r,\text{large}}$ and $\theta_{r,\text{small}}$ are sufficiently accurate, and additionally, Elim eliminates a sufficiently large fraction of arms. The following observation, due to a simple union bound, lower bounds the probability of each good event.

**Observation 4.1.** $\Pr[\mathcal{E}_r^{\text{good}}] \geq 1 - 5\delta_r$. 

9
Valid executions. We say that an execution of Bilateral-Elimination is valid at round $r$, if and only if the following two conditions are satisfied:

- For each $1 \leq i < r$, event $E^\text{good}_i$ happens. (i.e., all calls to subroutines return correctly in previous rounds.)
- The union of $T_r$ and the best $k_r^\text{large}$ arms in $S_r$ is the correct answer of the Best-$k$-Arm instance. In other words, no arms have been incorrectly eliminated in previous rounds.

Moreover, an execution is valid if it is valid at every round before it terminates. We define $E^{\text{valid}}$ to be the event that an execution of Bilateral-Elimination is valid.

Thresholds. In the following, we bound the thresholds $\theta^\text{large}_r$ and $\theta^\text{small}_r$ returned by subroutine EstMean conditioning on $E^\text{good}_r$. Let $\mu^\text{large}_r$ and $\mu^\text{small}_r$ denote the means of the $k_r^\text{large}$-th and the $(k_r^\text{large} + 1)$-th largest arms in $S_r$. We show that $\theta^\text{large}_r$ and $\theta^\text{small}_r$ are $O(\varepsilon_r)$-approximations of $\mu^\text{small}_r$ and $\mu^\text{large}_r$ conditioning on the good event $E^\text{good}_r$. The proof of the following observation is postponed to Appendix D.

Observation 4.2. Conditioning on $E^\text{good}_r$,

\[
\theta^\text{large}_r \in [\mu^\text{small}_r - \varepsilon_r/8, \mu^\text{small}_r + \varepsilon_r/4],
\]

\[
\theta^\text{small}_r \in [\mu^\text{large}_r - \varepsilon_r/4, \mu^\text{large}_r + \varepsilon_r/8].
\]

Number of remaining arms. Finally, we show that conditioning on the validity of an execution, the number of remaining arms at the beginning of each round can be upper bounded in terms of $|G^\text{large}_{\geq r}|$ and $|G^\text{small}_{\geq r}|$. The following observation, proved in Appendix D, is crucial to analyzing the sample complexity of our algorithm.

Observation 4.3. Conditioning on $E^{\text{valid}}$, it holds that $k_r^\text{large} \leq 2|G^\text{large}_{\geq r}|$ and $k_r^\text{small} \leq 2|G^\text{small}_{\geq r}|$.

4.4 Correctness

Recall that $E^{\text{valid}}$ denotes the event that the execution of Bilateral-Elimination is valid. The following lemma, proved in Appendix D, shows that event $E^{\text{valid}}$ happens with high probability.

Lemma 4.4. $Pr[E^{\text{valid}}] \geq 1 - \delta$.

We show that Bilateral-Elimination always returns the correct answer conditioning on $E^{\text{valid}}$, thus proving that Bilateral-Elimination is $\delta$-correct.

Lemma 4.5. Bilateral-Elimination returns the correct answer with probability at least $1 - \delta$.

Proof of Lemma 4.5. It suffices to show that conditioning on $E^{\text{valid}}$, the algorithm always returns the correct answer. In fact, if Bilateral-Elimination terminates at round $r$, it either returns $T_r$ at Line 4 or returns $T_r \cup S_r$ at Line 6. According to the second property guaranteed by the validity at round $r$, the answer returned by Bilateral-Elimination must be correct.

It remains to show that Bilateral-Elimination does not run forever. Recall that $\Delta_{[k]} = \mu_{[k]} - \mu_{[k+1]}$ is the gap between the $k$-th and the $(k + 1)$-th largest means in the original instance $I$. We choose a sufficiently large $r^*$ that satisfies $\varepsilon_{r^*} < \Delta_{[k]}$. By definition, we have $G^\text{large}_{\geq r^*} = G^\text{small}_{\geq r^*} = \emptyset$. Then Observation 4.3 implies that $k_{r^*}^\text{large} = k_{r^*}^\text{small} = 0$, if the algorithm does not terminate before round $r^*$. Therefore the algorithm either terminates at or before round $r^*$. This completes the proof.
4.5 Sample Complexity

We prove the following Lemma 4.6, which bounds the sample complexity of Bilateral-Elimination conditioning on $\mathcal{E}^{\text{valid}}$. Then Theorem 1.2 directly follows from Lemma 4.5 and Lemma 4.6. The proof of Theorem 1.3 is postponed to the appendix.

**Lemma 4.6.** Conditioning on event $\mathcal{E}^{\text{valid}}$, Bilateral-Elimination takes $O(H \ln \delta^{-1} + H_{\text{large}} + H_{\text{small}} + \bar{H})$ samples.

**Proof of Lemma 4.6.** We consider the $r$-th round of the algorithm. Recall that $k_r^{\text{large}} + k_r^{\text{small}} = |S_r|$. According to Lemmas 4.1 through 4.3 PAC-Best-k takes

$$O(|S_r| \varepsilon_r^{-2} \ln \delta^{-1} + \ln \min (k_r^{\text{large}}, k_r^{\text{small}}))$$

samples. EstMean-Large and EstMean-Small take

$$O((k_r^{\text{large}} + k_r^{\text{small}}) \varepsilon_r^{-2} \ln \delta^{-1}) = O(|S_r| \varepsilon_r^{-2} \ln \delta^{-1})$$

samples in total, while Elim-Large and Elim-Small take

$$O(k_r^{\text{large}} \varepsilon_r^{-2} \ln \delta_r^{-1}) + O(k_r^{\text{small}} \varepsilon_r^{-2} \ln \delta_r^{-1})$$

$$= O(|S_r| \varepsilon_r^{-2} \ln \delta^{-1} + \ln \min (k_r^{\text{large}}, k_r^{\text{small}}))$$

samples conditioning on $\mathcal{E}^{\text{valid}}$. Clearly the sample complexity in round $r$ is dominated by (7).

**Simplify and split the sum:** By Observation 4.3, conditioning on event $\mathcal{E}^{\text{valid}}$, $k_r^{\text{large}}$ and $k_r^{\text{small}}$ are bounded by $2 |C_r^{\text{large}}|$ and $2 |G_r^{\text{small}}|$ respectively. Thus it suffices to bound the sum of $H_r^{(1)} + H_r^{(2, \text{large})} + H_r^{(2, \text{small})}$, where

$$H_r^{(1)} = (|C_r^{\text{large}}| + |G_r^{\text{large}}|) \varepsilon_r^{-2} (\ln \delta^{-1} + \ln r),$$

$$H_r^{(2, \text{large})} = \varepsilon_r^{-2} |C_r^{\text{large}}| \ln |G_r^{\text{small}}|,$$

$$H_r^{(2, \text{small})} = \varepsilon_r^{-2} |G_r^{\text{small}}| \ln |C_r^{\text{large}}|.$$  

In fact, since

$$\ln \delta_r^{-1} = \ln \delta^{-1} + \ln (20r^2) = O(\ln \delta^{-1} + \ln r),$$

the $|S_r| \varepsilon_r^{-2} \ln \delta^{-1}$ term in (7) is bounded by $H_r^{(1)}$. Moreover, the $|S_r| \varepsilon_r^{-2} \ln k_r^{\text{large}} k_r^{\text{small}}$ term is smaller than or equal to

$$\varepsilon_r^{-2} (k_r^{\text{large}} \ln k_r^{\text{small}} + k_r^{\text{small}} \ln k_r^{\text{large}}),$$

and is thus upper bounded by $H_r^{(2, \text{large})} + H_r^{(2, \text{small})}$.

In Appendix D, we show with a straightforward calculation that

$$\sum_{r=1}^{\infty} H_r^{(1)} = O\left( H \ln \delta^{-1} + \bar{H} \right),$$

$$\sum_{r=1}^{\infty} H_r^{(2, \text{large})} = O\left( \bar{H}_{\text{large}} \right),$$

and

$$\sum_{r=1}^{\infty} H_r^{(2, \text{small})} = O\left( \bar{H}_{\text{small}} \right).$$

Then the lemma directly follows. \qed
Finally, we prove our main result on the upper bound side.

**Proof of Theorem 1.2.** Let

\[ T = H \ln \delta^{-1} + \tilde{H} + \tilde{H}_{\text{large}} + \tilde{H}_{\text{small}}. \]

Lemma 4.5 and Lemma 4.6 together imply that conditioning on an event that happens with probability \(1 - \delta\), Bilateral-Elimination returns the correct answer and takes \(O(T)\) samples. Using the parallel simulation trick in [CL15, Theorem H.5], we can obtain an algorithm which uses \(O(T)\) samples in expectation (unconditionally), thus proving Theorem 1.2. \(\square\)

**References**

[AB10] Jean-Yves Audibert and Sébastien Bubeck. Best arm identification in multi-armed bandits. In *COLT*, 2010.

[ABC09] Peyman Afshani, Jérémy Barbay, and Timothy M Chan. Instance-optimal geometric algorithms. In *FOCS*, 2009.

[Bec54] Robert E. Bechhofer. A single-sample multiple decision procedure for ranking means of normal populations with known variances. *The Annals of Mathematical Statistics*, pages 16–39, 1954.

[BWV12] Sébastien Bubeck, Tengyao Wang, and Nitin Viswanathan. Multiple identifications in multi-armed bandits. *arXiv preprint arXiv:1205.3181*, 2012.

[CGL16] Lijie Chen, Anupam Gupta, and Jian Li. Pure exploration of multi-armed bandit under matroid constraints. In *29th Annual Conference on Learning Theory*, pages 647–669, 2016.

[CL15] Lijie Chen and Jian Li. On the optimal sample complexity for best arm identification. *arXiv preprint arXiv:1511.03774*, 2015.

[CL16a] Alexandra Carpentier and Andrea Locatelli. Tight (lower) bounds for the fixed budget best arm identification bandit problem. *arXiv preprint arXiv:1605.09004*, 2016.

[CL16b] Lijie Chen and Jian Li. Open problem: Best arm identification: Almost instance-wise optimality and the gap entropy conjecture. In *COLT*, 2016.

[CLK+14] Shouyuan Chen, Tian Lin, Irwin King, Michael R Lyu, and Wei Chen. Combinatorial pure exploration of multi-armed bandits. In *NIPS*, pages 379–387, 2014.

[CLQ16] Lijie Chen, Jian Li, and Mingda Qiao. Towards instance optimal bounds for best arm identification. *arXiv preprint arXiv:1608.06031*, 2016.

[CLTL15] Wei Cao, Jian Li, Yifei Tao, and Zhiye Li. On top-k selection in multi-armed bandits and hidden bipartite graphs. In *NIPS*, pages 1036–1044, 2015.

[Duc07] John Duchi. Derivations for linear algebra and optimization. *Berkeley, California*, 2007.

[EDMM02] Eyal Even-Dar, Shie Mannor, and Yishay Mansour. Pac bounds for multi-armed bandit and markov decision processes. In *COLT*, pages 255–270. Springer, 2002.

[EDMM06] Eyal Even-Dar, Shie Mannor, and Yishay Mansour. Action elimination and stopping conditions for the multi-armed bandit and reinforcement learning problems. *JMLR*, 7:1079–1105, 2006.

[GGL12] Victor Gabillon, Mohammad Ghavamzadeh, and Alessandro Lazaric. Best arm identification: A unified approach to fixed budget and fixed confidence. In *NIPS*, pages 3212–3220, 2012.

[GGLB11] Victor Gabillon, Mohammad Ghavamzadeh, Alessandro Lazaric, and Sébastien Bubeck. Multibandit best arm identification. In *NIPS*, pages 2222–2230, 2011.
[GK16] Aurélien Garivier and Emilie Kaufmann. Optimal best arm identification with fixed confidence. In Conference on Learning Theory (COLT), 2016.

[GLG+16] Victor Gabillon, Alessandro Lazaric, Mohammad Ghavamzadeh, Ronald Ortner, and Peter Bartlett. Improved learning complexity in combinatorial pure exploration bandits. In Proceedings of the 19th International Conference on Artificial Intelligence and Statistics, pages 1004–1012, 2016.

[JMNB14] Kevin Jamieson, Matthew Malloy, Robert Nowak, and Sébastien Bubeck. lil’ucb: An optimal exploration algorithm for multi-armed bandits. COLT, 2014.

[KCG15] Emilie Kaufmann, Olivier Cappé, and Aurélien Garivier. On the complexity of best arm identification in multi-armed bandit models. The Journal of Machine Learning Research, 2015.

[KK13] Emilie Kaufmann and Shivaram Kalyanakrishnan. Information complexity in bandit subset selection. In COLT, pages 228–251, 2013.

[KKS13] Zohar Karnin, Tomer Koren, and Oren Somekh. Almost optimal exploration in multi-armed bandits. In ICML, pages 1238–1246, 2013.

[KS10] Shivaram Kalyanakrishnan and Peter Stone. Efficient selection of multiple bandit arms: Theory and practice. In ICML, pages 511–518, 2010.

[KTAS12] Shivaram Kalyanakrishnan, Ambuj Tewari, Peter Auer, and Peter Stone. Pac subset selection in stochastic multi-armed bandits. In ICML, pages 655–662, 2012.

[MT04] Shie Mannor and John N Tsitsiklis. The sample complexity of exploration in the multi-armed bandit problem. JMLR, 5:623–648, 2004.

[Rob85] Herbert Robbins. Some aspects of the sequential design of experiments. In Herbert Robbins Selected Papers, pages 169–177. Springer, 1985.

[SJR16] Max Simchowitz, Kevin Jamieson, and Benjamin Recht. Towards a richer understanding of adaptive sampling in the moderate-confidence regime. 2016.

[ZCL14] Yuan Zhou, Xi Chen, and Jian Li. Optimal pac multiple arm identification with applications to crowdsourcing. In ICML, pages 217–225, 2014.
Organization of the Appendix

In the appendix, we present the missing proofs in this paper. In Appendix A, we first discuss a specific instance mentioned in Section 1, showing that our upper bound strictly improves previous algorithms. In Appendix B, we prove Fact 2.2 in Section 2. In Appendix C, we prove the Instance Embedding lemma (Lemma 3.1) and the relatively technical Lemma 3.3 which relates a general instance of Best-1-Arm to a symmetric instance. In Appendix D, we discuss the implementation of the building blocks of our algorithm, prove a few useful and observations, and finally complete the missing proofs of other lemmas and theorems.

A Specific Best-\(k\)-Arm Instance

We show that our upper bound results (Theorem 1.2 and Theorem 1.3) strictly improve the state-of-the-art algorithm for Best-\(k\)-Arm obtained in [CGL16] by calculating the sample complexity of both algorithms on a specific Best-\(k\)-Arm instance.

We consider a family of instances parametrized by integer \(n\) and \(\varepsilon \in (0, 1/4)\). Each instance consists of \(n\) arms with mean 0, \(n\) arms with mean \(1/2\), along with two arms with means \(1/4 + \varepsilon\) and \(1/4 - \varepsilon\) respectively. We are required to identify the top \(n + 1\) arms. By definition, the gap of every arm with mean 0 or 1/2 is \(1/4 + \varepsilon\), while the gaps of the remaining two arms are \(2\varepsilon\). As \(\varepsilon\) tends to zero, the arms with gap \(1/4 + \varepsilon\) become relatively simple: an algorithm can decide whether to include them in the answer or not with few samples. The hardness of the instance is then concentrated on the two arms with close means.

For simplicity, we assume that the confidence level, \(\delta\), is set to a constant. Then the \(O(H \ln \delta^{-1})\) term in the upper bounds are dominated by the \(O(\tilde{H})\) term. By a direct calculation, we have

\[
\tilde{H} = \Theta(n + \varepsilon^{-2} \ln \ln \varepsilon^{-1}).
\]

Let \(m\) be the integer that satisfies \(2\varepsilon \in (\varepsilon_{m+1}, \varepsilon_m]\). Then we have

\[
|G_1^{\text{large}}| = |G_1^{\text{small}}| = n, \text{ and } |C_m^{\text{large}}| = |C_m^{\text{small}}| = 1.
\]

It follows from the definition of \(H^{\text{large}}\) and \(H^{\text{small}}\) that

\[
H^{\text{large}} = H^{\text{small}} = O(n \ln n + \varepsilon^{-2}).
\]

By Theorem 1.2 for constant \(\delta\), our algorithm takes

\[
O(\tilde{H} + \tilde{H}^{\text{large}} + \tilde{H}^{\text{small}}) = O(n \ln n + \varepsilon^{-2} \ln \ln \varepsilon^{-1})
\]
samples on this instance.

On the other hand, the upper bound achieved by PAC-SamplePrune algorithm is

\[
O(H + H \ln n) = O(n \ln n + \varepsilon^{-2} \ln \ln \varepsilon^{-1} + \varepsilon^{-2} \ln n).
\]

Note that if \(\varepsilon = 1/n\), our algorithm takes \(O(n^2 \ln \ln n)\) samples, while PAC-SamplePrune takes \(O(n^2 \ln n)\) samples. This indicates that there is a logarithmic gap between the state-of-the-art upper bound and the instance-wise lower bound, while we narrow down the gap to a doubly-logarithmic factor.

B Missing Proof in Section 2

Fact 2.2 (restated) For \(0 \leq y \leq y_0 \leq x_0 \leq x \leq 1\), \(d(x, y) \geq d(x_0, y_0)\).
Proof of Fact 2.3 Taking the partial derivative yields
\[
\frac{\partial d(x, y)}{\partial x} = \ln \frac{x(1 - y)}{y(1 - x)},
\]
\[
\frac{\partial d(x, y)}{\partial y} = \frac{y - x}{y(1 - y)}.
\]
Therefore when \( x \geq y \), \( d(x, y) \) is increasing in \( x \) and decreasing in \( y \), which proves the fact.

C  Missing Proofs in Section 3

C.1  Proof of Lemma 3.1

Lemma 3.1 (restated) Let \( I \) be a Best-k-Arm instance. Let \( A \) be an arm among the top \( k \) arms, and \( I^{emb} \) be a Best-1-Arm instance consisting of \( A \) and a subset of arms in \( I \) outside the top \( k \) arms. If some algorithm \( \mathbb{A} \) solves \( I \) with probability \( 1 - \delta \) while taking less than \( N \) samples on \( A \) in expectation, there exists another algorithm \( \mathbb{A}^{emb} \) that solves \( I^{emb} \) with probability \( 1 - \delta \) while taking less than \( N \) samples on \( A \) in expectation.

Proof of Lemma 3.1 We construct the following algorithm \( \mathbb{A}^{emb} \) for \( I^{emb} \). Given the instance \( I^{emb} \), \( \mathbb{A}^{emb} \) first augments the instance into \( I \) by adding a fictitious arm for each arm in \( I \setminus I^{emb} \). Then \( \mathbb{A}^{emb} \) simulates \( \mathbb{A} \) on the Best-k-Arm instance \( I \). When \( \mathbb{A} \) requires a sample from an arm in \( I^{emb} \), \( \mathbb{A}^{emb} \) draws a sample and sends it to \( \mathbb{A} \). If \( \mathbb{A} \) requires a sample from an arm outside \( I^{emb} \), \( \mathbb{A}^{emb} \) generates a fictitious sample on its own and then sends it to \( \mathbb{A} \). When \( \mathbb{A} \) terminates and returns a subset \( S \) of \( k \) arms, \( \mathbb{A}^{emb} \) terminates and returns an arbitrary arm in \( S \cap I^{emb} \).

Note that when \( \mathbb{A}^{emb} \) runs on instance \( I^{emb} \), the algorithm \( \mathbb{A} \) simulated by \( \mathbb{A}^{emb} \) effectively runs on the instance \( I \). It follows that with probability \( 1 - \delta \), \( \mathbb{A} \) returns the correct answer of the Best-k-Arm instance \( I \), and thus \( A \) is the only arm in both \( I^{emb} \) and the set \( S \) returned by \( \mathbb{A} \). Therefore, \( \mathbb{A}^{emb} \) correctly solves the Best-1-Arm instance \( I^{emb} \) with probability at least \( 1 - \delta \). Moreover, the expected number of samples drawn from arm \( A \) is less than \( N \) by our assumptions.

C.2  Proof of Lemma 3.3

Lemma 3.3 (restated) Let \( I \) be an instance of Best-1-Arm consisting of one arm with mean \( \mu \) and \( n \) arms with means on \( [\mu - \Delta, \mu] \). There exist universal constants \( \delta \) and \( c \) (independent of \( n \) and \( \Delta \)) such that for all algorithm \( \mathbb{A} \) that correctly solves \( I \) with probability \( 1 - \delta \), the expected number of samples drawn from the optimal arm is at least \( c\Delta^{-2} \ln n \).

Proof of Lemma 3.3 Let \( \delta_0 \) and \( c_0 \) be the constants in Lemma 3.1. We claim that Lemma 3.3 holds for constants \( \delta = \delta_0/3 \) and \( c = c_0\delta_0/30 \).

Suppose for a contradiction that when algorithm \( \mathbb{A} \) runs on Best-1-Arm instance \( I \), it outputs the correct answer with probability \( 1 - \delta \) and the optimal arm \( A_0 \) is sampled less than \( c\Delta^{-2} \ln n \) times in expectation.

Overview. Our proof follows the following five steps.

Step 1. We apply Instance Embedding to obtain a smaller yet denser (in the sense that all suboptimal arms have almost identical means) instance \( I^{dense} \), together with a new algorithm \( \mathbb{A}^{new} \) that solves \( I^{dense} \) by taking few samples on the optimal arm with high probability.

Step 2. We obtain a symmetric instance \( I^{sym} \) from \( I^{dense} \) by making the suboptimal arms identical to each other. We also define an algorithm \( \mathbb{A}^{sym} \) for instance \( I^{sym} \).

Step 3. To analyze algorithm \( \mathbb{A}^{sym} \) on instance \( I^{sym} \), we define the notion of “mixed arms”, which return a fixed number of samples from one distribution, and then switch to another distribution permanently. We transform \( I^{dense} \) into an instance \( I^{mix} \) with mixed arms.
Step 4. We show by Change of Distribution that when $\mathcal{A}_{\text{new}}$ runs on $T_{\text{mix}}$, it also returns the correct answer with few samples on the optimal arm.

Step 5. We show that the execution of $\mathcal{A}_{\text{sym}}$ on $T_{\text{sym}}$ is, in a sense, equivalent to the execution of $\mathcal{A}_{\text{new}}$ on $T_{\text{mix}}$. This finally leads to a contradiction to Lemma 3.4.

The reductions involved in the proof is illustrated in Figure 1.

**Step 1: Construct $T_{\text{dense}}$ and $\mathcal{A}_{\text{new}}$.** We first construct a new Best-1-Arm instance $T_{\text{dense}}$ in which the sub-optimal arms have almost identical means. Let $\mu_0$ denote the mean of the optimal arm $A_0$. We divide the interval $[\mu_0 - \Delta, \mu_0]$ into $n^{0.9}$ segments, each with length $\Delta/n^{0.9}$. Set $m = n^{0.1}$. By the pigeonhole principle, we can assume that $A_1, A_2, \ldots, A_m$ are $m$ arms with means in the same interval. Let $\mu_i$ denote the mean of arm $A_i$. By construction, $\mu_0 - \mu_i \leq \Delta$ for all $1 \leq i \leq m$ and $|\mu_i - \mu_j| \leq \Delta/n^{0.9}$ for all $1 \leq i, j \leq m$.

We simply let $T_{\text{dense}} = \{A_0, A_1, A_2, \ldots, A_m\}$. By Instance Embedding (Lemma 3.1), there exists an algorithm $\mathcal{A}_{\text{new}}$ that solves $T_{\text{dense}}$ with probability $1 - \delta$ while taking less than $c\Delta^{-2}\ln n$ samples on $A_0$ in expectation. We will focus on instance $T_{\text{dense}}$ in the rest of our proof.

Recall that $Pr_{\mathcal{A}, T}$ and $E_{\mathcal{A}, T}$ denote the probability and expectation when algorithm $\mathcal{A}$ runs on instance $T$ respectively. Let $\tau_i$ denote the number of samples taken on $A_i$. Then we have

$$E_{\mathcal{A}_{\text{new}}, T_{\text{dense}}}[\tau_0] \leq c\Delta^{-2}\ln n.$$  

Let $N = c\delta^{-1}\Delta^{-2}\ln n$. By Markov’s inequality,

$$Pr_{\mathcal{A}_{\text{new}}, T_{\text{dense}}}[\tau_0 \geq N] \leq \frac{c\Delta^{-2}\ln n}{N} = \delta.$$  

Let $E$ denote the event that the algorithm returns the correct answer while taking at most $N$ samples on arm $A_0$. The union bound implies that

$$Pr_{\mathcal{A}_{\text{new}}, T_{\text{dense}}}[E] \geq 1 - 2\delta.$$  

**Step 2: Construct $T_{\text{sym}}$ and $\mathcal{A}_{\text{sym}}$.** Let $T_{\text{sym}}$ be the Best-1-Arm instance consisting of arm $A_0$ and $m = n^{0.1}$ copies of arm $A_1$. We define algorithm $\mathcal{A}_{\text{sym}}$ as follows. Given instance $T_{\text{sym}}$, $\mathcal{A}_{\text{sym}}$ simulates algorithm $\mathcal{A}_{\text{new}}$ as if $\mathcal{A}_{\text{new}}$ is running on instance $T_{\text{dense}}$. When $\mathcal{A}_{\text{new}}$ requires a sample from an arm $A$ that has not been pulled $N$ times (recall that $N = c\delta^{-1}\Delta^{-2}\ln n$), $\mathcal{A}_{\text{sym}}$ draws a sample from $A$ and sends it to $\mathcal{A}_{\text{new}}$. When the number of pulls on $A$ exceeds $N$ for the first time, $\mathcal{A}_{\text{sym}}$ assigns a random number $\pi(A)$ from $\{1, 2, \ldots, m\}$ to arm $A$, such that $\pi(A)$ is different from every number that has already been assigned to another arm. If this step cannot be performed because all numbers in $\{1, 2, \ldots, m\}$ have been used up, $\mathcal{A}_{\text{sym}}$ simply terminates without returning an answer. After that, upon each pull of $A$, $\mathcal{A}_{\text{sym}}$ sends a sample drawn from $N(\mu_{\pi(A)}, 1)$ to $\mathcal{A}_{\text{new}}$. (Recall that $\mu_i$ denotes the mean of arm $A_i$ in $T_{\text{dense}}$.) Finally, $\mathcal{A}_{\text{sym}}$ outputs what $\mathcal{A}_{\text{new}}$ outputs.

**Step 3: Construct mixed arms and $T_{\text{mix}}$.** In order to analyze the execution of $\mathcal{A}_{\text{sym}}$ on instance $T_{\text{sym}}$, it is helpful to define $m$ “mixed arms”. For $1 \leq i \leq m$, the $i$-th mixed arm, denoted by $M_i$, returns a sample drawn from $N(\mu_i, 1)$ (i.e., the reward distribution of arm $A_1$) when it is pulled for the first $N$ times. After $N$ pulls, $M_i$ returns samples from $N(\mu_i, 1)$ as $A_i$ does. For ease of notation, we also let $M_0$ denote $A_0$. Let $T_{\text{mix}}$ denote the Best-1-Arm instance $\{M_0, M_1, M_2, \ldots, M_m\}$.

---

As shown in the analysis in Step 5, we only care the behavior of $A_{\text{sym}}$ when the labels are not used up.
Step 4: Run $A_{\text{new}}$ on $\mathcal{I}^{\text{mix}}$. Now suppose we run $A_{\text{new}}$ on instance $\mathcal{I}^{\text{mix}}$. In fact, we may view each arm (either $A_i$ or $M_i$) as two separate ‘semi-arms’. When $A_{\text{new}}$ samples arm $A_i$ in the first $N$ times, it pulls the first semi-arm of $A_i$. After $A_i$ has been pulled $N$ times, $A_{\text{new}}$ pulls the second semi-arm. From this perspective, $\mathcal{I}^{\text{mix}}$ is simply obtained from $\mathcal{I}^{\text{dense}}$ by changing the first semi-arm of each arm $A_i$ ($1 \leq i \leq m$) from $\mathcal{N}(\mu_i, 1)$ to $\mathcal{N}(\mu_1, 1)$. Since the first semi-arm is sampled at most $N$ times by $A_{\text{new}}$, it follows from Change of Distribution (Lemma 2.1) that

$$d \left( \Pr_{A_{\text{new}}, \mathcal{I}^{\text{dense}}} [\mathcal{E}], \Pr_{A_{\text{new}}, \mathcal{I}^{\text{mix}}} [\mathcal{E}] \right)$$

$$\leq \sum_{i=1}^{m} N \cdot \text{KL} (\mathcal{N}(\mu_i, 1), \mathcal{N}(\mu_1, 1))$$

$$= \frac{N}{2} \sum_{i=1}^{m} (\mu_i - \mu_1)^2$$

$$\leq \frac{c_0}{2} n^{-1.7} \ln n.$$

Here the second step follows from

$$\text{KL}(\mathcal{N}(\mu_1, 1), \mathcal{N}(\mu_2, 1)) = (\mu_1 - \mu_2)^2 / 2.$$

The third step is due to $N = c_0^{-1} \Delta^{-2} \ln n$, $m = n^{0.1}$, and $|\mu_1 - \mu_i| \leq \Delta / n^{0.9}$.

For sufficiently large $n$, we have

$$\frac{c_0}{2} n^{-1.7} \ln n < d(1 - 2\delta, 1 - 3\delta).$$

Recall that $\Pr_{A_{\text{new}}, \mathcal{I}^{\text{dense}}} [\mathcal{E}] \geq 1 - 2\delta$. It follows from the monotonicity of $d(\cdot, \cdot)$ (Fact 2.2) that

$$\Pr_{A_{\text{new}}, \mathcal{I}^{\text{mix}}} [\mathcal{E}] \geq 1 - 3\delta.$$

Step 5: Analyze $A_{\text{sym}}$ and derive a contradiction to Lemma 3.4. For clarity, let $\text{Expr}^{\text{mix}}$ denote the experiment that $A_{\text{new}}$ runs on $\mathcal{I}^{\text{mix}}$, and $\text{Expr}^{\text{sym}}$ denote the experiment that $A_{\text{sym}}$ runs on $\mathcal{I}^{\text{sym}}$. Step 4 implies that event $\mathcal{E}$ happens with probability at least $1 - 3\delta$ in experiment $\text{Expr}^{\text{mix}}$.

In the following, we derive the likelihood of an arbitrary execution of $\text{Expr}^{\text{mix}}$ in which event $\mathcal{E}$ happens, and prove that this execution has the same likelihood in experiment $\text{Expr}^{\text{sym}}$. As a result, $A_{\text{sym}}$ also returns the correct answer with probability at least $1 - 3\delta$. Moreover, according to our construction, $A_{\text{sym}}$ always takes at most $N$ samples on arm $A_0$. On the other hand, since $\mu_0 - \mu_1 \leq \Delta$, Lemma 3.4 implies that no algorithm can solve $A_{\text{sym}}$ correctly with probability $1 - \delta_0 = 1 - 3\delta$ while taking less than

$$c_0 \Delta^{-2} \ln m = 30 c_0^{-1} \Delta^{-2} \cdot (0.1 \ln n) = N$$

samples on $A_0$ in expectation. This leads to a contradiction and finishes the proof.

Technicalities: equivalence between $\text{Expr}^{\text{mix}}$ and $\text{Expr}^{\text{sym}}$. For ease of notation, we assume in the following that algorithm $A_{\text{new}}$ is deterministic\footnote{In fact, this assumption is without loss of generality: the argument still holds conditioning on the randomness of $A_{\text{new}}$.}. Then the only randomness in experiment $\text{Expr}^{\text{mix}}$ stems from the random permutation of arms at the beginning, and the samples drawn from the arms.

We consider an arbitrary run of experiment $\text{Expr}^{\text{mix}}$ in which event $\mathcal{E}$ happens (i.e., $A_{\text{new}}$ returns the optimal arm before taking more than $N$ samples from it). For $0 \leq i \leq m$, let $\sigma(i)$ denote the index of the $i$-th arm received by algorithm $A_{\text{new}}$. (i.e., the $i$-th arm received by $A_{\text{new}}$ is $M_{\sigma(i)}$.). By definition, $\sigma$ is a uniformly random permutation of $\{0, 1, \ldots, m\}$. Let $\text{obs}_i$ denote the sequence of samples that $A_{\text{new}}$ observes from the $i$-th arm. Then the likelihood of this execution is given by

$$\frac{1}{(m + 1)!} \sum_{\sigma} \prod_{i=0}^{m} f_{M_{\sigma(i)}} (\text{obs}_i).$$
Here we sum over all random permutations $\sigma$ on $\{0, 1, 2, \ldots, m\}$, and $f_{M_{\pi(i)}}(\text{obs}_i)$ denote the probability density of observing $\text{obs}_i$ on arm $M_{\pi(i)}$.

Now we compute the likelihood that in experiment $\text{Expr}^{\text{sym}}$, the algorithm $A^{\text{new}}$ simulated by $A^{\text{sym}}$ observes the same sequence of samples. Let $\lambda$ denote the random permutation of arms given to $A^{\text{sym}}$. We define

$$p^* = \lambda^{-1}(0),$$

$$\text{Long} = \{i \in \{0, 1, 2, \ldots, m\} : |\text{obs}_i| > N\},$$

$$\text{Short} = \{0, 1, \ldots, m\} \setminus (\text{Long} \cup \{p^*\}).$$

In other words, $p^*$ is the position of the optimal arm $A_0$ in $A^{\text{sym}}$. Long denote the positions of suboptimal arms that have been sampled more than $N$ times, while Short denote the remaining suboptimal arms. Note that since less than $N$ samples are taken on the optimal arm, $p^*$ is excluded from both sets.

Another source of randomness in $\text{Expr}^{\text{sym}}$ is the random numbers $\pi(\cdot)$ that $A^{\text{sym}}$ assigns to different arms. In this specific execution, function $\pi(\cdot)$ chosen by $A^{\text{sym}}$ is a random injection from $\text{Long}$ to $\{1, 2, \ldots, m\}$. By our construction of $A^{\text{sym}}$, for each $i \in \text{Long}$, the algorithm $A^{\text{new}}$ simulated by $A^{\text{sym}}$ first observes $N$ samples drawn from $\mathcal{N}(\mu_1, 1)$ (i.e., the reward distribution of arm $A_1$) on the $i$-th arm. After that, $A^{\text{new}}$ starts to observe samples drawn from $\mathcal{N}(\mu_{\pi(i)}, 1)$. Recall that the mixed arm $M_{\pi(i)}$ also returns samples in this pattern. Therefore, the likelihood of observations on the $i$-th arm is exactly

$$f_{M_{\pi(i)}}(\text{obs}_i).$$

In fact, we may express the likelihood for all arms as in (9) by extending $\pi$ into a permutation on $\{0, 1, 2, \ldots, m\}$. First, we set $\pi(p^*) = 0$. Recall that the optimal arm is sampled less than $N$ times, all the samples observed from it are drawn from $\mathcal{N}(\mu_0, 1)$, which is exactly the reward distribution of $M_0 = M_{\pi(p^*)}$. Therefore the likelihood of observations on the $i$-th arm is given by

$$f_{M_{\pi(p^*)}}(\text{obs}_{p^*}).$$

Second, we let $R = \{1, 2, \ldots, m\} \setminus \pi(\text{Long})$ denote the available labels among $\{1, 2, \ldots, m\}$. We define $\pi$ on Short by matching Short with $R$ uniformly at random. Note that since all arms in Short are sampled at most $N$ times, $A^{\text{new}}$ simulated by $A^{\text{sym}}$ always observes samples drawn from $\mathcal{N}(\mu_1, 1)$, which agrees with the first $N$ samples from every mixed arm $M_i (i \neq 0)$. Therefore, the likelihood of observations on the $i$-th arm where $i \in \text{Short}$ is also given by

$$f_{M_{\pi(i)}}(\text{obs}_i).$$

According to our analysis above, the samples from the $i$-th arm observed by the simulated $A^{\text{new}}$ in experiment $\text{Expr}^{\text{sym}}$ follows the same distribution as samples drawn from $M_{\pi(i)}$. Moreover, $\pi$ is a uniformly random permutation with the only condition that $\pi(p^*) = 0$, which is equivalent to $\pi^{-1}(0) = p^* = \lambda^{-1}(0)$. Therefore, the likelihood is given by

$$\frac{1}{m! \cdot (m + 1)!} \sum_{\pi^{-1}(0) = \lambda^{-1}(0)} \prod_{i=0}^{m} f_{M_{\pi(i)}}(\text{obs}_i).$$

Note that conditioning on $\lambda^{-1}(0) = \pi^{-1}(0)$, $\pi$ is still a uniformly random permutation on $\{0, 1, 2, \ldots, m\}$. Therefore the two likelihoods in (9) and (10) are equal. This finishes the proof of the equivalence. \qed

\section*{D Missing Proofs in Section 4}

\subsection*{D.1 Building Blocks}

\subsubsection*{D.1.1 PAC algorithm for Best-$k$-Arm}

On an instance of Best-$k$-Arm with $n$ arms, the PAC-SamplePrune algorithm in \cite{CGL16} is guaranteed to return a $\varepsilon$-optimal answer of Best-$k$-Arm with probability $1 - \delta$, using

$$O(n\varepsilon^{-2}(\ln \delta^{-1} + \ln k)).$$
samples. Here a subset of \( k \) arms \( T \subseteq \mathcal{I} \) is called \( \varepsilon \)-optimal, if after adding \( \varepsilon \) to the mean of each arm in \( T \), \( T \) becomes the best \( k \) arms in \( \mathcal{I} \).

We implement our PAC-Best-\( k(S,k,\varepsilon,\delta) \) subroutine as follows. Recall that PAC-Best-\( k \) is expected to return a partition \( (S^{\text{large}}, S^{\text{small}}) \) of the arm set \( S \). If \( k \leq |S|/2 \), we directly run PAC-SamplePrune on the Best-k-Arm instance \( S \). Otherwise, we negate the mean of all arms in \( S \) and run PAC-SamplePrune to find the top \( |S| - k \) arms in the negated instance. Finally, we return the output of PAC-SamplePrune as \( S^{\text{small}} \) and let \( S^{\text{large}} = S \setminus S^{\text{small}} \). In the following we prove Lemma 4.1.

**Proof of Lemma 4.1** By construction, the algorithm PAC-Best-\( k(S,k,\varepsilon,\delta) \) takes
\[
O(|S|\varepsilon^{-2}[\ln \delta^{-1} + \ln \min(k,|S| - k)])
\]
samples. In the following we prove that if \( k \leq |S|/2 \), the set \( T \) returned by PAC-SamplePrune is \( \varepsilon \)-optimal with probability \( 1 - \delta \). The case \( k > |S|/2 \) can be proved by an analogous argument.

Let \( S' \) denote the instance in which the mean of every arm in \( T \) is increased by \( \varepsilon \). By definition of \( \varepsilon \)-optimality, \( T \) contains the best \( k \) arms in \( S' \). Note that the \( k \)-th largest mean is \( S' \) is at least \( \mu_{[k]} \). Thus for each arm \( A \in T \), \( \mu_A \) must be at least \( \mu_{[k]} - \varepsilon \), since otherwise even after \( \mu_A \) increases by \( \varepsilon \), \( A \) is still not among the best \( k \) arms.

It also holds that every arm in \( S \setminus T \) must have a mean smaller than or equal to \( \mu_{[k+1]} + \varepsilon \). Suppose for a contradiction that \( A \in S \setminus T \) has a mean \( \mu_A > \mu_{[k+1]} + \varepsilon \). Then every arm with mean less than or equal to \( \mu_{[k+1]} \) in \( S \) still have a mean smaller than \( \mu_A \) in \( S' \). This implies that \( A \) is among the best \( k \) arms in \( S' \), which contradicts our assumption that \( A \notin T \).

**D.1.2 PAC algorithms for Best-1-Arm**

By symmetry, it suffices to implement the subroutine EstMean-Large and prove its property. In order to estimate the mean of the largest arm in \( S \), we first call PAC-Best-\( k(S,1,\varepsilon/2,\delta/2) \) to find an approximately largest arm. Then we sample the arm \( 2\varepsilon^{-2}\ln(4/\delta) \) times, and finally return its empirical mean. We prove Lemma 4.2 as follows.

**Proof of Lemma 4.2** Let \( A^* \) denote the largest arm in \( S \), and let \( A_0 \) denote the arm returned by PAC-Best-\( k(S,1,\varepsilon/2,\delta/2) \). According to Lemma 4.1, with probability \( 1 - \delta/2 \), \( \mu_{A_0} \in [\mu_{A^*} - \varepsilon/2, \mu_{A^*}] \). It follows that, with probability \( 1 - \delta/2 \),
\[
\left| \mu_{A_0} - \max_{A \in S} \mu_A \right| \leq \varepsilon/2.
\]

Let \( \hat{\mu} \) denote the empirical mean of arm \( A_0 \). By a Chernoff bound, with probability \( 1 - \delta/2 \),
\[
|\hat{\mu} - \mu_{A_0}| \leq \varepsilon/2.
\]

It follows from a union bound that with probability \( 1 - \delta/2 \),
\[
\left| \hat{\mu} - \max_{A \in S} \mu_A \right| \leq \varepsilon.
\]

Finally, we note that PAC-Best-\( k \) consumes \( O(|S|\varepsilon^{-2}\ln \delta^{-1}) \) samples as \( k = 1 \), while sampling \( A_0 \) takes \( O(\varepsilon^{-2}\ln \delta^{-1}) \) samples. This finishes the proof.

---

6More precisely, when the algorithm requires a sample from an arm, we draw a sample and return the opposite.
D.1.3 Elimination procedures

We use the Elimination procedure defined in \cite{CL15} as our subroutine Elim-Small\((S, \theta_{small}, \theta_{large}, \delta)\). The other building block Elim-Large\((S, \theta_{small}, \theta_{large}, \delta)\) can be implemented either using a procedure symmetric to Elimination, or simply by running Elim-Small\((S', -\theta_{large}, -\theta_{small}, \delta)\), where \(S'\) is obtained from \(S\) by negating the arms. In the following, we prove Lemma 4.3.

**Proof of Lemma 4.3.** Let \(T\) denote the set of arms returned by Elim-Small\((S, \theta_{small}, \theta_{large}, \delta)\). Lemma B.4 in \cite{CL15} guarantees that with probability \(1 - \delta\), the following three properties are satisfied: (1) Elim-Small takes \(O(|S|\varepsilon^{-2}\ln\delta^{-1})\) samples, where \(\varepsilon = \theta_{large} - \theta_{small}\); (2) \[
|\{A \in T : \mu_A < \theta_{small}\}| \leq |T|/10;
\]
(3) Let \(A^\ast\) be the largest arm in \(S\). If \(\mu_{A^\ast} > \theta_{large}\), then \(A^\ast \in T\).

In fact, the proof of Lemma B.4 does not rely on the fact that \(A^\ast\) is the largest arm in \(S\). Thus property (3) holds for any fixed arm in \(S\). This proves the properties of Elim-Small. The properties of Elim-Large hold due to the symmetry.

D.2 Observations

D.2.1 Proof of Observation 4.2

**Proof of Observation 4.2.** Let \(A\) denote the arm with the largest mean in \(S_{small}\). Recall that \(\mu_{small}\) denote the mean of the \((k_{large} + 1)\)-th largest mean in \(S_r\). The correctness of PAC-Best-\(k\) and Lemma 4.1 guarantee that \(\mu_A \leq \mu_{small} + \varepsilon_r/8\). Note that \(\mu_{small}\) is the \(k_{small}\)-th smallest mean in \(S_r\), while \(\mu_A\) is the largest mean among the \(k_{small}\) arms in \(S_{small} \subseteq S_r\). So it also holds that \(\mu_A \geq \mu_{small}\). Thus we have

\[
\mu_A \in [\mu_{small}^r, \mu_{small}^r + \varepsilon_r/8].
\]

Moreover, as EstMean-Large returns correctly conditioning on \(\varepsilon_{good}^r\), by Lemma 4.2 we have

\[
\theta_{large}^r \in [\mu_{small}^r - \varepsilon_r/8, \mu_{small}^r + \varepsilon_r/4].
\]

The second property follows from a symmetric argument.

D.2.2 Proof of Observation 4.3

**Proof of Observation 4.3.** Recall that \(\varepsilon_{valid}^r\) denotes the event that the execution of Bilateral-Elimination is valid. We condition on \(\varepsilon_{valid}^r\) in the following proof. In particular, conditioning on \(\varepsilon_{valid}^r, \varepsilon_{good}^r_{r-1}\) happens and \(T_{r-1}\) along with the best \(k_{large}\) arms in \(S_{r-1}\) constitute the correct answer of the original instance.

Let \(\mu_{large}^{r-1}\) and \(\mu_{small}^{r-1}\) be the \(k_{large}\)-th and the \((k_{large} + 1)\)-th largest mean in \(S_{r-1}\). As the arm with mean \(\mu_{large}^{r-1}\) is among the correct answer, we have \(\mu_{large}^{r-1} \geq \mu[k]\), where \(\mu[k]\) is the \(k\)-th largest mean in the original instance. We also have \(\mu_{small}^{r-1} \leq \mu[k+1]\) for the same reason.

Since \(\varepsilon_{good}^r_{r-1}\) happens, by Observation 4.2 we have

\[
\theta_{large}^{r-1} \leq \mu_{small}^{r-1} + \varepsilon_{r-1}/4 \leq \mu[k+1] + \varepsilon_{r-1}/4.
\]

Then the larger threshold used in Elim-Large is upper bounded by

\[
\theta_{large}^{r-1} + \varepsilon_{r-1}/4 \leq \mu[k+1] + \varepsilon_{r-1}/2 = \mu[k+1] + \varepsilon_r.
\]

Let \(T\) denote the set of arms returned Elim-Large in round \(r - 1\). We partition \(T\) into the following three parts:

\[
T^{(1)} = \{A \in T : \mu_A > \mu[k+1] + \varepsilon_r\}.
\]
\[ T(2) = \{ A \in T : \mu_{[k]} \leq \mu_A \leq \mu_{[k+1]} + \varepsilon_r \}, \]
\[ T(3) = \{ A \in T : \mu_A \leq \mu_{[k+1]} \}. \]

By Lemma 4.3 and the correctness of Elim conditioning on \( \mathcal{E}_{r-1}^{good} \), we have
\[ |T(1)| \leq |T|/10. \]

It follows that
\[ |T(2)| + |T(3)| \geq 9|T|/10 \geq |T|/2. \]

By definition of arm groups, every arm in \( T(2) \) is in \( G_{\geq r}^{large} \). In order to bound \( T(3) \), we say that an arm is misclassified into \( S_{r-1}^{large} \), if the arm is not among the best \( k_{r-1}^{large} \) arms in \( S_{r-1} \), but is included in \( S_{r-1}^{large} \). We may define misclassification into \( S_{r-1}^{small} \) similarly. As \( |S_{r-1}^{large}| = k_{r-1}^{large} \), the numbers of arms misclassified into both sides are the same.

Since the arms in \( T(3) \) are misclassified into \( S_{r-1}^{large} \), there are at least \( |T(3)| \) other arms misclassified into \( S_{r-1}^{small} \). Lemma 4.1 (along with the correctness of PAC-Best-k) guarantees that all arms misclassified into \( S_{r-1}^{small} \) have means smaller than or equal to \( \mu_{[k+1]} + \varepsilon_r/8 \). Thus by definition of arm groups, all these \( |T(3)| \) arms are also in \( G_{\geq r}^{large} \). Therefore, we have
\[ |G_{\geq r}^{large} | \geq |T(2)| + |T(3)| \geq |T|/2. \]

Note that \(|T| = k_r^{large}\). Therefore we conclude that \( k_r^{large} \leq 2|G_{\geq r}^{large}| \). The bound on \( k_r^{small} \) can be proved using a symmetric argument. \( \square \)

### D.3 Proof of Lemma 4.4

**Lemma 4.4** (restated) \( \Pr[\mathcal{E}_{r}^{valid}] \geq 1 - \delta \).

**Proof of Lemma 4.4** We prove the lemma by upper bounding the probability of \( \overline{\mathcal{E}_{r}^{valid}} \), the complement of \( \mathcal{E}_{r}^{valid} \).

**Split \( \overline{\mathcal{E}_{r}^{valid}} \).** Let \( \mathcal{E}_{r}^{bad} \) denote the event that Bilateral-Elimination is valid at round \( r \), yet it becomes invalid at round \( r + 1 \). Then we have
\[ \Pr[\overline{\mathcal{E}_{r}^{valid}}] = \sum_{r=1}^{\infty} \Pr[\mathcal{E}_{r}^{bad}]. \]

By definition of validity, event \( \mathcal{E}_{r}^{bad} \) happens in one of the following two cases:

- **Case 1:** \( \mathcal{E}_{r}^{good} \) does not happen.
- **Case 2:** \( \mathcal{E}_{r}^{good} \) happens, yet \( T_{r+1} \) together with the best \( k_{r+1}^{large} \) arms in \( S_{r+1} \) is no longer the correct answer.

The probability of Case 1 is upper bounded by \( 5\delta_r \) according to Observation 4.1. We focus on bounding the probability of Case 2 in the following.

**Misclassified arms.** Recall that \( \mu_r^{large} \) and \( \mu_r^{small} \) denote the means of the \( k_r^{large} \)-th and the \( (k_r^{large} + 1) \)-th largest arms in \( S_r \) respectively. Conditioning on the validity of the execution at round \( r \), the arm with mean \( \mu_r^{large} \) is among the best \( k \) arms in the original instance, while the arm with mean \( \mu_r^{small} \) is not. Thus we have
\[ \mu_r^{large} \geq \mu_{[k]} \geq \mu_{[k+1]} \geq \mu_r^{small}. \]

Define
\[ U_r^{large} = \{ A \in S_r^{large} : \mu_A \leq \mu_r^{small} \}. \]
and

\[ U_r^{\text{small}} = \{ A \in S_r^{\text{small}} : \mu_A \geq \mu_r^{\text{large}} \}. \]

In other words, \( U_r^{\text{large}} \) and \( U_r^{\text{small}} \) denote the set of arms “misclassified” by the PAC-Best-k subroutine into \( S_r^{\text{large}} \) and \( S_r^{\text{small}} \) in round \( r \).

**Bound the number of misclassified arms.** Note that since \( |U_r^{\text{large}}| \leq |S_r^{\text{large}}| = k_r^{\text{large}} \), and in addition, less than \( k_r^{\text{small}} \) arms in \( S_r \) have means smaller than or equal to \( \mu_r^{\text{small}} \),

\[ |U_r^{\text{large}}| \leq \min(k_r^{\text{large}}, k_r^{\text{small}}). \]

For the same reason, it holds that

\[ |U_r^{\text{small}}| \leq \min(k_r^{\text{large}}, k_r^{\text{small}}). \]

**With high probability, no misclassified arms are removed.** By Observation 4.2 conditioning on \( E_{\text{good}}^r \), we have

\[ \theta_r^{\text{large}} \geq \mu_r^{\text{small}} - \varepsilon_r / 8. \]

Therefore, when Elim-Large in Line 11 is called at round \( r \), the smaller threshold is at least

\[ \theta_r^{\text{large}} + \varepsilon_r / 8 \geq \mu_r^{\text{small}}, \]

which is larger than the mean of every arm in \( U_r^{\text{large}} \). By Lemma 4.3 and a union bound, with probability

\[ 1 - |U_r^{\text{large}}| \delta_r' \geq 1 - \min(k_r^{\text{large}}, k_r^{\text{small}}) \delta_r' = 1 - \delta_r, \]

no arms in \( U_r^{\text{large}} \) are removed by Elim-Large. For the same reason, with probability \( 1 - \delta_r \), no arms in \( U_r^{\text{small}} \) are removed by Elim-Small.

**Bound the probability of Case 2.** Thus, with probability at least \( 1 - 2\delta_r \), conditioning on \( E_{\text{good}}^r \), Elim-Large only removes arms with means larger than or equal to \( \mu_r^{\text{large}} \), and Elim-Small only removes arms with means smaller than or equal to \( \mu_r^{\text{small}} \). Consequently, every arm in \( S_r \) with mean greater than or equal to \( \mu_r^{\text{large}} \) either moves to \( T_{r+1} \) or stays in \( S_{r+1} \), which implies that Case 2 does not happen.

Therefore, the Case 2 happens with probability at most \( 2\delta_r \), and it follows that

\[ \Pr[\delta_{\text{bad}}^r] \leq 5\delta_r + 2\delta_r = 7\delta_r. \]

Finally, we have

\[ \Pr[\delta_{\text{valid}}^r] \leq \sum_{r=1}^{\infty} 7\delta_r \leq \sum_{r=1}^{\infty} \frac{7\delta}{20r^2} \geq \delta. \]

\[ \square \]

**D.4 Missing Calculation in the Proof of Lemma 4.6**

**Lemma 4.6** (restated) Conditioning on event \( E_{\text{valid}}^r \), Bilateral-Elimination takes \( O(H \ln \delta^{-1} + \bar{H}_r^{\text{large}} + \bar{H}_r^{\text{small}} + \bar{H}) \) samples.

**Proof (continued).** Recall that

\[ H_r^{(1)} = (|G_r^{\text{large}}| + |G_r^{\text{small}}|) \varepsilon_r^{-2} (\ln \delta^{-1} + \ln r), \]

\[ H_r^{(2,\text{large})} = \varepsilon_r^{-2} |G_r^{\text{large}}| \ln |G_r^{\text{small}}|, \]

\[ H_r^{(2,\text{small})} = \varepsilon_r^{-2} |G_r^{\text{small}}| \ln |G_r^{\text{large}}|. \]

Our goal is to show that

\[ \sum_{r=1}^{\infty} H_r^{(1)} = O \left( H \ln \delta^{-1} + \bar{H} \right), \]
\[
\sum_{r=1}^{\infty} H_r^{(2, \text{large})} = O(H_{\text{large}}), \text{ and } \\
\sum_{r=1}^{\infty} H_r^{(2, \text{small})} = O(H_{\text{small}}).
\]

Upper bound the \(H^{(1)}\) term: It follows from a directly calculation that
\[
\sum_{r=1}^{\infty} H_r^{(1)} = \sum_{r=1}^{\infty} \sum_{i=r}^{\infty} \left( |G_{i+1}^{\text{large}}| + |G_{i}^{\text{small}}| \right) \varepsilon_r^{-2} (\ln \delta - 1 + \ln r)
\]
\[
= \sum_{i=1}^{\infty} \left( |G_{i+1}^{\text{large}}| + |G_{i}^{\text{small}}| \right) \sum_{r=1}^{\infty} \varepsilon_r^{-2} (\ln \delta - 1 + \ln i)
\]
\[
= O\left( \sum_{i=1}^{n} \Delta_i^{-2} \left( \ln \delta - 1 + \ln \Delta_i^{-1} \right) \right).
\]

Here the second step interchanges the order of summation. The third step holds since the inner summation is always dominated by the last term. Finally, the last step is due to the fact that \(\Delta_A = \Theta(\varepsilon(i))\) for every arm \(A \in G_{i}^{\text{large}} \cup G_{i}^{\text{small}}\). Therefore we have
\[
\sum_{r=1}^{\infty} H_r^{(1)} = O(H \ln \delta^{-1} + \bar{H}).
\]

Upper bound \(H_{r}^{(2, \text{large})}\) and \(H_{r}^{(2, \text{small})}\): By definition of \(H_r^{(2, \text{large})}\), we have
\[
\sum_{r=1}^{\infty} H_r^{(2, \text{large})} = \sum_{r=1}^{\infty} \sum_{i=r}^{\infty} \varepsilon_r^{-2} |G_{i+1}^{\text{large}}| \ln |G_{i}^{\text{small}}| \ln |G_{i}^{\text{small}}|
\]
\[
= \sum_{i=1}^{\infty} |G_{i+1}^{\text{large}}| \sum_{r=1}^{\infty} \varepsilon_r^{-2} \ln |G_{i}^{\text{small}}|.
\]

Therefore we conclude that
\[
\sum_{r=1}^{\infty} H_r^{(2, \text{large})} = O(H_{\text{large}}).
\]

The bound on the sum of \(H_{r}^{(2, \text{small})}\) follows from an analogous calculation.

D.5 Proof of Theorem 1.3

Theorem 1.3 (restated) For every Best-k-Arm instance, the following statements hold:

1. \(\bar{H}^{\text{large}} + \bar{H}^{\text{small}} = O((H^{\text{large}} + H^{\text{small}}) \ln \ln n)\).

2. \(\bar{H}^{\text{large}} + \bar{H}^{\text{small}} = O(H \ln k)\).

Proof of Theorem 1.3 First Upper Bound. Recall that
\[
H^{\text{large}} = \sum_{i=1}^{\infty} |G_{i}^{\text{large}}| \cdot \max_{j \leq i} \varepsilon_j^{-2} \ln |G_{j}^{\text{small}}|, \text{ and }
\]
For brevity, let $N_r$ denote $\varepsilon_r^{-2} \ln |G_{\geq r}| = 4^r \ln |G_{\geq r}|$. We fix the value $i$. Then the $i$-th term in $\tilde{H}^\text{large}$ reduces to $|G_{i=1}^{\text{large}}| \sum_{r=1}^i N_r$. Let $r^* = \arg\max_{1 \leq r \leq N_r}$. Thus the $i$-th term in $H^\text{large}$ is simply $|G_{i=1}^{\text{large}}| N_{r^*}$, which is in general smaller than $|G_{i=1}^{\text{large}}| \sum_{r=1}^i N_r$. However, we will show that the ratio between the two terms is bounded by $O(\ln \ln n)$.

By definition of $r^*$, we have $N_{r^*} \geq N_i$. Substituting $N_{r^*}$ and $N_i$ yields

$$4^{r^*} \ln |G_{\geq r^*}^\text{small}| \geq 4^i \ln |G_{\geq i}^\text{small}|.$$

It follows that

$$4^{i-r^*} \ln |G_{\geq i}^\text{small}| \leq \ln |G_{\geq r^*}^\text{small}| \leq \ln n,$$

and thus $i - r^* = O(\ln \ln n)$.

Let $1 \leq r_1 \leq r^*$ be the smallest integer such that $N_{r_1} \geq 2^{r_1-r^*} N_{r^*}$. By substituting $N_{r_1}$ and $N_{r^*}$, we obtain

$$4^{r_1} \ln |G_{\geq r_1}^\text{small}| \geq 2^{r_1-r^*} \cdot 4^{r^*} \ln |G_{\geq r^*}^\text{small}|,$$

which further implies that

$$2^{r^*-r_1} \ln |G_{\geq r^*}^\text{small}| \leq \ln |G_{\geq r_1}^\text{small}| \leq \ln n$$

and thus $r^* - r_1 = O(\ln \ln n)$.

Therefore we have $i - r_1 = O(\ln \ln n)$, and we can bound the sum of $N_r$ as follows:

$$\sum_{r=1}^i N_r = \sum_{r=1}^{r_1-1} N_r + \sum_{r=r_1}^i N_r$$

$$\leq N_{r^*} \sum_{r=1}^{r_1-1} 2^{r-r^*} + (i - r_1 + 1) N_{r^*}$$

$$\leq (i - r_1 + 2) N_{r^*} = O(N_{r^*} \ln \ln n).$$

Here the second step follows from $N_r < 2^{r-r^*} N_{r^*}$ for $r < r_1$ (by definition of $r_1$) and $N_r \leq N_{r^*}$ for $r \geq r_1$ (by definition of $r^*$).

It then follows from a direct summation over all $i$ that

$$\tilde{H}^\text{large} = O(\tilde{H}^\text{large} \ln \ln n).$$

The bound on $\tilde{H}^\text{small}$ can be proved similarly.

**Second Upper Bound.** Note that

$$\tilde{H}^\text{large} = \sum_{i=1}^\infty |G_{i=1}^{\text{large}}| \sum_{j=1}^i \varepsilon_j^{-2} \ln |G_{\geq j}^\text{small}|$$

$$= \sum_{j=1}^\infty \varepsilon_j^{-2} \ln |G_{\geq j}^\text{small}| \sum_{i=j}^\infty |G_{i=1}^{\text{large}}|$$

$$= \sum_{i=1}^\infty \varepsilon_i^{-2} |G_{i=1}^{\text{large}}| \ln |G_{\geq i}^\text{small}|.$$

Here the second step interchanges the order of summation. By symmetry we also have

$$\tilde{H}^\text{small} = \sum_{i=1}^\infty \varepsilon_i^{-2} |G_{i=1}^\text{large}| \ln |G_{\geq i}^\text{small}|.$$  

24
It can be easily verified that for $1 \leq x \leq y$, we have

$$x \ln y + y \ln x \leq (x + y)(2 \ln x + 1).$$

(13)

Note that $\min \left( |G_{\geq i}^{\text{large}}|, |G_{\geq i}^{\text{small}}| \right) \leq k$ for all $i$. Therefore we can bound $\bar{H}_{\text{large}} + \bar{H}_{\text{small}}$ as follows:

$$\bar{H}_{\text{large}} + \bar{H}_{\text{small}} \leq \sum_{i=1}^{\infty} \varepsilon_i^{-2} \left( |G_{\geq i}^{\text{large}}| + |G_{\geq i}^{\text{small}}| \right) \ln \min \left( |G_{\geq i}^{\text{large}}|, |G_{\geq i}^{\text{small}}| \right)$$

$$= O \left( \sum_{i=1}^{\infty} \varepsilon_i^{-2} \left( |G_{\geq i}^{\text{large}}| + |G_{\geq i}^{\text{small}}| \right) \ln \left( \min \left( |G_{\geq i}^{\text{large}}|, |G_{\geq i}^{\text{small}}| \right) \ln k \right) = O(H \ln k).$$

The first step follows from (11) and (12). The second step is due to (13). The third step is due to the observation that $\min \left( |G_{\geq i}^{\text{large}}|, |G_{\geq i}^{\text{small}}| \right) \leq k$. Finally, the last step follows from a simple rearrangement of the summation:

$$\sum_{i=1}^{\infty} \varepsilon_i^{-2} \left( |G_{\geq i}^{\text{large}}| + |G_{\geq i}^{\text{small}}| \right)$$

$$= \sum_{i=1}^{\infty} \varepsilon_i^{-2} \sum_{j=i}^{\infty} \left( |G_{j}^{\text{large}}| + |G_{j}^{\text{small}}| \right)$$

$$= \sum_{j=1}^{\infty} \left( |G_{j}^{\text{large}}| + |G_{j}^{\text{small}}| \right) \sum_{i=1}^{j} \varepsilon_i^{-2}$$

$$= O \left( \sum_{j=1}^{\infty} \varepsilon_j^{-2} \left( |G_{j}^{\text{large}}| + |G_{j}^{\text{small}}| \right) \right) = O(H).$$