Optimal Simple Regret in Bayesian Best Arm Identification

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1 Abstract

We consider Bayesian best arm identification in the multi-armed bandit problem. Assuming certain continuity conditions of the prior, we characterize the rate of the Bayesian simple regret. Differing from Bayesian regret minimization (Lai, 1987), the leading factor in Bayesian simple regret derives from the region where the gap between optimal and sub-optimal arms is smaller than $\sqrt{\log T / T}$. We propose a simple and easy-to-compute algorithm with its leading factor matches with the lower bound up to a constant factor; simulation results support our theoretical findings.

2 Introduction

We consider finding the best treatment among $K$ treatments and $T$ sample size. In this problem, each arm (treatment) $i \in [K] = \{1, 2, \ldots, K\}$ is associated with (unknown) parameter $\mu_i \in [0, 1]$. We use $\mu = (\mu_1, \mu_2, \ldots, \mu_K)$ to denote the set of parameters. At each round $t = 1, 2, \ldots, T$, the forecaster, who follows some adaptive algorithm, selects an arm $I(t) \in [K]$ and receives the corresponding reward $X_{I(t)}(t) \sim \text{Bernoulli}(\mu_{I(t)})$, where 1 and 0 represent the success and the failure of the selected treatment. Let $i^* = \arg\max_i \mu_i$ and $\mu^* = \mu_{i^*}$ be the optimal (best) arm and its corresponding mean, respectively.\textsuperscript{1}

The extant literature has mainly considered two different objectives. The first involves maximizing the total reward (Robbins, 1952; Lai and Robbins, 1985), which is equivalent to minimizing the draw of suboptimal arms. Letting $N_i(T)$ be the number of draws on arm $i$ up to round $T$, the (frequentist) regret is defined as

$$\text{Reg}_\mu(T) := \sum_{i=1}^{K} \mathbb{E}_\mu[N_i(T)](\mu^* - \mu_i),$$

where $\mu$ is unknown but fixed, and the expectation here is over the randomness of the rewards and (possibly randomized) choices $I(t)$.

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\textsuperscript{1}Ties are broken arbitrarily.
The second objective is identifying the best arm. In this case, the forecaster at the end of round $T$ recommends an arm $J(T)$. The performance of the forecaster is measured by the simple regret

$$R_{\mu}(T) := \mu^* - E_{\mu}[\mu_{J(T)}],$$

(2)

which is the expected difference between the means of the best arm and recommended arm $J(T)$. The two objectives are very different. Where minimizing regret (Eq. (1)) concerns minimizing the number of draws of suboptimal arms, demanding balancing the exploration (i.e., drawing all the arms uniformly) and exploitation (i.e., drawing the empirical optimal arm), in minimizing the simple regret, the rewards received from the arms $I(t)$ ($1 \leq t \leq T$) do not matter; thus, Eq. (2) is minimized by pure exploration (Bubeck et al., 2011).

The simple regret of Eq. (2) is frequentist; it assumes that $\mu$ is (unknown but) fixed. On the other hand, we may consider a distribution of $\mu \in [0,1]^K$ and take expectation of the frequentist simple regret over the distribution. We can call this the Bayesian simple regret, which is defined as

$$R_H(T) = E_{\mu \sim H}[R_{\mu}(T)],$$

(3)

where $E_{\mu \sim H}$ marginalizes $\mu$ over the prior $H$ on $\Theta$. In this paper, we consider the problem of minimizing the Bayesian simple regret of Eq. (3). We drop the term “Bayesian” when it clearly refers Bayesian simple regret.

### 2.1 Regularity Condition

We assume the following regularity condition for the prior distribution. For $i \in [K]$, let $\mu_{\setminus i}$ be the set of $K - 1$ parameters other than $\mu_i$. For $i,j \in [K]$, let $\mu_{\setminus ij}$ be the set of $K - 2$ parameters other than $\mu_i, \mu_j$. Let $H_i(\mu_{\setminus i})$ be the joint cumulative density function of $\mu_{\setminus i}$, and $H_i(\mu_{\setminus i}|\mu_{\setminus i})$ be the conditional cumulative density function of $\mu_i$ given $\mu_{\setminus i}$. Define $H_{ij}(\mu_{\setminus ij})$, $H_{ij}(\mu_{\setminus i}|\mu_{\setminus ij})$, $H_{ij}(\mu_{\setminus i}|\mu_{\setminus ij})$ in the same way. The following assumption concerns the existence of continuous derivatives of $H_i(\mu_{\setminus i})$ and $H_{ij}(\mu_{\setminus i}|\mu_{\setminus ij})$.

**Assumption 1.** (Uniform continuity of the conditional probability density functions) There exist conditional probability density functions $h_i(\mu_i|\mu_{\setminus i})$ and $h_{ij}(\mu_i, \mu_j|\mu_{\setminus ij})$ that are uniformly continuous. Namely, for every $\epsilon > 0$ there exists $\delta(\epsilon) > 0$ such that

$$\forall |\mu_i - \lambda_i| \leq \delta, \quad |h_i(\mu_i|\mu_{\setminus i}) - h_i(\lambda_i|\mu_{\setminus i})| \leq \epsilon,$$

$$\forall |\mu_i - \lambda_i|, |\mu_j - \lambda_j| \leq \delta, \quad |h_{ij}(\mu_i, \mu_j|\mu_{\setminus ij}) - h_{ij}(\lambda_i, \lambda_j|\mu_{\setminus ij})| \leq \epsilon. \quad (4)$$

**Remark 1.** (Uniform continuity) Assumption 1 is similar to that of Lai (1987)\(^2\); however, it is slightly stronger. Namely, we assume the uniform continuity; $\delta$ in Eq. (4) does not depend on $\mu$. We also assume the uniform continuity of $h_{ij}(\mu_i, \mu_j|\mu_{\setminus ij})$, which is required to bound the probability that three or more arms have very similar means.

We consider Assumption 1 to be satisfied by most distributions of interests. For example, it is satisfied when the joint distribution is Lipshitz continuous, as in the case that each $\mu_i$ is i.i.d. as the uniform prior. However, the following demonstrates a situation in which Assumption 1 does not hold.

\(^2\)Eq. (3.17) in Theorem 3 of Lai (1987).
Example 1. (Corner case excluded by Assumption 1) Let there be three arms, \( \mu_1, \mu_2 \sim \text{Unif}(0,1) \) are independent each other, and \( \mu_3 = 1 - \mu_1 \). That is, the variables are redundant. This case violates Assumption 1 because \( h_3(\mu_3|\mu_1,\mu_2) \) has point mass on \( 1 - \mu_1 \) and is not continuous.

Nonetheless, in the rest of this paper, we adopt Assumption 1.

2.2 Main Results

Table 1 compares our results and existing results. Subsequently, we characterize the optimal rate of the Bayesian simple regret.

Table 1: Optimal rate in an undiscounted Bernoulli MAB problem with regret minimization (RM) setting and simple regret minimization (SRM) setting. The optimality presented in each column indicates that the leading factor of the corresponding measure (RM or SRM) matches the lower bound. Carpentier and Locatelli (2016) derived a lower bound for frequentist simple regret that matches with known upper bound (Audibert et al., 2010) up to constant or \( O(\log K) \), depending on model parameters.

|       | RM                        | SRM                        |
|-------|---------------------------|---------------------------|
| Frequentist | Lai and Robbins (1985) | Carpentier and Locatelli (2016) (up to \( O(\log K) \)) |
| Bayesian | Lai (1987)                | This paper (up to constant) |

According to Theorem 3 in Lai (1987), an asymptotically optimal algorithm’s Bayesian regret is

\[
\text{Reg}(T) := \mathbb{E}_{\mu \sim H} [\text{Reg}_{\mu}(T)] = \frac{1}{2} \sum_{i=1}^{K} \int_{[0,1]^{K-1}} h_i(\mu^*_{\mu,i}|\mu_{\mu,i})dH_{\mu,i}(\mu_{\mu,i}) + o((\log T)^2),
\]

where \( \mu^*_{\mu,i} = \max_{j \neq i} \mu_j \).

This paper shows that the expected Bayesian simple regret is at most

\[
R_H(T) \leq \frac{1}{T} \sum_{i=1}^{K} \int_{[0,1]^{K-1}} \mu^*_{\mu,i}(1 - \mu^*_{\mu,i}) h_i(\mu^*_{\mu,i}|\mu_{\mu,i})dH_{\mu,i}(\mu_{\mu,i}) + o\left(\frac{1}{T}\right)
\]

and derive the corresponding lower bound that matches up to a constant factor. That is, we characterize the optimal rate of Bayesian simple regret under the continuity assumption of the prior.

Among the greatest challenges for establishing the Bayesian simple regret bound is the absence of any notion for characterizing “good” algorithm. In the case of regret minimization (RM), Lai and Robbins (1985) proposed a notion of “uniformly good”; an algorithm is uniformly good if it has \( o(T^c) \) regret for any \( c > 0 \) and for any fixed parameter \( \mu \). Almost all meaningful algorithms in RM setting are uniformly good.\(^3\) The bound of Eq. (5) can be explained by (some of) the asymptotically optimal algorithms among the uniformly good algorithms. In contrast, an optimal algorithm in the context of Bayesian simple regret minimization (SRM) remains relatively unexplored. Although certain frequentist characterizations are known (Audibert et al., 2010; Carpentier and Locatelli, 2016), there remain no notions corresponding to RM’s notions of “uniformly good” or “asymptotical optimality.” Accordingly, this paper demonstrates that a minimal assumption on the prior distribution can sufficiently derive the asymptotic rate of Bayesian simple regret.

\(^3\)For example, \( \epsilon \)-greedy (Auer et al., 2002), UCB (Lai and Robbins, 1985; Auer et al., 2002), Thompson sampling (Thompson, 1933), and Minimum Empirical Divergence (Honda and Takemura, 2015) are uniformly good.
2.3 Intuitive derivation of the Bound

This section provides an informal derivation of Eq. (6). Section 3 presents the formal results.

Consider the parameters $\mu : \mu_i > \mu_i^*$ where arm $i$ is the best arm. The Kullback-Leibler (KL) divergence between parameters $(\mu_i, \mu_i^*)$ and $(\frac{\mu_i^* + \mu_i}{2}, \frac{\mu_i^* + \mu_i}{2})$ characterizes the difficulty of confirming that $\mu_i$ is larger that $\mu_i^*$. That is, the frequentist simple regret for parameter $\mu$ is approximately

$$\frac{\mu_i - \mu_i^*}{2} \exp\left(-T d_{KL}\left(\mu_i^*, \frac{\mu_i^* + \mu_i}{2}\right)\right),$$

where $d_{KL}(p, q) = p \log(p/q) + (1 - p) \log((1 - p)/(1 - q))$ is the KL divergence between two Bernoulli distributions with parameters $p, q \in (0, 1)$. Integrating this over the prior yields

$$\int_{[0,1]}^{|\mu^*_i|} \int_{[0,1]}^{|\mu_i|} \frac{\mu_i - \mu_i^*}{2} \exp\left(-T d_{KL}\left(\mu_i^*, \frac{\mu_i^* + \mu_i}{2}\right)\right) dH_i(\mu_i^*|\mu_i) dH_i(\mu_i) \approx \int_{[0,1]}^{|\mu^*_i|} \left[ -2\mu_i^*(1 - \mu_i^*) T \exp\left(-T d_{KL}\left(\mu_i^*, \frac{\mu_i^* + \mu_i}{2}\right)\right) \right]^{1-\mu_i^*} h_i(\mu_i^*|\mu_i) dH_i(\mu_i) = \int_{[0,1]}^{|\mu^*_i|} \frac{2\mu_i^*(1 - \mu_i^*) T}{T} h_i(\mu_i^*|\mu_i) dH_i(\mu_i) + o\left(\frac{1}{T}\right),$$

which is twice as Eq. (6). A more elaborated analysis removes the factor of two and yields Eq. (6). The derivation implies

- The region that matters is $\mu_i - \mu_i^* = O(1/\sqrt{T})$, which is small when $T$ is large. By Assumption 1, $h_i(\mu_i^*|\mu_i)$ is sufficiently flat in this region.

- When $|\mu_i - \mu_j| \approx O(1/\sqrt{T})$ and the other arms are substantially suboptimal, the optimal strategy invests most of the $T$ rounds into the two arms. Eq. (7) represents the information-theoretic bound of identifying the parameters $(\mu_i, \mu_j)$ (i.e., arm $i$ is better) from $(\frac{\mu_i + \mu_j}{2}, \frac{\mu_i + \mu_j}{2})$ (i.e., both arms are the same).

- Eq. (6) states that the regret is $O(K/T)$ for most of the priors. Moreover, the term $\mu_i^*(1 - \mu_i^*)$ implies that the closer the best arm to 0, 1, the more identifiable it is. This is intuitive because the KL divergence diverges around 0, 1 in Bernoulli distributions.

2.4 Dynamic Programming

Bayesian simple regret (i.e., Eq. (3)) is exactly minimized by solving the corresponding dynamic programming. However, computing such dynamic programming does not scale for moderate $K$ and $T$. The number of possible states characterizes the amount of computation required. In the Bernoulli MAB problem, the number of possible states is proportional to the number of rewards 0 and 1 for each arm, which is $O(T^{2K-1})$. Instead of computing the solution of the dynamic programming, Section 3 introduces an alternative algorithm that is easy to compute.
2.5 Related Work

The MAB problem has garnered much attention in the machine learning community because it is useful in several crucial applications such as online advertisements and A/B testings. The goal in the standard MAB problem is to maximize the sum of the rewards, which boils down to regret minimization (RM). On the other hand, there is another established branch of bandit problems, called best arm identification (BAI, Audibert et al., 2010). In BAI, the goal is to find the best treatment arm with the highest expected reward; this relates closely to classical sequential testing (Chernoff, 1959). Finding the best treatment boils down to simple regret minimization (SRM). The different goals of the two approaches mean that RM and SRM algorithms differ considerably in terms of balancing exploration and exploitation.

Best arm identification (simple regret minimization) Although the term “best arm identification” was coined in early 2010s (Audibert et al., 2010; Bubeck et al., 2011), similar ideas have attracted substantial attention in various fields (Paulson, 1964; Maron and Moore, 1997; Even-Dar et al., 2006). Audibert et al. (2010) proposed the successive rejects algorithm, which has frequentist simple regret that matches up to a constant or up to an $O(\log K)$ factor, depending on the model parameters $\mu$ (Carpentier and Locatelli, 2016).

Ordinal optimization: A particularly interesting strand of literature concerns the ordinal optimization (Ho et al., 1992; Chen et al., 2000), for which Glynn and Juneja (2004) provides a rigorous modern foundation. Although ordinal optimization and BAI are both interested in finding optimal arms, the two approaches differ markedly. The framework of Glynn and Juneja (2004) assumes that the model parameters $\mu$ are known, BAI assumes the parameters are unknown. In practice, these parameters are often unknown, necessitating the use of plug-in estimators. However, the convergence of the plug-in estimators to the true parameters is not the primal concern in ordinal optimization.

Bayesian bandit algorithms for regret minimization: Thompson sampling (Thompson, 1933), among the oldest heuristics, is known to be asymptotically optimal in terms of the frequentist regret (Granmo, 2008; Agrawal and Goyal, 2012; Kaufmann et al., 2012). One of the seminal results regarding Bayesian regret is the Gittins index theorem (Gittins, 1989; Weber, 1992), which states that minimizing the discounted Bayesian regret is achieved by computing the Gittins index of each arm. However, the Gittins index is no longer optimal in the context of undiscounted regret. Note also that there are some similarities between the frequentist method and the Gittins index (Russo, 2021).

Bayesian bandit algorithms for simple regret minimization: Russo (2020) presented a version of Thompson sampling and derived its posterior convergence in a frequentist sense. Elsewhere, Shang et al. (2020) extended the algorithm of Russo (2020) to demonstrate asymptotic optimality in the sense of the frequentist lower bound for the fixed confidence setting. The expected improvement algorithm, a well-known myopic heuristic, is known to be suboptimal in the context of SRM (Ryzhov, 2016). However, Qin et al. (2017) demonstrated that a modification of the algorithm enables good posterior convergence. Note that the Bayesian algorithms discussed have been evaluated in terms of frequentist simple regret or posterior convergence; that is, the scholarship includes very limited discussion of Bayesian simple regret.

Gaussian process bandits: Finally, it is necessary to introduce Gaussian process bandits, also known as Bayesian optimization (Frazier, 2018). While Gaussian process bandits originally aimed to minimize Bayesian simple regret, seminal papers have analyzed a worst-case (minimax) simple regret (Bull, 2011) or high-probability bound for simple regret (Srinivas et al., 2010; Vakili et al., 2021).

4Sometimes, the probability of error, which behaves very similarly to simple regret (Audibert et al., 2010, Section 2), is used to measure a BAI algorithm.
Algorithm 1 Two-Stage Exploration Algorithm

Require: $q \in (0, 1)$

Draw each arm $qT/K$ times.

At the end of round $qT$, calculate the lower $L_i = \mu_i - B_{\text{conf}}$ and upper confidence bounds $U_i = \mu_i + B_{\text{conf}}$ for each arm $i \in [K]$.

Compute a candidate $\hat{J}^* := \{ i : U_i \geq \max_j L_j \}$.

if $|\hat{J}^*| = 1$ then
  Immediately return the unique arm in $\hat{J}^*$.
else
  Draw each arm in $\hat{J}^*$ for $(1 - q)T/|\hat{J}^*|$ times.
  Return $J(T) = \arg\max_{i \in \hat{J}^*} \hat{\mu}_i$.
end if

3 Proposed Algorithm: Two-Stage Exploration

This section proposes the Two-Stage Exploration (TSE) Algorithm and derives its simple regret upper bound.

3.1 Two-Stage Exploration Procedure

Instead of the computationally prohibitive dynamic programming procedure, we introduce the two-stage exploration (TSE) algorithm (Algorithm 1), which requires only summary statistics, which are easy computed. The TSE algorithm conducts uniform exploration during the first $qT$ rounds, based on which it finalizes the best arm candidate $\hat{J}^*$. Using the confidence bound of width

$$B_{\text{conf}}(T) = \sqrt{\frac{K \log T}{qT}},$$

the true best arm is found in $\hat{J}^*$ with high probability. The rest of the $(1 - q)T$ rounds are exclusively dedicated to the arms in $\hat{J}^*$. Following round $T$, the TSE algorithm recommends the arm with the largest empirical mean.

3.2 Regret Analysis of Two-Stage Exploration

Theorem 1. (Simple regret upper bound of TSE) For any $q > 0$, the Bayesian simple regret of Algorithm 1 is bounded as follows:

$$R_H(T) \leq \frac{C_{\text{opt}}}{T'} + o\left(\frac{1}{T}\right),$$

where

$$C_{\text{opt}} = \sum_{i \in [K]} \int_{[0, 1]^{K-1}} \mu_i^{*}(1 - \mu_i^{*}) h_i(\mu_i^{*} | \mu_{\setminus i}) dH_{\setminus i}(\mu_{\setminus i})$$

$$T' = \left(q/K + (1 - q)\right)T.$$

Remark 2. (Hyperparameter $q$) Theorem 1 assumes $q > 0$ to be a constant so that $B_{\text{conf}} = O(\sqrt{(\log T)/T})$. While $T' \to T$ as $q \to 0$, a small value for $q$ increases the probability that $|\hat{J}^*| \geq 3$ (Lemma 3). Alternatively, $q$ can be set as a function of $T$ that decays slowly, such that $q^3 = o(T^{-1/6})$.

\footnote{The value $q = T^{-1/20}$ suffices.}
We use the following lemmas to derive Theorem 1. The proof of all lemmas are in the appendix. For two events \( \mathcal{A} \) and \( \mathcal{B} \), let \( \mathcal{A} \cap \mathcal{B} \). Let us define an event for which the true parameters lie within the confidence bounds as

\[
S = \bigcap_{i \in [K]} \{ L_i \leq \mu_i \leq U_i \}.
\]

Let \( \Delta_{J(T)} = \mu^* - \mu_{J(T)} \) be the loss of recommending arm \( J(T) \).

**Lemma 2** (\( S \) occurs with high-probability).

\[
P[S] \geq 1 - \frac{2K}{T^2}.
\]

**Lemma 3.**

\[
\mathbb{E}_{\mu \sim \mathcal{H}} \left[ \mathbb{E}_{\mu} \left[ 1 \left[ S, |\hat{J}^*| \geq 3 \right] \right] \right] = o \left( \frac{1}{T} \right),
\]

where \( 1[\mathcal{A}] = 1 \) if \( \mathcal{A} \) holds or 0 otherwise.

**Lemma 4.** The following inequality holds:

\[
\mathbb{E}_{\mu \sim \mathcal{H}} \left[ \mathbb{E}_{\mu} \left[ 1 \left[ S, |\hat{J}^*| = 2 \right] \Delta_{J(T)} \right] \right] \leq \frac{C_{\text{opt}}}{T} + o \left( \frac{1}{T} \right).
\]

Lemma 2 states that the true parameters lie in the confidence bounds with high probability. Lemma 3 states that the case of \( |\hat{J}^*| \geq 3 \) is negligible with a large \( T \), and Lemma 4 states the leading factor stems from the case of \( |\hat{J}^*| = 2 \).

**Proof of Theorem 1.** The simple regret of TSE is bounded as

\[
R_H(T) := \mathbb{E}_{\mu \sim \mathcal{H}} [R_\mu(T)]
\]

\[
\leq \mathbb{E}_{\mu \sim \mathcal{H}} \left[ \mathbb{E}_{\mu} [1[S] \Delta_{J(T)}] \right] + \frac{2K}{T^2} \quad \text{(by Lemma 2)}
\]

\[
= \mathbb{E}_{\mu \sim \mathcal{H}} \left[ \mathbb{E}_{\mu} [1[S, |\hat{J}^*| = 1] \Delta_{J(T)}] \right] + \mathbb{E}_{\mu \sim \mathcal{H}} \left[ \mathbb{E}_{\mu} [1[S, |\hat{J}^*| = 2] \Delta_{J(T)}] \right] + \frac{2K}{T^2}
\]

\[
= \mathbb{E}_{\mu \sim \mathcal{H}} \left[ \mathbb{E}_{\mu} [1[S, |\hat{J}^*| \geq 3] \Delta_{J(T)}] \right] + \mathbb{E}_{\mu \sim \mathcal{H}} \left[ \mathbb{E}_{\mu} [1[S, |\hat{J}^*| = 3] \Delta_{J(T)}] \right] + \frac{2K}{T^2}
\]

\[
(\text{by } S \text{ implies } i^* \in \hat{J}^*)
\]

\[
= \mathbb{E}_{\mu \sim \mathcal{H}} \left[ \mathbb{E}_{\mu} [1[S, |\hat{J}^*| = 2] \Delta_{J(T)}] \right] + o \left( \frac{1}{T} \right) + \frac{2K}{T^2} \quad \text{(by Lemma 3)}
\]

\[
\leq \frac{C_{\text{opt}}}{T} + o \left( \frac{1}{T} \right) + \frac{2K}{T^2}. \quad \text{(by Lemma 4)}
\]

**Example 2.** (Uniform prior) In the case of the uniform prior where each \( \mu_i \) is independently drawn from \( \text{Unif}(0,1) \),

\[
h_i(\mu_i | \mu_i) = 1
\]

\[
dH_i(\mu_i) = K(\mu_i^*)^{K-1}d\mu_i^*.
\]
and the constant $C_{\text{opt}}$ in Theorem 1 is

$$C_{\text{opt}} = \frac{K^2}{(K + 1)(K + 2)}.$$ 

Section 5 confirms that the empirical performance of the TSE algorithm matches this constant.

4 Lower Bound of Bayesian Simple Regret

4.1 Lower Bound

The following theorem characterizes the achievable performance of any algorithm.

**Theorem 5.** (Simple regret lower bound of an arbitrary algorithm) Under Assumption 1, for any BAI algorithm, we have

$$\mathbb{R}_H(T) \geq \frac{C_{\text{opt}}}{4.8T} - o\left(\frac{1}{T}\right),$$

where $C_{\text{opt}}$ is the constant that is defined in Theorem 1.\(^6\)

Theorem 5 states that TSE is optimal up to a constant factor. For any prior distribution,\(^7\) no algorithm,\(^8\) has a smaller order of simple regret than the TSE algorithm. Namely,

$$\limsup_{T \to \infty} \frac{\mathbb{R}_H(T)}{\mathbb{R}_{H^*}(T)} \leq 1,$$

where $\mathbb{R}_H(T)$ is the simple regret of TSE and $\mathbb{R}_{H^*}(T)$ is the simple regret of the optimal algorithm, which is produced by solving the dynamic programming (Section 2.4) at each round.

The rest of this section derives Theorem 5, which requires the introduction of some notation and several lemmas. Let

$$\Theta_i = \{\mu : \mu_i > \max_{j \neq i} \mu_j\},$$

$$\Theta_{i,1/6} = \{\mu : \mu_i > \max_{j \neq i} \mu_j, \mu_i \in [T^{-1/6}, 1 - T^{-1/6}]\},$$

$$\Theta_{i,j,1/6} = \{\mu \in \Theta_{i,1/6} : \mu_j + 2B_{\text{conf}}(T) > \mu_i > \mu_j > \mu_{ij}^*\}.$$ 

Namely, $\Theta_i$ is the parameter where $i$ is the best arm, $\Theta_{i,1/6}$ is a subset of $\Theta_i$ where $\mu_i$ is not very close\(^9\) to 0, 1. Moreover, $\Theta_{i,j,1/6}$ is a subset of $\Theta_{i,1/6}$ where $j$ is the second-best arm, such that $|\mu_i - \mu_j|$ is very small.\(^10\) Simple regret is characterized by this region. We use the following Lemmas to prove Theorem 5.

**Lemma 6.** (Exchangeable mass) Let $f(\mu_i, \mu_j, \mu_{ij})$ be any function on $[0, 1]$. Then,

$$\int_{\Theta_{i,j,1/6}} (\mu_i - \mu_j)f(\mu_i, \mu_j, \mu_{ij})dH(\mu) = (1 + o(1))\int_{\Theta_{i,1/6}} (\mu_j - \mu_i)f(\mu_j, \mu_i, \mu_{ij})dH(\mu).$$

\(^6\)Since $o(1)$ is a function $f(T)$ such that $\lim_{T \to \infty} |f(T)| = 0$, $+o(1)$ and $-o(1)$ are the same. For clarity, we use $+o(1)$ for upper bounds and $-o(1)$ for lower bounds, respectively.

\(^7\)The prior distribution of the arms can be correlated as long as Assumption 1 holds.

\(^8\)Regardless of knowledge of the prior.

\(^9\)The set $\Theta_{i,1/6}$ is introduced to avoid substantial KL divergence around $\mu_i \approx 0, 1$.

\(^10\)Remember that $B_{\text{conf}}(T) = O(\sqrt{\log T}/T)$. 

8
Lemma 7. For any $\eta > 0$, there exists $T_0$ such that the following inequality holds for all $T \geq T_0$, $\mu \in \Theta_{i,j,1/6}$:

$$
\max(\mathbb{P}_\mu[J(T) \neq i], \mathbb{P}_\nu[J(T) \neq j]) \geq \frac{1}{2.4} \exp \left( - (1 + \eta) T d_{KL}(\mu_j, \mu_i) \right),
$$

where

$$
\nu := (\mu_1, \mu_2, \ldots, \mu_{i-1}, \frac{\mu_j}{i\text{-th element}}, \mu_{i+1}, \ldots, \mu_{j-1}, \frac{\mu_i}{j\text{-th element}}, \mu_{j+1}, \ldots, \mu_{K}) \in \Theta_{j,i,1/6}
$$

be another set of parameters, such that $(\mu_i, \mu_j)$ are swapped from $\mu$.

Lemma 8. (Integration on the lower bound) The following inequality holds:

$$
\int_{[\rho, \rho + 2B_{\text{const}}]} (\mu - \mu_j^*) \exp \left( - (1 + \eta) T d_{KL}(\mu_j^*, \mu_i) \right) d\mu = \frac{\mu_j^*(1 - \mu_j^*)}{(1 + \eta)T} - o(1).
$$

Lemma 6 states that the area of $\Theta_{i,j,1/6}$ and $\Theta_{j,i,1/6}$ are approximately equal. Lemma 7, which utilizes a Lemma in Kaufmann et al. (2016), represents the performance tradeoff between identifying $J(T) = i$ and $J(T) = j$. Lemma 8 integrates frequentist simple regret over the conditional distribution of $\mu_i$ given $\mu_{\backslash i}$.

Proof of Theorem 5. By definition,

$$
R_H(T) = \int_{[0,1]^K} R_\mu(T) dH(\mu) = \int_{[0,1]^K} \left( \mu^* - \mathbb{E}_\mu[\mu_{J(T)}] \right) dH(\mu).
$$

We have,

$$
\int_{[0,1]^K} \left( \mu^* - \mathbb{E}_\mu[\mu_{J(T)}] \right) dH(\mu)
$$

$$
= \sum_{i \in [K]} \int_{[0,1]^K} 1[\mu \in \Theta_i](\mu_i - \mu_i^*) \mathbb{P}_\mu[J(T) \neq i] dH(\mu)
$$

$$
\geq \sum_{i \in [K]} \sum_{j \neq i} \int_{[0,1]^K} 1[\mu \in \Theta_{i,j,1/6}](\mu_i - \mu_j) \mathbb{P}_\mu[J(T) \neq i] dH(\mu)
$$

$$
= \sum_{i \in [K]} \sum_{j \neq i} \int_{[0,1]^K} 1[\mu \in \Theta_{i,j,1/6}](\mu_i - \mu_j) \frac{\mathbb{P}_\mu[J(T) \neq i] + \mathbb{P}_\nu[J(T) \neq j]}{2} dH(\mu) - o\left( \frac{1}{T} \right)
$$

(by Lemma 6 with $f = \mathbb{P}_\mu[J(T) \neq i]$)

$$
\geq \frac{1}{4.8} \sum_{i \in [K]} \sum_{j \neq i} \int_{[0,1]^K} 1[\mu \in \Theta_{i,j,1/6}](\mu_i - \mu_j) \exp \left( - (1 + \eta) T d_{KL}(\mu_j, \mu_i) \right) dH(\mu) - o\left( \frac{1}{T} \right)
$$

(by Lemma 7)

$$
= \frac{1}{4.8} \sum_{i \in [K]} \int_{[0,1]^K} \int_{[0,1]} 1[\mu \in \Theta_{i,1/6}](\mu_i - \mu_i^*) \exp \left( - (1 + \eta) T d_{KL}(\mu_i^*, \mu_i) \right) dH_i(\mu_i) dH_{\backslash i}(\mu_{\backslash i}) - o\left( \frac{1}{T} \right)
$$

$$
= \frac{1}{4.8} \sum_{i \in [K]} \int_{[0,1]^{K-1}} h(\mu_i^*) \left( \int_{[\rho, \rho + 2B_{\text{const}}]} (\mu_i - \mu_i^*) \exp \left( - (1 + \eta) T d_{KL}(\mu_i^*, \mu_i) \right) d\mu_i \right) dH_{\backslash i}(\mu_{\backslash i}) - o\left( \frac{1}{T} \right)
$$

(by uniform continuity)
\[ \frac{1}{4.8(1 + \eta)T} \sum_{i \in [K]} \int_{[0,1]} \mu_i^*(1 - \mu_i^*)h_i(\mu_i^*|\mu_i) dH_i(\mu_i) - o \left( \frac{1}{T} \right), \]

(by Lemma 8)

which holds for any \( \eta > 0 \), and thus, the proof is completed. \( \square \)

**Remark 3.** (Finite-time analysis) Theorems 1 and 5 are asymptotics. The only point at which we lose the finite-time property is on the continuity of the conditional cumulative density function \( h_i(\mu_i|\mu_i^*) \): We do not specify how fast \( h_i(\mu_i|\mu_i^*) \) changes as a function of \( \mu_i \). It is not very difficult to derive a finite-time bound for specific models where the sensitivity of \( h_i(\mu_i|\mu_i^*) \) is known, as in the case of the uniform prior of Example 2, where \( h_i(\mu_i|\mu_i^*) = 1 \). In this case, the \( o(1) \) term in Theorems 1 and 5 can be replaced by a factor \( CT^{-1/6}(\log T)^3 \) for the constant \( C > 0 \).

### 4.2 Towards a Tight Bound

Although there is a constant factor in the lower bound (i.e., \( 1/4.8 \)), we hypothesize the upper bound (Theorem 1) is tight in the following reasons.

- The TSE algorithm only spends \( q \) fraction of rounds identifying \( \hat{\mathcal{J}}^* \), and we may set small \( q \) with a large \( T \). When \( |\hat{\mathcal{J}}^*| = 2 \) (which holds with high probability), it spends approximately \( T/2 \) rounds on each candidate of \( \hat{\mathcal{J}}^* \); this appears to produce little to no space for improvements.

- The simulation results, which we present in Section 5, empirically match the bound of Theorem 1. Although we can increase factor \( 1/4.8 \) to some extent, making it to 1 is highly non-trivial. Let \( i, j \) be the best two arms and \( \mu_i - \mu_j = \Delta \). Among the largest challenges is the determination of Bayesian simple regret in the region where \( \Delta = O \left( \frac{1}{\sqrt{T}} \right) \). In this case, \( d_{KL}(\mu_j, \mu_i) = O(\Delta^2) \) and

\[ Td_{KL}(\mu_j, \mu_i) = O(1). \]

Meanwhile, the estimation error of \( \mu_i \) with \( T \) sample is \( O(1/\sqrt{T}) \); thus,

\[ T(d_{KL}(\mu_j, \mu_i) - d_{KL}(\mu_j, \hat{\mu}_i)) \approx T \frac{\partial d_{KL}(\mu_j, \mu_i)}{\partial \mu_i} (\mu_i - \hat{\mu}_i) = T \times O \left( \frac{1}{\sqrt{T}} \right) \times O \left( \frac{1}{\sqrt{T}} \right) = O(1) \]

matters here. That is, a high-probability bound of the form \( (1 + \eta)Td_{KL}(\mu_j, \mu_i) \) is unavailable for deriving an optimal Bayesian simple regret lower bound.

### 5 Simulation

We conducted a set of simulations to support our theoretical findings. We empirically tested the TSE algorithm (Algorithm 1, with \( q = 0.5 \)) with the uniform prior (Example 2) and measured its simple regret with the aim of verifying the tightness of the upper bound of Theorem 1 with its leading order \( C_{opt}/T' \). To improve the finite performance, the lower and upper confidence bounds of Algorithm 1 are replaced by the Chernoff bound (Lemma 10) of confidence level \( 1/T^2 \), which is sharper than \( B_{cont} \); Namely,

\[ L_i = \inf \{ q \in (0, \hat{\mu}_i) : N_i(qT)d_{KL}(\hat{\mu}_i, q) \leq 2 \log(T) \} \]
Figure 1: Comparison of $C_{\text{opt}} (= K^2/((K + 1)(K + 2)))$, Theory and its estimated value using the TSE algorithm ($= R_H(T)T'$) with several different values of $K$. Here, the value of $T$ is set to $10^5K$ for each $K$. TSE_three indicates the simple regret when $|\hat{J}^*| \geq 3$, with each bar representing two sigma of the corresponding plug-in variance.

Figure 2: Comparison of $C_{\text{opt}}$ (Theory) and its estimated value using the TSE algorithm ($= R_H(T)T'$) with several different values $T$. Here, $K$ is fixed to be 5. The decreasing value of TSE_three implies that the probability of $|\hat{J}^*| \geq 3$ is small if $T$ is large. Each bar represents two sigma of the corresponding plug-in variance.

$$U_i = \sup\{q \in (\hat{\mu}_i, 1) : N_i(qT)d_{KL}(\hat{\mu}_i, q) \leq 2\log(T)\}.$$ 

Moreover, to effectively sample small-gap cases, $R_H(T)$ should be computed by a Monte Carlo rejection sampling of the prior $\mu$ with acceptance ratio

$$\max\left(\min\left(\frac{1}{2\Delta\sqrt{T}}, 1\right), 0.01\right),$$

where $\Delta$ is the gap between the best arm and the second-best arm. Our simulation is implemented in the Python 3 programming language.$^{11}$

Figure 1 compares the performance of the TSE with the lower bound with several values of $K = \{2, 3, 5, 10\}$. The results are averaged over $5 \times 10^4$ runs. The TSE performs very closely to $C_{\text{opt}}/T'$, which implies the tightness of Theorem 1. The value $R_H(T)$ is slightly larger than $C_{\text{opt}}/T'$ because the case of $|\hat{J}^*| \geq 3$ is non-negligible unless $T$ is infinitely large. Furthermore, Figure 2 sets $K = 5$ and compares several different values of $T$. Larger $T$ values increase the probability of $|\hat{J}^*| = 2$. Consequently, the simple regret of the TSE algorithm approaches the theoretical bound.

Note that this section does not aim to compare Algorithm 1 with existing algorithms. Although the TSE algorithm approaches the optimal bound by choosing a $q$ of $o(1)$, its practical performance has the capacity to improve.

6 Conclusion and Discussion

We have analyzed the Bayesian BAI in the context of the $K$-armed MAB problem, which concerns identifying the Bayes-optimal treatment allocation. We derived a lower bound of the Bayesian simple regret and introduced a simple algorithm that matches the lower bound under a mild regularity condition.

$^{11}$The source code of the simulation is available at https://github.com/jkomiyama/bayesbai_paper.
Our results is a counterpart of the Bayesian regret minimization (RM) of Lai (1987) for the Bayesian simple regret minimization (SRM). Upon deriving a lower bound for Bayesian simple regret, we introduced a simple algorithm to match the lower bound under a mild regularity condition. Our results constitute the counterpart of the Bayesian RM of Lai (1987) in the context of Bayesian SRM. Several particular differences between RM and SRM can be summarized:

- In RM, certain asymptotically optimal algorithms adopting a frequentist perspective are also optimal in terms of Bayesian RM and vice versa,\(^\text{12}\) whereas optimality in frequentist SRM remains inadequately characterized (Carpentier and Locatelli, 2016).

- The leading factor of Bayesian RM derives from the region of \(\Delta > \sqrt{\frac{\log T}{T}}\), whereas the leading factor of Bayesian SRM derives from \(\Delta < \sqrt{\frac{\log T}{T}}\). This makes analyzing Bayesian simple regret challenging (Section 4.2). At the high level, Bayesian SRM involves quickly discarding clearly suboptimal arms and concentrating the rest of the samples on the competitive candidates of the best arm.

This paper has considered Bernoulli distributions, which are important for optimal treatment allocation because the simplest case we consider involves binary outcomes. Extending our results to other classes of distributions, such as the Gaussian distributions, would represent an interesting future research direction.

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A General Lemmas

**Proposition 9.** (Stirling’s approximation) For any \( n \in \mathbb{N} \), the following inequality holds:

\[
\sqrt{2\pi n^{n+\frac{1}{2}}e^{-n}} \frac{1}{n!} < n! < \sqrt{2\pi n^{n+\frac{1}{2}}e^{-n}} \frac{1}{n!}.
\]

By using \( e^{1/n} \leq 1 + 2/n \) for \( n \geq 2 \), we have

\[
\sqrt{2\pi n^{n+\frac{1}{2}}e^{-n}} < n! < \sqrt{2\pi n^{n+\frac{1}{2}}e^{-n}} \left(1 + \frac{1}{6n}\right).
\]

**Lemma 10** (Chernoff bound). Let \( x_1, x_2, \ldots, x_n \) be Bernoulli random variables with their common mean \( \mu \). Let \( \hat{\mu}_n = (1/n) \sum_{t=1}^{n} x_t \). Then,

\[
\begin{align*}
\Pr[\hat{\mu}_n - \mu & \geq \epsilon] \leq e^{-nd_{KL}(\mu + \epsilon, \mu)}, \\
\Pr[\hat{\mu}_n - \mu & \leq -\epsilon] \leq e^{-nd_{KL}(\mu - \epsilon, \mu)}.
\end{align*}
\]

Moreover, using the Pinsker’s inequality \( d_{KL}(p, q) \geq 2(p - q)^2 \) and taking a union bound yields

\[
\Pr[|\hat{\mu}_n - \mu| \geq \epsilon] \leq 2e^{-2n\epsilon^2}.
\]  

(11)

B Bounds on KL Divergence

Let \( l \in [T^{-1/6}, 1 - T^{-1/6}] \). Let \( h(T) = o(T^{-1/6}) \), and \( T_0 > 0 \) be such that \( 2h(T) < T^{-1/6} \) and \( T^{1/6} < 1/2 \) for all \( T \geq T_0 \). Let \( u \) be such that \( h(T) + l > u > l \). Let \( m = (l + u)/2 \) and \( \Delta_k = (u - l)/2 \).

Roughly speaking, Lemmas 11 and 12, which are below, state that

\[
d_{KL}(l, u) \approx 4d_{KL}(l, m) \approx 4d_{KL}(m, l) \approx \frac{(u - l)^2}{2l(1 - l)} \approx \frac{(u - l)^2}{2m(1 - m)} \approx \frac{(u - l)^2}{2u(1 - u)}
\]  

(12)
when $\Delta_h$ is sufficiently small. We show the formal version of Eq. (12) in Lemma 13.

**Lemma 11.** (Bound on the KL divergence around $l$)

For all $T \geq T_0$, the following inequality holds:

\[
\left| d_{KL}(l, u) - \frac{(u - l)^2}{2l(1 - l)} \right| \leq C_{KL}(h(T))^{3T^{1/3}},
\]

**Proof of Lemma 11.** Letting $\eta = \max\left(\frac{u - l}{T}, \frac{1 - l}{T}\right) \leq 4h(T)^{T^{1/6}}$, we have

\[
d_{KL}(l, u) := \int_{x=0}^{u-l} d\left(d_{KL}(l, l + x)\right) \, dx
\]

\[
= \int_{x=0}^{u-l} \frac{x}{(l + x)(1 - l - x)} \, dx
\]

\[
\leq (1 + 2\eta) \int_{x=0}^{u-l} \frac{x}{l(1 - l)} \, dx
\]

\[
= (1 + 2\eta) \frac{(u - l)^2}{2l(1 - l)}
\]

\[
+ 2\eta \times \left(\frac{(u - l)^2}{2l(1 - l)}\right) = \frac{(u - l)^2}{2l(1 - l)} + 2\eta \times \left((h(T))^{3T^{1/6}}\right)
\]

Another inequality $\frac{(u - l)^2}{2l(1 - l)} - 8 \times (h(T))^{3T^{1/3}} \leq d_{KL}(l, u)$ is derived in the same manner.

**Lemma 12.** For all $T \geq T_0$, the following inequalities hold:

\[
|d_{KL}(m, u) - d_{KL}(l, m)| \leq C_{KL}(h(T))^{3T^{1/3}}
\]

\[
|d_{KL}(m, u) - d_{KL}(u, m)| \leq C_{KL}(h(T))^{3T^{1/6}},
\]

for some universal constant $C_{KL} > 0$.

**Proof of Lemma 12.**

\[
|d_{KL}(m, u) - d_{KL}(l, m)| = \left| \int_{x=l}^{m} \frac{d(d_{KL}(x, x + \Delta_h))}{dx} \, dx \right|
\]

\[
\leq \Delta_h \max_{x \in [m, m + \Delta_h]} \left| \frac{d(d_{KL}(x, x + \Delta_h))}{dx} \right|.
\]

We have

\[
\frac{d}{dx}d_{KL}(x, x + \Delta_h) = \frac{d}{dx} \left( x \log \left( \frac{x}{x + \Delta_h} \right) + (1 - x) \log \left( \frac{1 - x}{1 - x - \Delta_h} \right) \right)
\]

\[
= \left[ \log \left( \frac{x}{x + \Delta_h} \right) - \log \left( \frac{1 - x}{1 - x - \Delta_h} \right) \right] + \frac{\Delta_h}{x + \Delta_h} + \frac{\Delta_h}{1 - x - \Delta_h}
\]

\[
= \log \left( 1 - \frac{\Delta_h}{(x + \Delta_h)(1 - x)} \right) + \frac{\Delta_h}{(x + \Delta_h)(1 - x - \Delta_h)}.
\]

---

15
By using \( \left| \frac{\Delta_h}{(x + \Delta_h)(1-x)} \right| < 1/2 \) and \(-y - y^2 \leq \log(1-y) \leq -y \) for \( y \in [0, 1/2] \), we have

\[
\left| \frac{d}{dx} d_{KL}(x, x + \Delta_h) \right| \leq \left| -\frac{\Delta_h}{(x + \Delta_h)(1-x)} + \frac{\Delta_h}{(x + \Delta_h)(1-x - \Delta_h)} \right| + \left| \left( \frac{\Delta_h}{(x + \Delta_h)(1-x)} \right)^2 \right|
\]

\[
= \frac{\Delta_h^2}{(x + \Delta_h)(1-x)(1-x - \Delta)} + \left( \frac{\Delta_h}{(x + \Delta_h)(1-x)} \right)^2
\]

which, by using \( \Delta_h < h(T)/2 = o(\log T) \) and \( x, 1 - x > T^{-1/6} \), can be easily bounded by \( C \Delta_h^2 T^{1/3} \) for some \( C > 0 \), which is Eq. (13).

We next derive Eq. (14).

\[
d_{KL}(m, u) - d_{KL}(m, l) = \int_{x=0}^{\Delta_h} \frac{x}{(m + x)(1-m - x)} dx - \int_{x=0}^{\Delta_h} \frac{x}{(m-x)(1-m + x)} dx
\]

\[
= \int_{x=0}^{\Delta_h} \frac{2x^2(2m-1)}{(m^2 - x^2)((1-x)^2 - m^2)} dx
\]

and thus

\[
|d_{KL}(m, u) - d_{KL}(m, l)| \leq \Delta_h \times \max \left| \frac{2\Delta_h^2(2m-1)}{(m^2 - x^2)((1-x)^2 - m^2)} \right|
\]

\[
= C \Delta_h^3 T^{1/6}
\]

for some \( C > 0 \), which is Eq. (14). \( \square \)

**Lemma 13.** (Bound on the KL divergence) Let \( h(T) = \sqrt{\log T/T} \) for some constant \( C_h > 0 \). Then, there exist \( C_a > 0, T_0 \) for all \( T \geq T_0 \),

\[
\frac{(u-l)^2}{2m(1-m)} - C_a T^{-1/6} (\log T)^3 \leq d_{KL}(l, u), d_{KL}(u, l) \leq \frac{(u-l)^2}{2m(1-m)} + C_a T^{-1/6} (\log T)^3
\]

and

\[
\frac{(u-l)^2}{8m(1-m)} - C_a T^{-1/6} (\log T)^3 \leq d_{KL}(m, u), d_{KL}(u, m), d_{KL}(m, l), d_{KL}(l, m) \leq \frac{(u-l)^2}{8m(1-m)} + C_a T^{-1/6} (\log T)^3.
\]

The proof of Lemma 13 is straightforward from Lemmas 11 and 12.

**C Lemmas for Upper Bound**

**C.1 Proof of Lemma 2**

*Proof of Lemma 2.* At the end of round \( qT \), TSE draws each arm for \( N_i(qT) = qT/K \) times. Eq. (9) is derived by using the union bound of the Hoeffding inequality (Eq. (11)) over \( K \) arms. \( \square \)
C.2 Proof of Lemma 3

Proof of Lemma 3.

\[
\begin{align*}
E_{\mu \sim H} \left[ E_\mu [1[S, |\hat{\mathbf{J}}^*| \geq 3]] \right] \\
\leq 2B_{\text{conf}} \sum_{i,j,k} \int 1[|\mu_i - \mu_k| \leq 2B_{\text{conf}}, |\mu_j - \mu_k| \leq 2B_{\text{conf}}] dH(\mu) \\
= 2B_{\text{conf}} \sum_{i,j,k} \int 1[|\mu_i - \mu_k| \leq 2B_{\text{conf}}, |\mu_j - \mu_k| \leq 2B_{\text{conf}}] h_{ij}(\mu_i, \mu_j | \mu_{\backslash ij}) d\mu_i d\mu_j dH_{\backslash ij}(\mu_{\backslash ij})
\end{align*}
\]

By choosing \( \epsilon = 1 \) in Eq. (4), for any \( T \) such that \( B_{\text{conf}}(T) \leq \delta(\epsilon)/4 \), for each \( \mu_{\backslash ij} \), we have

\[
\int 1[|\mu_i - \mu_k| \leq 2B_{\text{conf}}, |\mu_j - \mu_k| \leq 2B_{\text{conf}}] d\mu_i d\mu_j \leq \int 1 \left[ \sqrt{(\mu_i - \mu_k)^2 + (\mu_j - \mu_k)^2} \leq \delta(\epsilon) \right] d\mu_i d\mu_j \quad (15)
\]

By using this, we have

\[
\begin{align*}
2B_{\text{conf}} \int 1[|\mu_i - \mu_k| \leq 2B_{\text{conf}}, |\mu_j - \mu_k| \leq 2B_{\text{conf}}] h(\mu_i, \mu_j; \mu_{\backslash ij}) d\mu_i d\mu_j dH_{\backslash ij}(\mu_{\backslash ij}) \\
\leq 2B_{\text{conf}} \int 1[|\mu_i - \mu_k| \leq 2B_{\text{conf}}, |\mu_j - \mu_k| \leq 2B_{\text{conf}}] (h(\mu_k, \mu_k; \mu_{\backslash ij}) + 1) d\mu_i d\mu_j dH_{\backslash ij}(\mu_{\backslash ij}) \\
\quad \text{(by uniform continuity and Eq. (15))} \\
= O \left( (B_{\text{conf}})^3 \right) = o \left( \frac{1}{T} \right).
\end{align*}
\]

\( \square \)

C.3 Lemmas on the Main Term

Lemma 14. (Tight Bayesian bound) Let \( m = (\mu_i + \mu_j)/2 \). Let \( \hat{\mu}_{i,n} \) is the empirical mean of arm \( i \) with the first \( n \) samples. Then,

\[
\begin{align*}
\int_{\mu_j}^{\min(\mu_j + 2B_{\text{conf}}, 1 - T^{-1/6})} & (\mu_i - \mu_j) \mathbb{P}_\mu [\hat{\mu}_{i,T_h} < \mu_i, T_h, \mathcal{S}] d\mu_i \\
\leq & \mathbb{P} [\hat{\mu}_i(T) \leq \hat{\mu}_j(T)] \leq \mathbb{P} [\hat{\mu}_i(T) \leq m] + \mathbb{P} [\hat{\mu}_j(T) \geq m] \approx 2e^{-T_h^2 \Delta^2 L(\mu_j, m)}
\end{align*}
\]

Remark 4. (Lemma 14 is tighter than the Chernoff bound) In the proof of Lemma 14, we carefully use the change-of-measure argument to derive a tight bound. Alternatively, we may use the concentration inequality (Chernoff bound, Lemma 10) in bounding the regret, which yields

\[
\mathbb{P}[\hat{\mu}_i(T) \leq \hat{\mu}_j(T)] \leq \mathbb{P}[\hat{\mu}_i(T) \leq m] + \mathbb{P}[\hat{\mu}_j(T) \geq m] \approx 2e^{-T_h^2 \Delta^2 L(\mu_j, m)}
\]

which, integrated over the prior, is four times larger than Lemma 14.

Lemma 15. (Tight frequentist bound) Let \( m = (\mu_i + \mu_j)/2 \) and \( \Delta = \mu_i - \mu_j > 0 \). Let \( \mu_{\backslash ij}^* \) is \( \mu_j < \mu_i < \min(\mu_j + 2B_{\text{conf}}, 1 - T^{-1/6}) \). Then,

\[
\mathbb{P}_\mu [\hat{\mu}_{i,T_h} \leq \hat{\mu}_j, T_h, \mathcal{S}] = (1 + o(1)) \sqrt{\frac{T'}{8\pi m(1-m)}} \int_{s_2=0}^{\infty} e^{-\frac{T'}{8\pi m(1-m)}(\Delta^2 + 2s_2\Delta + s_2^2)} ds_2,
\]
where the $o(1)$ term does not depend on $\mu_i, \mu_j$.

Particular care is required in Lemma 15 because a high-probability bound on the KL divergence is not tight (c.f., Section 4.2); we can upper-bound a simple regret based on a high-probability bound on the KL divergence, which simplify the analysis of Lemma 15. However, such a high-probability bound compromises the leading constant.\(^{13}\) In the following proof, we use Proposition 9, Lemma 13, and manual calculation on the number of combinations because these operations are tight with respect to the leading constant.

**Proof of Lemma 15.** Let

$$\lambda := (\mu_1, \mu_2, \ldots, \mu_{i-1}, \hat{m}, \mu_{i+1}, \ldots, \mu_{j-1}, \hat{m}, \mu_{j+1}, \ldots, \mu_K)$$

be the set of parameters where \((\mu_i, \mu_j)\) is replaced by \((m, m)\). Let \(\hat{\mu}_{i,n}\) be the empirical mean of arm \(i\) with \(n\) samples.

Under \(\mu_j + 2B_{\text{conf}} > \mu_i > \mu_j > \mu_{i,j}^\ast\), we have

$$\{\hat{\mu}_{i,T_h} \leq \hat{\mu}_{j,T_h}, S\}$$

$$= \{T_h' \hat{\mu}_{i,T_h} \leq T_h' \hat{\mu}_{j,T_h}, S\}$$

$$= (T_h' \hat{\mu}_{i,T_h}, T_h' \hat{\mu}_{j,T_h}) \subseteq \{(T_1, T_2) \in \mathbb{N}^2 : -4TB_{\text{conf}} \leq T_1 - T_h'm \leq T_2 - T_h'm \leq 4TB_{\text{conf}}\}$$

$$= S_{i,j}$$

Let \((D_1, D_2) = (T_1 - T_h'm, T_2 - T_h'm)\). We have

$$\mathbb{P}_\mu[\hat{\mu}_{i,T_h} \leq \hat{\mu}_{j,T_h}, S]$$

$$= \sum_{(T_1, T_2) \in S_{i,j}} \mathbb{P}_\mu[T_h' \hat{\mu}_{i,T_h} = T_1, T_h' \hat{\mu}_{j,T_h} = T_2]$$

$$= \sum_{(T_1, T_2) \in S_{i,j}} e^{(D_1 + T_h'm) \log(\frac{\hat{m}}{m}) + (T_h'(1 - m) - D_1) \log(\frac{1 - \hat{m}}{1 - m}) + (D_2 + T_h'm) \log(\frac{\hat{m}}{m}) + (T_h'(1 - m) - D_2) \log(\frac{1 - \hat{m}}{1 - m})}$$

$$\times \mathbb{P}_\lambda[T_h' \hat{\mu}_{i,T_h} = T_1, T_h' \hat{\mu}_{j,T_h} = T_2]$$

(change of measure)

$$= \sum_{(T_1, T_2) \in S_{i,j}} e^{-T_h'(\text{dKL}(m, \mu_i) + \text{dKL}(m, \mu_j))} + (D_1 \log(\frac{\hat{m}}{m}) - D_1 \log(\frac{1 - \hat{m}}{1 - m}) + D_2 \log(\frac{\hat{m}}{m}) - D_2 \log(\frac{1 - \hat{m}}{1 - m}))$$

$$\times \mathbb{P}_\lambda[T_h' \hat{\mu}_{i,T_h} = T_1, T_h' \hat{\mu}_{j,T_h} = T_2]$$

$$= \sum_{(T_1, T_2) \in S_{i,j}} e^{-(1-o(1))\left(\frac{\hat{m}}{m} - \frac{1 - \hat{m}}{1 - m}\right)} + (D_1 \log(\frac{\hat{m}}{m}) - D_1 \log(\frac{1 - \hat{m}}{1 - m}) + D_2 \log(\frac{\hat{m}}{m}) - D_2 \log(\frac{1 - \hat{m}}{1 - m}))$$

$$\times \mathbb{P}_\lambda[T_h' \hat{\mu}_{i,T_h} = T_1, T_h' \hat{\mu}_{j,T_h} = T_2]$$

(By Lemma 13)

$$= \sum_{(T_1, T_2) \in S_{i,j}} e^{-(1-o(1))\left(\frac{\hat{m}}{m} - \frac{1 - \hat{m}}{1 - m}\right)} + (D_1 \log(\frac{\hat{m}}{m}) - D_1 \log(\frac{1 - \hat{m}}{1 - m}) + D_2 \log(\frac{\hat{m}}{m}) - D_2 \log(\frac{1 - \hat{m}}{1 - m}))$$

$$\times \mathbb{P}_\lambda[T_h' \hat{\mu}_{i,T_h} = T_1, T_h' \hat{\mu}_{j,T_h} = T_2]$$

\(^{13}\)Remember that Eq. (8) is twice as large as our bound.
\[(\text{By } |\log(1 + x) - x| = O(x^2) \text{ and } \frac{\mu_1(1 - m)}{m(1 - \mu_1)} - 1 - \frac{\Delta}{2m(1 - m)} = o(\Delta))
= \sum_{(T_1, T_2) \in S_{i,j}} e^{-(1-o(1))\left(\frac{T'_h \Delta^2}{\tilde{m}(1-m)} + D_1 \frac{\Delta}{\tilde{m}(1-m)} - D_2 \frac{\Delta}{\tilde{m}(1-m)}\right)}
\times \frac{T'_h}{T'_1(T'_h - T'_1)} \cdot m^{T'_1(1-m)T'_h - T'_1} \cdot \frac{T'_h}{T'_2(T'_h - T'_2)} \cdot m^{T'_2(1-m)T'_h - T'_2}
\] (by number of combinations)
\[= \sum_{(T_1, T_2) \in S_{i,j}} e^{-(1-o(1))\left(\frac{T'_h \Delta^2}{\tilde{m}(1-m)} + D_1 \frac{\Delta}{\tilde{m}(1-m)} - D_2 \frac{\Delta}{\tilde{m}(1-m)}\right)}
\times \frac{1}{\sqrt{2\pi}} e^{\left(1+o(1)\right)\left(T'_h \log(T'_h) - \left(T'_h - T'_1 + \frac{1}{2}\right) \log(T'_h - T'_1) + T_1 \log(m) + (T'_h - T'_1) \log(1-m)\right)}
\times \frac{1}{\sqrt{2\pi}} e^{\left(1+o(1)\right)\left(T'_h \log(T'_h) - \left(T'_h - T'_2 + \frac{1}{2}\right) \log(T'_h - T'_2) + T_2 \log(m) + (T'_h - T'_2) \log(1-m)\right)}.
\tag{16} \]
(by Proposition 9)

Here, letting \((t_1, t_2) = (T_1/T'_h, T_2/T'_h)\), we have
\[e^{\left(1+o(1)\right)\left(T'_h \log(T'_h) - \left(T'_h - T'_1 + \frac{1}{2}\right) \log(T'_h - T'_1) + T_1 \log(m) + (T'_h - T'_1) \log(1-m)\right)} = \sqrt{\frac{T'_h}{T'_1(T'_h - T'_1)}} e^{\left(1+o(1)\right)\left(T'_h \log(T'_h) - \left(T'_h - T'_1\right) \log(T'_h - T'_1) + T_1 \log(m) + (T'_h - T'_1) \log(1-m)\right)}
= \sqrt{\frac{2}{m(1-m)T'_h}} e^{\left(1+o(1)\right)\left(T'_h \log(T'_h) - \left(t_1 \log(t_1) - (1-t_1) \log(1-t_1) + t_1 \log(m) + (1-t_1) \log(1-m)\right)}
= \sqrt{\frac{2}{m(1-m)T'_h}} e^{-(1-o(1))T'_h d_{\text{KL}}(m, t_1)} \tag{17}
\]
and thus, by letting \((d_1, d_2) = (D_1/T'_h, D_2/T'_h)\), we have
\[\text{Eq. (16)} = \frac{2}{\sqrt{2\pi}} \frac{2}{m(1-m)T'_h} \sum_{(T_1, T_2) \in S_{i,j}} e^{-(1-o(1))\left(\frac{T'_h \Delta^2}{\tilde{m}(1-m)} + D_1 \frac{\Delta}{\tilde{m}(1-m)} - D_2 \frac{\Delta}{\tilde{m}(1-m)} + T'_h d_{\text{KL}}(m, t_1) + T'_h d_{\text{KL}}(m, t_2)\right)}
\text{(by Eq. (17))}
= \frac{1}{\pi m(1-m)T'_h} \sum_{(T_1, T_2) \in S_{i,j}} e^{-(1-o(1))\left(\frac{T'_h \Delta^2}{\tilde{m}(1-m)} + D_1 \frac{\Delta}{\tilde{m}(1-m)} - D_2 \frac{\Delta}{\tilde{m}(1-m)} + T'_h d_{\text{KL}}(m, t_1) + T'_h d_{\text{KL}}(m, t_2)\right)}
= \frac{1}{\pi m(1-m)T'_h} \sum_{(T_1, T_2) \in S_{i,j}} e^{-(1-o(1))\left(\frac{T'_h \Delta^2}{\tilde{m}(1-m)} + T'_h d_{\text{KL}}(m, t_1) + T'_h d_{\text{KL}}(m, t_2)\right)}
\text{(By Lemma 13)}
= \frac{1 + o(1)}{\pi m(1-m)T'_h} \sum_{(T_1, T_2) \in S_{i,j}} e^{-\frac{T'_h \Delta^2}{\tilde{m}(1-m)}(\Delta^2 + 2d_1 \Delta - 2d_2 \Delta + 2d_1^2 + 2d_2^2)}
\]
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Proof of Lemma 14. An integration of Lemma 15 over \( C \) This concludes the proof. Note that the \( o(1) \) term is derived by applying Lemma 13, where the term \( C_a T^{-1/6} (\log T)^3 \) does not depend on \( \mu_i, \mu_j \).

\[ \text{by } \int_{-\infty}^{\infty} \exp(-x^2) dx = \sqrt{\pi} \]
C.4 Proof of Lemma 4

Proof of Lemma 4. Event \( S \) implies that \( i^* \in \hat{J}^* \). Let \( T' := qT/K + (1 - q)T/2 \) and \( T_h = T'/2 \). Under \( \hat{J}^* = \{i, j\} \), we have \( N_i(T) = N_j(T) = T_h \).

\[
E_{\mu \sim H} \left[ E_{\mu}[1[S, \hat{J}^* = 2|\Delta_J(T)]] \right] \\
\leq \sum_{i,j} E_{\mu \sim H} \left[ 1[S, \mu_i > \mu_j > \mu_{ij}^*, |E_{\mu}[1[S, \hat{J}^* = \{i, j\}]|] \Delta_J(T) \right] \\
\leq \sum_{i,j} E_{\mu \sim H} \left[ 1[\mu_j + 2B_{\text{conf}}, \mu_i > \mu_j > \mu_{ij}^*, |E_{\mu}[1[S, \hat{J}^* = \{i, j\}]|] \Delta_J(T) \right] \\
= \sum_{i,j} E_{\mu \sim H} \left[ 1[\mu_j + 2B_{\text{conf}}, \mu_i > \mu_j > \mu_{ij}^*, (\mu_i - \mu_j)P_{\mu}[\hat{\mu}_i, T_h \leq \hat{\mu}_j, T_h, S] \right] \\
+ \sum_{i,j} 2B_{\text{conf}} O \left( P_{\mu \sim H} [\mu_i > 1 - T^{-1/6}, |\mu_i - \mu_j| \leq 2B_{\text{conf}}] \right). \\
\text{(by uniform continuity)} \\
\leq \sum_{i} E_{\mu \sim H} \left[ 1[\mu_i + 2B_{\text{conf}}, \mu_i > \mu_{ij}^*, 1 - T^{-1/6}, \mu_i] (\mu_i - \mu_{ij}^*) P_{\mu}[\hat{\mu}_i, T_h \leq \hat{\mu}_j, T_h, S] \right] + o \left( \frac{1}{T} \right). \quad (18)
\]

Here, the first term of Eq. (18) is bounded as:

\[
E_{\mu \sim H} \left[ 1[\mu_i + 2B_{\text{conf}}, \mu_i > \mu_{ij}^*, 1 - T^{-1/6}, \mu_i] (\mu_i - \mu_{ij}^*) P_{\mu}[\hat{\mu}_i, T_h \leq \hat{\mu}_j, T_h, S] \right] \\
\leq \int_{[0,1]} h_i(\mu_{ij}^*, \mu_i) \int_{[0,1]} \min(\mu_{ij}^*, 2B_{\text{conf}}, 1 - T^{-1/6}) d\mu_i dH_i(\mu_i) \\
\leq (1 + o(1)) \int_{[0,1]} h_i(\mu_{ij}^*, \mu_i) \int_{[0,1]} \min(\mu_{ij}^*, 2B_{\text{conf}}, 1 - T^{-1/6}) d\mu_i dH_i(\mu_i) \\
\text{(by uniform continuity)} \\
\leq (1 + o(1)) \int_{[0,1]} h_i(\mu_{ij}^*, \mu_i) \frac{\mu_{ij}^*(1 - \mu_{ij}^*)}{T} dH_i(\mu_i),
\]

which completes the proof. \( \square \)

D Lemmas for Lower Bound

D.1 Lower Bound on the Error

Proposition 16. (Lemma 1 in Kaufmann et al. (2016)) Let \( \mu, \nu \in [0, 1]^K \) be two set of model parameters.
Then, for any event $E$, the following inequality holds:

$$\sum_{i \in [K]} \mathbb{E}_\nu[N_i(T)]d_{KL}(\nu_i, \mu_i) \geq d_{KL}(\mathbb{P}_\nu(E), \mathbb{P}_\mu(E)).$$

Moreover,

$$\forall x \in [0, 1]d_{KL}(x, 1-x) \geq \log \frac{1}{2.4x}. \quad (19)$$

Proposition 16 describes the hardness of identifying two different sets of parameters. By using this proposition, we derive Lemma 7.

**Proof of Lemma 7.** We assume that Eq. (10) is false and derive a contradiction; that is, suppose that

$$\max(\mathbb{P}_\mu[J(T) \neq i], \mathbb{P}_\nu[J(T) \neq j]) < \frac{1}{2.4} \exp \left( -(1 + \eta)Td_{KL}(\mu_j, \mu_i) \right).$$

Let $p = \frac{1}{2.4} \exp \left( -(1 + \eta)Td_{KL}(\mu_j, \mu_i) \right)$. Then, Proposition 16 with $E = \{J(T) \neq i\}$ yields

$$T \max(d_{KL}(\mu_j, \mu_i), d_{KL}(\mu_i, \mu_j)) \geq \sum_{i \in [K]} \mathbb{E}_\nu[N_i(T)]d_{KL}(\nu_i, \mu_i)$$

$$\geq d_{KL}(\mathbb{P}_\nu[J(T) \neq i], \mathbb{P}_\mu[J(T) \neq i])$$

(by Proposition 16)

$$\geq d_{KL}(p, 1-p)$$

(by Eq. (10) is false)

$$\geq \log \frac{1}{2.4p}$$

(by Eq. (19))

$$\geq (1 + \eta)Td_{KL}(\mu_j, \mu_i)$$

$$\geq (1 + \eta)(1 - \eta')T \max(d_{KL}(\mu_j, \mu_i), d_{KL}(\mu_i, \mu_j)),$$

(for some constant $C > 0$ and $\eta' = C \times B_{\text{conf}}T^{1/3}$ by Lemma 12)

which contradicts for some $C_2 > 0$ and $\eta = C_2 \times B_{\text{conf}}T^{1/3}$ such that $(1 + \eta)(1 - \eta') > 1$, and thus Eq. (10) holds.

**D.2 Exchangeable Mass**

**Proof of Lemma 6.** Letting $m = (\mu_i + \mu_j)/2$, we have

$$\int_{\Theta_{i,j,1/6}} (\mu_i - \mu_j) f(\mu_i, \mu_j, \mu_{\setminus ij}) dH(\mu)$$

$$= \int_{\Theta_{i,j,1/6}} (\mu_i - \mu_j) f(\mu_i, \mu_j, \mu_{\setminus ij}) h_{ij}(\mu_i, \mu_j) d\mu_i d\mu_j dH_{\setminus ij}(\mu_{\setminus ij})$$

$$= (1 + o(1)) \int_{\Theta_{i,j,1/6}} h_{ij}(m, m) d\mu_i d\mu_j dH_{\setminus ij}(\mu_{\setminus ij})$$

(by uniform continuity and the diameter of $\Theta_{i,j,1/6}$ is $o(1)$)
\[= (1 + o(1)) \int_{\Theta_{j,i,1/6}} h_{ij}(m, m|\mu_{\setminus ij})(\mu_j - \mu_i) f(\mu_j, \mu_i, \mu_{\setminus ij}) d\mu_j d\mu_i dH_{\setminus ij}(\mu_{\setminus ij})\]

(by symmetry)

\[= (1 + o(1)) \int_{\Theta_{j,i,1/6}} (\mu_j - \mu_i) f(\mu_j, \mu_i, \mu_{\setminus ij}) dH(\mu).\]

(by uniform continuity)

\[\]

D.3 Integration on the Lower Bound

Proof of Lemma 8.

\[\int_{[\mu_{\setminus i}, \mu_{\setminus i} + 2B_{\text{conf}}]} (\mu_i - \mu_{\star i}) \exp \left( -(1 + \eta) T d_{\text{KL}}(\mu_{\star i}, \mu_i) \right) d\mu_i \]

\[= (1 - o(1)) \int_{[\mu_{\setminus i}, \mu_{\setminus i} + 2B_{\text{conf}}]} (\mu_i - \mu_{\star i}) \exp \left( -(1 + \eta) T \frac{(\mu_i - \mu_{\star i})^2}{2\mu_{\star i}(1 - \mu_{\star i})} \right) d\mu_i \]

(by Lemma 13)

\[= (1 - o(1)) \left[ \frac{\mu_{\star i}(1 - \mu_{\star i})}{T} \exp \left( -(1 + \eta) T \frac{(\mu_i - \mu_{\star i})^2}{2\mu_{\star i}(1 - \mu_{\star i})} \right) \right]_{\mu_{\setminus i} + 2B_{\text{conf}}}^{\mu_{\setminus i}} \]

\[= \frac{\mu_{\star i}(1 - \mu_{\star i})}{(1 + \eta)T} - o \left( \frac{1}{T} \right).\]

(by \exp \left( -(1 + \eta) T \frac{(\mu_i - \mu_{\star i})^2}{2\mu_{\star i}(1 - \mu_{\star i})} \right) = o(1) \text{ for } \mu_i - \mu_{\star i} = 2B_{\text{conf}})\]