Bandit Learning Through Biased Maximum Likelihood Estimation

Xi Liu*  
Electrical and Computer Engineering  
Texas A&M University  
xiliu@tamu.edu

Ping-Chun Hsieh*  
Department of Computer Science  
National Chiao Tung University  
pinghsieh@cs.nctu.edu.tw

Anirban Bhattacharya  
Department of Statistics  
Texas A&M University  
anirbanb@stat.tamu.edu

P. R. Kumar  
Electrical and Computer Engineering  
Texas A&M University  
prk@tamu.edu

Abstract

We propose BMLE, a new family of bandit algorithms, that are formulated in a general way based on the Biased Maximum Likelihood Estimation method originally appearing in the adaptive control literature. We design the cost-bias term to tackle the exploration and exploitation tradeoff for stochastic bandit problems. We provide an explicit closed form expression for the index of an arm for Bernoulli bandits, which is trivial to compute. We also provide a general recipe for extending the BMLE algorithm to other families of reward distributions. We prove that for Bernoulli bandits, the BMLE algorithm achieves a logarithmic finite-time regret bound and hence attains order-optimality. Through extensive simulations, we demonstrate that the proposed algorithms achieve regret performance comparable to the best of several state-of-the-art baseline methods, while having a significant computational advantage in comparison to other best performing methods. The generality of the proposed approach makes it possible to address more complex models, including general adaptive control of Markovian systems.

1 Introduction

Sequential decision making in an unknown environment [1] has historically been a challenging task in engineering systems since a control action taken on a dynamic system serves the “dual” purposes [2,3] of controlling the system to reduce immediate cost incurred and also simultaneously exploring system behavior by exciting it. To learn an optimal policy, the decision maker needs to simultaneously handle parameter estimation from stochastic observations as well as adaptive policy design based on these estimates. In a statistical parameter estimation problem, maximum likelihood estimation (MLE) is among the most powerful and commonly-used estimation techniques. However, when directly applied to learning an optimal policy, MLE and least-squares parametric methods have been shown to suffer from the “closed-loop identifiability” problem: the system is ever evolving in a closed-loop with the adaptive control law, and as the control law converges to a limiting control law, it ceases to learn about other possibly better control laws [4,7]. Specifically, given its greedy nature, MLE can converge to a sub-optimal set of parameters due to insufficient exploration. To resolve this issue, in the community of adaptive control for unknown Markov decision processes (MDPs), is to introduce a multiplicative cost-bias into the likelihood in favor of candidate models with higher optimal rewards [8,17], so as to encourage exploration. It exploits the specific property that the limit points of the

*Equal contribution.

Preprint. Under review.
MLE correspond to parameters which have higher optimal cost than the true one \(\theta\). This makes possible directed exploration. Specifically, the biased maximum likelihood estimator (BMLE) is designed to take the following form

\[
\hat{\theta}^{\text{BMLE}} = \arg\max_{\theta} J(\theta)^{-\alpha(t)} L(\mathcal{H}; \theta),
\]

where \(J(\theta)\) is the optimal long-term average cost achievable under the environment parameter \(\theta\), \(\alpha(t) : [1, \infty) \rightarrow \mathbb{R}_+\) is a function that satisfies \(\lim_{t \rightarrow \infty} \alpha(t) = \infty\) and \(\lim_{t \rightarrow \infty} \alpha(t)/t = 0\), \(\mathcal{H}\) is the history of all observations, and \(L(\mathcal{H}; \theta)\) denotes the likelihood of \(\mathcal{H}\) under \(\theta\). The cost-bias term \(J(\theta)^{-\alpha(t)}\) employed in (1) has two salient features: (i) \(J(\theta)^{-\alpha(t)}\) achieves active exploration by favoring the models with lower cost, and (ii) the effect of the bias term gradually diminishes as \(\alpha(t)\) grows indefinitely with time. For a properly chosen bias term, the resulting BMLE estimate combined with standard dynamic programming has been shown to achieve asymptotically optimal long-term average cost, i.e., regret of order \(\alpha(t)\), for a variety of stochastic dynamic systems \([8, 17]\).

In this paper, we revisit the BMLE approach in the context of bandit learning to address the more demanding issue of minimizing regret and to demonstrate performance in comparison to the best of existing methods. Different from the asymptotic consistency results in \([8, 17]\), our goal is to tailor the BMLE to the stochastic multi-armed bandit problem and perform finite-time analysis in terms of regret. The proposed BMLE can be thought of as a generic approach to implement the principle of optimism in the face of uncertainty. Different from the popular Upper Confidence Bound (UCB) family of algorithms, whose indices usually consist of two components: a maximum likelihood estimator and a confidence interval, BMLE directly operates with the likelihood function to guide the exploration instead of using concentration inequalities. This feature allows the BMLE algorithm to better exploit the collected information of the underlying reward distributions. The BMLE has one additional advantage: It provides a trivial-to-compute index for each arm that considerably saves computation time. We provide a comparison of computational time with respect to other methods.

The main contributions of this paper can be summarized as follows: (i) Motivated by the classic adaptive control literature, we present a new family of bandit algorithms from the perspective of biased maximum likelihood estimation. (ii) As the first step, we design BMLE algorithms for the Bernoulli reward case as well as the more general exponential family reward distributions. By designing proper bias terms for the likelihood function, we can derive simple closed-form expressions for the indices of BMLE algorithms. The presented procedure can be easily extended to other parametric families of reward distributions. (iii) For Bernoulli bandits, we provide the first logarithmic regret bound for the BMLE algorithm and thereby characterize the interplay between the bias term and the regret. (iv) Finally, we conduct extensive numerical simulations and show that the BMLE algorithm can achieve state-of-the-art regret performance while being computationally efficient. (v) Present comparative computation time results that show the superiority of the BMLE method.

Related work. Algorithm design for the stochastic multi-armed bandit problem has been studied extensively in the existing literature. Most of the prior work can be categorized into two main groups, namely frequentist approaches and Bayesian approaches. In the frequentist settings, the family of UCB algorithms \([18–22]\) are among the most popular ones given their simplicity in implementation and good theoretical guarantees. An upper confidence bound can be directly derived from concentration inequalities or constructed with the help of other information measures, such as the Kullback–Leibler divergence used by the KL-UCB algorithm \([23, 26]\). The concept of upper confidence bound has later been extended to various types of models, such as contextual linear bandits \([27, 29]\), Gaussian process bandit optimization \([30]\), and model-based reinforcement learning \([31]\). The above list is by no means exhaustive but is mainly meant to illustrate the wide applicability of the UCB approach in different settings. While being a simple and generic index-type algorithm, UCB-based methods sometimes suffer from much higher regret than their counterparts \([32, 33]\). This mainly results from the fact that the upper confidence bound itself only uses moment assumptions on the true distribution and hence does not fully exploit the underlying information structure. Different from the UCB solutions, the proposed BMLE algorithm addresses the exploration and exploitation tradeoff by directly operating with the likelihood function to navigate the exploration, and therefore it makes better use of the information of the parametric distributions.

On the other hand, the Bayesian approach studies the setting where the unknown reward parameters are drawn from an underlying prior distribution. As one of the most popular Bayesian bandit

\footnote{Due to space limitation, please refer to Appendix J.2 for the results.}
We consider the stochastic $N$-armed bandit problem, where each arm $i$ is characterized by its reward distribution $D_i$ with mean $\theta_i$. Without loss of generality, we assume that $\theta_1 > \theta_2 > \cdots > \theta_N \geq 0$, and hence arm 1 is the optimal arm. For each arm $i$, we define $\Delta_i := \theta_1 - \theta_i$ to be the negative of the gap between its mean reward and that of the optimal arm. For ease of notation, we also use $\Delta$ to denote the minimum gap $\Delta_2$. We use $\theta$ to denote the vector $(\theta_1, \cdots, \theta_N)$. At each time $t = 1, \cdots, T$, the decision maker chooses an arm $\pi_t \in \{1, \cdots, N\}$ and observes the corresponding reward $X_t$, which is independently drawn from the distribution $D_{\pi_t}$. Let $N_t(t)$ and $S_t(t)$ be the total number of trials of arm $i$ and the total reward collected from pulling arm $i$ up to time $t$, respectively. We also use $H_t := (\pi_1, X_1, \pi_2, X_2, \cdots, \pi_t, X_t)$ to denote the history of all the choices of the decision maker and the reward observations up to time $t$. We let $L(H_t; \{D_i\})$ denote the likelihood of the history $H_t$ under the reward distributions $\{D_i\}$. Based on the multi-armed bandit convention, our objective is to minimize the pseudo regret defined as $\text{Regret}(T) := T \theta_1 - E[\sum_{t=1}^{T} X_t]$, where the expectation is taken with respect to the randomness of the rewards and the employed policy. The employed policy should not depend on $T$ and should perform well for all $T$.

2 Problem Setup

We consider the stochastic $N$-armed bandit problem, where each arm $i$ is characterized by its reward distribution $D_i$ with mean $\theta_i$. Without loss of generality, we assume that $\theta_1 > \theta_2 > \cdots > \theta_N \geq 0$, and hence arm 1 is the optimal arm. For each arm $i$, we define $\Delta_i := \theta_1 - \theta_i$ to be the negative of the gap between its mean reward and that of the optimal arm. For ease of notation, we also use $\Delta$ to denote the minimum gap $\Delta_2$. We use $\theta$ to denote the vector $(\theta_1, \cdots, \theta_N)$. At each time $t = 1, \cdots, T$, the decision maker chooses an arm $\pi_t \in \{1, \cdots, N\}$ and observes the corresponding reward $X_t$, which is independently drawn from the distribution $D_{\pi_t}$. Let $N_t(t)$ and $S_t(t)$ be the total number of trials of arm $i$ and the total reward collected from pulling arm $i$ up to time $t$, respectively. We also use $H_t := (\pi_1, X_1, \pi_2, X_2, \cdots, \pi_t, X_t)$ to denote the history of all the choices of the decision maker and the reward observations up to time $t$. We let $L(H_t; \{D_i\})$ denote the likelihood of the history $H_t$ under the reward distributions $\{D_i\}$. Based on the multi-armed bandit convention, our objective is to minimize the pseudo regret defined as $\text{Regret}(T) := T \theta_1 - E[\sum_{t=1}^{T} X_t]$, where the expectation is taken with respect to the randomness of the rewards and the employed policy. The employed policy should not depend on $T$ and should perform well for all $T$.

3 The BMLE Algorithm

In this section, we formally present the general BMLE algorithm. The main components of the BMLE algorithm can be summarized as follows:

1. Design a bias term that favors the model with larger achievable optimal long-term average reward.

2. At each time $t$, derive the biased maximum likelihood estimator $\hat{\theta}^{\text{BMLE}}_t = (\hat{\theta}^{\text{BMLE}}_{t,i})$ as detailed in the subsequent subsections, and then select an arm as

$$\pi^{\text{BMLE}}_t = \arg\max_{i \in \{1, \cdots, N\}} \hat{\theta}^{\text{BMLE}}_{t,i}.$$  

(We assume here and throughout that there is some arbitrary order on the argument of “argmax” used to break ties, so that “argmax” always yields a single choice).
3.1 BMLE Algorithm for Bernoulli Rewards

To begin with, we consider the simpler case of Bernoulli rewards to illustrate the rationale of the BMLE algorithm. Recall that \( N_i(t) \) denotes the number of trials of arm \( i \) up to time \( t \). In the Bernoulli case, the total reward \( S_i(t) \) collected from arm \( i \) follows a Binomial distribution with parameters \( N_i(t) \) and \( \theta_i \). Moreover, for Bernoulli rewards, we can simplify the notation for likelihood as \( L(\mathcal{H}_t; \{D_i\}) \equiv L(\mathcal{H}_t; \theta) \). Under any set of parameter \( \mu = (\mu_1, \cdots, \mu_N) \in [0, 1]^N \), we have

\[
L(\mathcal{H}_t; \mu) = \prod_{i=1}^{N} \mu_i^{S_i(t)} (1 - \mu_i)^{N_i(t) - S_i(t)}.
\]

By taking partial derivative with respect to each \( \mu_i \), it is easy to verify that the maximum likelihood estimator for \( \mu_i \) is simply the empirical mean, i.e., \( \hat{\mu}_i^{\text{MLE}} = S_i(t)/N_i(t) \). To construct the cost-bias term of (1) for the bandit setting, we consider an analogy using the mean reward. Recall that the selected arm at each time

\[
\text{Proposition 1}
\]

\[
\text{Remark 1}
\]

\[
\text{Definition 2}
\]

\[
3.1 \text{ BMLE Algorithm for Bernoulli Rewards}
\]

\[
\text{To begin with, we consider the simpler case of Bernoulli rewards to illustrate the rationale of the BMLE algorithm. Recall that } N_i(t) \text{ denotes the number of trials of arm } i \text{ up to time } t. \text{ In the Bernoulli case, the total reward } S_i(t) \text{ collected from arm } i \text{ follows a Binomial distribution with parameters } N_i(t) \text{ and } \theta_i. \text{ Moreover, for Bernoulli rewards, we can simplify the notation for likelihood as } L(\mathcal{H}_t; \{D_i\}) \equiv L(\mathcal{H}_t; \theta). \text{ Under any set of parameter } \mu = (\mu_1, \cdots, \mu_N) \in [0, 1]^N, \text{ we have}
\]

\[
L(\mathcal{H}_t; \mu) = \prod_{i=1}^{N} \mu_i^{S_i(t)} (1 - \mu_i)^{N_i(t) - S_i(t)}.
\]

By taking partial derivative with respect to each \( \mu_i \), it is easy to verify that the maximum likelihood estimator for \( \mu_i \) is simply the empirical mean, i.e., \( \hat{\mu}_i^{\text{MLE}} = S_i(t)/N_i(t) \). To construct the cost-bias term of (1) for the bandit setting, we consider an analogy using the mean reward. Recall that the selected arm at each time

\[
\text{Proposition 1}
\]

\[
\text{Remark 1}
\]

\[
\text{Definition 2}
\]

\[
L(\mathcal{H}_t; \mu) = \prod_{i=1}^{N} \mu_i^{S_i(t)} (1 - \mu_i)^{N_i(t) - S_i(t)}.
\]

By taking partial derivative with respect to each \( \mu_i \), it is easy to verify that the maximum likelihood estimator for \( \mu_i \) is simply the empirical mean, i.e., \( \hat{\mu}_i^{\text{MLE}} = S_i(t)/N_i(t) \). To construct the cost-bias term of (1) for the bandit setting, we consider an analogy using the mean reward. Recall that

\[
\text{Remark 1}
\]

\[
\text{Definition 2}
\]

\[
L(\mathcal{H}_t; \mu) = \prod_{i=1}^{N} \mu_i^{S_i(t)} (1 - \mu_i)^{N_i(t) - S_i(t)}.
\]

By taking partial derivative with respect to each \( \mu_i \), it is easy to verify that the maximum likelihood estimator for \( \mu_i \) is simply the empirical mean, i.e., \( \hat{\mu}_i^{\text{MLE}} = S_i(t)/N_i(t) \). To construct the cost-bias term of (1) for the bandit setting, we consider an analogy using the mean reward. Recall that

\[
\text{Remark 1}
\]

\[
\text{Definition 2}
\]

\[
L(\mathcal{H}_t; \mu) = \prod_{i=1}^{N} \mu_i^{S_i(t)} (1 - \mu_i)^{N_i(t) - S_i(t)}.
\]

By taking partial derivative with respect to each \( \mu_i \), it is easy to verify that the maximum likelihood estimator for \( \mu_i \) is simply the empirical mean, i.e., \( \hat{\mu}_i^{\text{MLE}} = S_i(t)/N_i(t) \). To construct the cost-bias term of (1) for the bandit setting, we consider an analogy using the mean reward. Recall that

\[
\text{Remark 1}
\]

\[
\text{Definition 2}
\]

\[
L(\mathcal{H}_t; \mu) = \prod_{i=1}^{N} \mu_i^{S_i(t)} (1 - \mu_i)^{N_i(t) - S_i(t)}.
\]
• An arm that has not been sufficiently explored: If \( N_i(t) \) is much smaller than \( \alpha(t) \), then by the same first-order approximation, \( I(p_i(t), N_i(t), \alpha(t)) \) is approximately equal to \( (S_j(t) - N_i(t)) \log(\alpha(t)) \geq -N_i(t) \log(\alpha(t)) \). In this case, the BMLE index is again negative and its absolute value is on the order of \( O(N_i(t) \log(\alpha(t))) \).

• Based on the above discussion, if a pair of arms \( j \) and \( k \) satisfy \( N_j(t) \gg \alpha(t) \) and \( N_k(t) \ll \alpha(t) \), then the BMLE algorithm chooses arm \( k \) since the index of arm \( j \) is much smaller than that of arm \( k \). Hence, the bias \( \alpha(t) \) indeed encourages exploration. On the other hand, if \( N_j(t) \) and \( N_k(t) \) are fairly close, then a more careful examination of each term in the BMLE index is necessitated, which will be discussed in more detail in Section 4.

Remark 2 There is another equivalent index for the BMLE algorithm. Specifically, define

\[
\hat{I}(p_i(t), N_i(t), \alpha(t)) := \alpha(t) \log \tilde{p}_i(t) - N_i(t) \cdot \text{KL}(p_i(t) || \tilde{p}_i(t)),
\]

where \( \text{KL}(\beta_1 || \beta_2) \) denotes the Kullback–Leibler divergence between a Bernoulli(\( \beta_1 \)) and Bernoulli(\( \beta_2 \)) distribution. The derivation of this index is provided in Appendix \( F \). Through this alternative index, one may find some its connection with the KL-UCB algorithm \( [23–26] \), which selects the arm with index: \( \arg\max_q \max\{q \in [0, 1]: N_i(t) \cdot \text{KL}(p_i(t) || q) \leq \log t + 3 \log \log t\} \). The index of (11) however has two salient distinctions: (i) The BMLE index is derived from the machinery of maximum likelihood estimation, while KL-UCB originates from the idea of introducing more smoothness to the UCB-type algorithms. (ii) Instead of solving a convex optimization problem as KL-UCB, the BMLE index enjoys a simple closed-form expression. For convenience of analysis in later sections, we stick to the expression of (8)-(9) for the rest of the paper.

Remark 3 The expression for \( \tilde{p}_i(t) \) resembles that of a Bayes estimator (under quadratic loss) for a Binomial likelihood with an improper Beta prior on the success probability. However, BMLE is not a Bayesian approach as it does not impose any prior on model parameters. Instead, BMLE achieves exploration entirely through the time-varying bias term.

### 3.2 BMLE Algorithm for Exponential Family Reward Distributions

In this section, we generalize the proposed BMLE index for exponential family reward distributions. To begin with, the density function of a canonical exponential family distribution can be expressed as

\[
p(x; \eta) = \exp(\eta x - b(\eta) - c(x)),
\]

where \( \eta \) is the canonical parameter, \( c(\cdot) \) is a real-valued function, and \( b(\cdot) \) is a real-valued twice-differentiable function. For example, for a Gaussian distributions with mean \( \mu_i \) and variance \( \sigma^2_i \), we can represent it in the form of (12) by letting \( \eta = \mu_i / \sigma^2_i \), \( b(\eta) = \sigma^2_i \eta^2 / 2 \), \( c(x) = (x^2) / 2 \sigma^2_i \) + \( \log \sqrt{2\pi \sigma^2_i} \). By calculating the moment generating function for \( p(x; \eta) \), we further know that \( \mathbb{E}[Y] = b'(\eta) \) for any random variable \( Y \) with a density function as (12). Therefore, we know the mean of an exponential family distribution is determined solely by \( \eta \).

Next, we turn to the derivation of the proposed BMLE index. Consider the case where the reward distribution of each arm \( i \) has the density function \( p(x; \eta) \) with mean \( \theta_i \), and the functions \( b(\cdot) \), \( c(\cdot) \), and \( v(\cdot, \cdot) \) are identical across all the arms. We use \( \eta \) to denote the vector \( \{\eta_1, \cdots, \eta_N\} \). Recall that \( \pi_t \) denotes the index of the arm chosen by the employed policy at time \( t \). Based on (12), we know that at each time \( t \), the likelihood of \( H_t \) under the distribution parameters \( \eta \) is

\[
L(H_t; \eta) = \prod_{s=1}^{t} \exp(\eta_{\pi_s} X_s - b(\eta_{\pi_s}) - c(X_s)).
\]

Next, we propose to construct the multiplicative bias term as \( \max_{i \in \{1, \cdots, N\}} \exp(g(b(\eta_i)) \alpha(t)) \), where \( g(\cdot) \) is a strictly increasing user-defined real-valued function. Following the same approach as (4), we propose the BMLE index for exponential family distribution as

\[
\eta^\text{BMLE}_t := \arg\max_{\eta \in \mathbb{R}^N} \left\{ L(H_t; \eta) \cdot \left( \max_{i \in \{1, \cdots, N\}} \exp(g(b(\eta_i)) \cdot \alpha(t)) \right) \right\},
\]

Similar to the procedure outlined in (5)-(7), based on (13) and the maximization problem of (14),

\[
\pi^\text{BMLE}_t = \arg\max_{i \in \{1, \cdots, N\}} \left\{ \arg\max_{\eta \in \mathbb{R}^N} \left\{ L(H_t; \eta) \cdot \left( \max_{i \in \{1, \cdots, N\}} \exp(g(b(\eta_i)) \cdot \alpha(t)) \right) \right\} \right\}
\]

\[
= \arg\max_{i \in \{1, \cdots, N\}} \left\{ \max_{\eta \in \mathbb{R}^N} \left\{ L(H_t; \eta) \cdot \exp(g(b(\eta_i)) \cdot \alpha(t)) \right\} \right\}.
\]
To further substantiate the above index, we examine the closed-form expression of the BMLE for Gaussian distributions. Suppose each arm $i$ has a Gaussian reward distribution with mean $\theta_i$ and variance $\sigma^2$. For simplicity, one can select $g(\cdot)$ as a linear map, i.e. $g(x) = x/\sigma^2$. In this case, $\eta_i = \theta_i/\sigma^2$, $b(\eta) = \sigma^2\eta^2/2$ and hence $b'(\eta) = \sigma^2\eta$ (note that $\eta_i$ and $\theta_i$ exhibit a one-to-one relationship in this case). Therefore, in the Gaussian case, we have
\[
\pi^{\text{BMLE}}_t = \arg\max_{i \in \{1, \ldots, N\}} \left\{ \max_{\eta \in \mathbb{R}^n} \left\{ L(H_i; \eta) \cdot \exp(\eta_i \cdot \alpha(t)) \right\} \right\}.
\] (17)

Again, the optimizer of the inner maximization problem of (17) can be derived by taking partial derivative with respect to $\eta$. After a series of calculations, we obtain the closed-form expression of BMLE index for Gaussian rewards as in the following Proposition 2 (the proof is in Appendix C).

**Proposition 2** For Gaussian reward distributions with the same variance $\sigma^2$ among arms, under the BMLE algorithm, the selected arm at each time $t$ is $\pi^{\text{BMLE}}_t = \arg\max_{i \in \{1, \ldots, N\}} \left\{ \frac{S_i(t)}{N_i(t)} + \frac{\alpha(t)}{2N_i(t)} \right\}$.

### 4 Analysis of the BMLE Algorithm for Bernoulli Rewards

In this section, we present the theoretical analysis of the proposed bandit algorithm. To begin with, we introduce several useful properties of the index $I(\nu, \alpha(t))$ in (8)-(9) to better demonstrate the behavior of the proposed BMLE algorithm.

**Lemma 1** For a fixed $\nu$ and $\alpha(t)$, $I(\nu, n, \alpha(t))$ is strictly decreasing with $n$.

**Lemma 2** For a fixed $n \geq 1$ and $\alpha(t)$, $I(\nu, n, \alpha(t))$ is strictly increasing with $\nu$, for all $\nu \geq 0$.

The proofs of Lemmas 1 and 2 are provided in Appendices A and B, respectively.

**Remark 4** Recall that the BMLE index for Bernoulli rewards is $I(p_i(t), N_i(t), \alpha(t))$, where $p_i(t) = S_i(t)/N_i(t)$ denotes the empirical mean. Then, it is reasonable to consider the index of an arm increases with its empirical mean reward, which is what Lemma 2 shows.

**Lemma 3** Given any pair of real numbers $\mu_1, \mu_2 \in [0, 1]$ with $\mu_1 > \mu_2$, for any real numbers $n_1, n_2$ that satisfy $n_1 \geq \frac{2\alpha(t)}{\mu_1 - \mu_2}$ and $n_2 \geq \frac{2\alpha(t)}{\mu_1 - \mu_2}$, we have $I(\mu_1, n_1, \alpha(t)) > I(\mu_2, n_2, \alpha(t))$.

To prepare for the following lemma, we first define a function $M^*(\mu_1, \mu_2) := \sup \left\{ K_1 : K_1 \log K_1 - K_1(K_1 + 1) \geq \log \left( \frac{\mu_1 + \mu_2}{2} \right) \right\}$.

**Lemma 4** Given any pair of real numbers $\mu_1, \mu_2 \in [0, 1]$ with $\mu_1 > \mu_2$, for any real numbers $n_1, n_2$ that satisfy $n_1 \leq M^*(\mu_1, \mu_2) \cdot \alpha(t)$ and $n_2 \geq \frac{2\alpha(t)}{\mu_1 - \mu_2}$, we have $I(0, n_1, \alpha(t)) > I(\mu_2, n_2, \alpha(t))$.

The proofs of Lemmas 3 and 4 are provided in Appendices C and D, respectively.

**Remark 5** Note that Lemma 3 shows that BMLE indeed tends to select the arm with a larger mean reward after sufficient exploration which is quantified in terms of $\alpha(t)$ by $n_j \geq \frac{2\alpha(t)}{\mu_1 - \mu_2}$ for $j = 1, 2$. On the other hand, Lemma 4 suggests that BMLE is designed to continue exploration even if the empirical mean reward is initially fairly low (which is reflected by the zero in $I(0, n_1, \alpha(t))$), when there has been insufficient exploration, as quantified by $n_1 \leq M^*(\mu_1, \mu_2) \cdot \alpha(t)$.

We are ready to present the main theoretical results as follows.

**Proposition 3** Under the BMLE algorithm with the bias term $\alpha(t) = \gamma(t) \log t$ with $\lim_{t \to \infty} \gamma(t) = \infty$, the pseudo regret is
\[
\text{Regret}(T) \leq \sum_{i=2}^{N} \left( \frac{32}{3\Delta_i} \alpha(t) + \Delta_i \left( 2 \log T + C_\gamma(\theta) \right) \right) = O(\gamma(T) \log T),
\] (18)

where $C_\gamma(\theta)$ is a constant that depends on $\theta$ and the choice of $\gamma(t)$, and is independent of $T$.

**Proposition 4** Given a lower bound $\Delta$ for the minimum gap $\Delta$, under the BMLE algorithm with $\gamma(t) = \max\left\{ \frac{4}{\Delta}, \frac{32}{\Delta^2 M^*(1, \theta) \cdot \frac{2}{\Delta^2}} \right\}$, the pseudo regret is $O(\log T)$.

**Proof Sketch:** We highlight the main idea of the proofs as follows: our target is to quantify the expected number of trials of a sub-optimal arm up to time $T$. The main challenge lies in characterizing the behavior of the BMLE index for both regimes where $N_i(t)$ is small compared to compared to $\alpha(t)$, as well as when it is large compared to $\alpha(t)$. Different from the straightforward confidence interval used by the conventional UCB-type policies, the dependency between the level of exploration and the bias term $\alpha(t)$ is technically more complex. We leverage the properties of the BMLE index in Lemma 4 to obtain a regret upper bound. The complete proof is provided in Appendix F. □
Remark 6 By Proposition[4] in the case of unknown minimum gap, the BMLE algorithm can achieve a regret arbitrarily close to $O(\log T)$ by configuring $\alpha(t)$ to be a slowly increasing function (e.g. $\alpha(t) = \log \log \log t$). However, the choice of $\gamma(t)$ also affects the constant $C_5(\theta)$. In Section[5] we will provide a more detailed discussion on the choice of the bias term based on empirical evaluation. In addition to the expected regret bounds, we also obtain a high-probability regret bound for Bernoulli bandits as presented in Appendix[4].

5 Simulation Results

A large-scale simulation experiment was implemented for Bernoulli bandits and Gaussian bandits to evaluate the performance of the proposed BMLE algorithm. In Bernoulli bandits, the reward of an arm $i$ is binary and drawn independently from a Bernoulli distribution with an unknown parameter $\theta_i \in (0, 1)$. For comparison, in the setting of Gaussian bandits, the reward distribution of arm $i$ is a Gaussian distribution with mean $\mu_i$ and standard deviation $\sigma_i$. For simplicity of presentation and to use the results of Proposition[4], we take $\sigma_i \equiv \sigma$ for all $i$ in the experiments with Gaussian bandits.

Figure 1: (a)-(b) Average cumulative regret of Bernoulli bandits over 80 trials with $(\theta_i)_{i=1}^{10} = (0.455, 0.46, 0.465, 0.47, 0.475, 0.48, 0.485, 0.49, 0.495, 0.5)$ and $T = 3 \times 10^4$. (c)-(d) Average cumulative regret of Bernoulli bandits over 80 trials with $(\theta_i)_{i=1}^{10} = (0.46, 0.47, 0.48, 0.49, 0.5, 0.41, 0.42, 0.43, 0.44, 0.45)$ and $T = 3 \times 10^4$ (Note: For (b) and (d), $\alpha(t) = (\log(t))^{1.5}$ for BMLE).

Table 1: Statistics of distribution of final regret over 80 trials for the Bernoulli bandits with true values: $(\theta_i)_{i=1}^{10} = (0.455, 0.46, 0.465, 0.47, 0.475, 0.48, 0.485, 0.49, 0.495, 0.5)$ and $T = 3 \times 10^4$ (We use TUCB and BUCB as the shorthand of UCB-Tuned and BayesUCB, respectively).

| Algorithm  | BMLE | V-IDS | IDS  | KG*  | KG   | UCB | UCB-Tuned | TS  | BUCB | MOSS |
|------------|------|-------|------|------|------|-----|-----------|-----|------|------|
| Mean Regret | 177.2| 235.0 | 251.4| 264.8| 340.3| 527.8| 318.1     | 308.0| 374.0| 305.6|
| Standard Error | 0.10 | 1.24  | 1.11  | 0.27 | 0.44 | 2.81 | 0.70      | 0.73 | 0.12  | 0.10 |
| Quantile .25 | 68.6 | 156.9 | 175.4| 42.9 | -    | 506.4| 257.3     | 246.5| 228.1| 244.9|
| Quantile .50 | 114.6| 201.5 | 233.1| 59.8 | 508.2| 528.5| 259.5     | 296.7| 366.0| 306.7|
| Quantile .75 | 233.2| 293.1 | 322.7| 451.4| 1049 | 547.4| 361.6     | 365.1| 415.1| 367.3|
| Quantile .90 | 391.7| 369.3 | 394.3| 615.8| 1197 | 565.2| 411.9     | 403.4| 440.2| 419.0|
| Quantile .95 | 465.1| 480.3 | 404.4| 876.5| 1198 | 574.3| 422.0     | 411.0| 443.8| 424.2|

Figures[1] (b) and (d) show the comparison of the performance of BMLE with many state-of-the-art baselines in terms of average cumulative regret. The UCB algorithm[19] selects an arm $i$ which maximizes the index $\hat{\theta}_i(t) + \sqrt{2 \log(t) / N_i(t)}$, where $\hat{\theta}_i(t)$ is the empirical mean reward received from samples of arm $i$. The index of UCB is constructed to facilitate regret bound analysis. To achieve better empirical performance, UCB-Tuned[19] replaces the index by $\hat{\theta}_i(t) + \sqrt{\min\{1/4, \nabla_i(t)\} \log(t) / N_i(t)}$, where $\nabla_i(t)$ is the upper bound on the variance of the reward of arm $i$. The MOSS algorithm[21][22] is a slightly different index from UCB and UCB–Tuned, and is known to achieve minimax-optimal-regret bounds up to a constant factor. The Thompson sampling (TS) algorithm[33][37][45] and BayesUCB[45] are proved to be optimal and observed to exhibit excellent performance in experiments with Bernoulli bandits. BayesUCB constructs upper confidence bounds based on the $1 - 1/t$ quantiles of posterior distribution. Their leading positions in empirical performance were displaced by Information Directed Sampling (IDS) and its variant - Variance Based IDS (V-IDS)[32][42]. It is not surprising that they are the closest competitors to BMLE. However, BMLE is found to be slightly better than IDS and V-IDS in the bandit setting as seen from Figure[1]. Moreover, in spite of their good performance, the determination of their indices suffers from high computational complexity, even under approximation. In contrast, the index suggested by BMLE with its simple closed-form expression is trivial to compute. We also compare BMLE with the Knowledge Gradient (KG) policy[39] method, although the regret of KG sometimes grows linearly as it may
explore insufficiently. Finally, comparison is also conducted with KG* [40], a heuristic KG-based method that was reported to offer better performance. In all the comparison, we sample 1000 points over [0, 1] interval in computation of IDS and V-IDS, use $\alpha = 1$ for explore-exploration balancing term in MOSS, and take $c = 0$ in BayesUCB. We repeat the experiment 80 times before taking average of the cumulative regret. We also compare their performance in terms of running time. Due to page limitation, please check Appendix J.2 for the discussion.

We compare the different choices of $\alpha(t)$ in Figures 2(a), and 2(c). We observe that $\alpha(t) = (\log(t))^{1.5}$ achieves the best empirical performance. This motivates us to choose $\alpha(t) = (\log(t))^{1.5}$ in the comparison between BMLE with state-of-the-art baselines. We observe BMLE performs slightly better performance than IDS and V-IDS and a lot better than other baselines. The advantage is especially obvious in more challenging tasks such as Figure 1(b), where the largest mean and the second largest mean is only 0.05, vs. 0.1 in Figure 1(d). We also summarize the standard error and quantile of the final regrets attained by those algorithms and highlighted the smallest number in Table 5. We observe that at many quantiles, BMLE attains smaller value than baselines. Its performance variation is smaller among different trials and more robust in experiments, although this advantage at lower quantiles versus high quantiles can be different.

Figure 2 presents the numerical results of BMLE for Gaussian bandits. In Figure 2(a) and 2(c), a comparison of different choices of $\alpha(t)$ is conducted. We noticed that the choice of $\alpha(t)$ that attains the best performance is $(\log(t))^2$, which is slightly different from the one that generally works well for Bernoulli bandits. Since we do not prove the regret bounds of BMLE in Gaussian bandits, we conjecture that this is because the function $J(\cdot)$ used in derivation of index for Gaussian bandits is different from the one used for Bernoulli bandits.\footnote{We experiment with $\alpha(t) = (\log(t))^\chi$ with various $\chi$, and $\chi = 1.5$ works the best. More work is required to arrive at a data-driven choice for $\chi$.}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{(a)-(b) Average cumulative regret of Gaussian bandits over 100 trials with 5 arms: \{\mu_i\}_{i=1}^{5} = \{0.48, 0.49, 0.5, 0.51, 0.52\} and $\sigma = 0.8$. (c)-(d) Average cumulative regret of Gaussian bandits over 100 trials with 5 arms: \{\mu_i\}_{i=1}^{5} = \{0.49, 0.495, 0.5, 0.505, 0.51\}, $\sigma = 0.8$ and $T = 3 \times 10^5$. (Note: For (b) and (d), $\alpha(t) = (\log(t))^2$ for BMLE).}
\end{figure}

A comparison between BMLE and several state-of-the-art baselines are illustrated in Figure 2(b) and 2(d). Similar with the comparison for Bernoulli bandits, we evaluate their performance under two sets of parameter values of different levels of difficulty. The GPUCB used in comparison was discussed in Gaussian process optimization [30] and used as baseline of bandit algorithm in [32]. Its index at time $t$ for arm $i$ is $\hat{\mu}_i(t) + \sqrt{2\sigma_i(t)}$, where $\hat{\mu}_i(t)$ and $\sigma_i(t)$ are the posterior mean and standard deviation and $\beta_i = 2 \log(Nt^2 T^2 / \delta_i)$. Its variant GPUCB-Tuned demonstrates better empirical performance and replaces the original $\beta_i$ by $\beta_i = 0.9 \log(t)$. We observe that, BMLE in general outperforms other baselines including the V-IDS, although the time horizon of the experiment is $3 \times 10^5$, ten times as long as the experiments with Bernoulli bandits. It needs to be emphasized here that we choose the parameter values to make the problem very challenging: the variance is 8 times of the value difference between the largest mean and second largest mean. We also summarize the quantiles statistics of the final regret in Table 5 (see Appendix J.2). Similar conclusions follow.

Remark 7 Like several baseline methods (e.g. IDS and BayesUCB), the BMLE algorithm takes a parametric approach to obtain its index. As BMLE makes good use of the information of the underlying distributions through the likelihood function, it is not surprising that BMLE achieves comparable performance compared to IDS and better regret than the UCB-type algorithms. On the other hand, we also expect some loss of efficiency if the likelihood is misspecified, and future work will focus on quantifying the effect of such (mild) model misspecification.\footnote{It remains an interesting direction to explore how $J(\cdot)$ influences the form of the empirically best $\alpha(t)$.}
6 Concluding Remarks

The Biased Maximum Likelihood method, developed in the study of general adaptive control, provides
a scheme for optimal control of general Markovian systems. However, it has not been explored with
respect to the finer notion of regret. Here we have explored the design of the bias term in the context
of bandit problems, and shown that it is a competitive method with performance often better than
other baseline schemes, and with a major computational advantage in terms of an easy-to-compute
index for each arm. It would be useful to extend precise regret and computational analysis to general
adaptive control of Markov chains, and to support such a study with detailed experiments.

References

[1] P. R. Kumar. A survey of some results in stochastic adaptive control. *SIAM Journal on Control and
    Optimization*, 23(3):329–380, 1985.
[2] A. A. Feldbaum. Dual control theory. I. *Avtomatika i Telemekhanika*, 21(9):1240–1249, 1960.
[3] A. A. Feldbaum. Dual control theory. II. *Avtomatika i Telemekhanika*, 21(11):1453–1464, 1960.
[4] Vivek Borkar and Pr. Varaiya. Adaptive control of Markov chains. I. Finite parameter set. *IEEE Transactions
    on Automatic Control*, 24(6):953–957, 1979.
[5] Vivek Borkar and Pravin Varaiya. Identification and adaptive control of Markov chains. *SIAM Journal on
    Control and Optimization*, 20(4):470–489, 1982.
[6] Woei Lin, P. R. Kumar, and T. I. Seidman. Will the self-tuning approach work for general cost criteria?
    *Systems & control letters*, 6(2):77–85, 1985.
[7] Arthur Becker, P. R. Kumar, and Ching-Zong Wei. Adaptive control with the stochastic approximation
    algorithm: Geometry and convergence. *IEEE Transactions on Automatic Control*, 30(4):330–338, 1985.
[8] P. R. Kumar and A. Becker. A new family of optimal adaptive controllers for Markov chains. *IEEE
    Transactions on Automatic Control*, 27(1):137–146, 1982.
[9] P. R. Kumar and Woei Lin. Optimal adaptive controllers for unknown Markov chains. *IEEE Transactions
    on Automatic Control*, 27(4):765–774, 1982.
[10] P. R. Kumar. Simultaneous identification and adaptive control of unknown systems over finite parameter
    sets. *IEEE Transactions on Automatic Control*, 28(1):68–76, 1983.
[11] P. R. Kumar. Optimal adaptive control of linear-quadratic-Gaussian systems. *SIAM Journal on Control
    and Optimization*, 21(2):163–178, 1983.
[12] V. S. Borkar. The Kumar-Becker-Lin scheme revisited. *Journal of Optimization Theory and Applications,
    66(2):289–309, 1990.
[13] V. S. Borkar. Self-tuning control of diffusions without the identifiability condition. *Journal of optimization
    theory and applications*, 68(1):117–138, 1991.
[14] Łukasz Stettner. On nearly self-optimizing strategies for a discrete-time uniformly ergodic adaptive model.
    *Applied Mathematics and Optimization*, 27(2):161–177, 1993.
[15] T. E. Duncan, B. Pasik-Duncan, and L. Stettner. Almost self-optimizing strategies for the adaptive control
    of diffusion processes. *Journal of optimization theory and applications*, 81(3):479–507, 1994.
[16] Marco C. Campi and P. R. Kumar. Adaptive linear quadratic Gaussian control: the cost-biased approach
    revisited. *SIAM Journal on Control and Optimization*, 36(6):1890–1907, 1998.
[17] Maria Prandini and Marco C. Campi. Adaptive LQG control of input-output systems—A cost-biased
    approach. *SIAM Journal on Control and Optimization*, 39(5):1499–1519, 2000.
[18] Tze Leung Lai and Herbert Robbins. Asymptotically efficient adaptive allocation rules. *Advances in
    applied mathematics*, 6(1):4–22, 1985.
[19] Peter Auer, Nicolo Cesa-Bianchi, and Paul Fischer. Finite-time analysis of the multiarmed bandit problem.
    *Machine learning*, 47(2-3):235–256, 2002.
[20] Jean-Yves Audibert and Sébastien Bubeck. Regret bounds and minimax policies under partial monitoring.
    *Journal of Machine Learning Research*, 11(Oct):2785–2836, 2010.
[21] Jean-Yves Audibert and Sébastien Bubeck. Minimax policies for adversarial and stochastic bandits. In COLT, pages 217–226, 2009.

[22] Rémy Degenne and Vianney Perchet. Anytime optimal algorithms in stochastic multi-armed bandits. In International Conference on Machine Learning, pages 1587–1595, 2016.

[23] Sarah Filippi, Olivier Cappe, and Aurélien Garivier. Optimism in reinforcement learning and Kullback-Leibler divergence. In 2010 48th Annual Allerton Conference on Communication, Control, and Computing (Allerton), pages 115–122, 2010.

[24] Aurélien Garivier and Olivier Cappe. The KL-UCB algorithm for bounded stochastic bandits and beyond. In Proceedings of the 24th Annual Conference On Learning Theory (COLT), pages 359–376, 2011.

[25] Emilie Kaufmann, Olivier Cappe, and Aurélien Garivier. On Bayesian upper confidence bounds for bandit problems. In Artificial intelligence and statistics (AISTATS), pages 592–600, 2012.

[26] Olivier Cappe, Aurélien Garivier, Odalric-Ambrym Maillard, Rémi Munos, Gilles Stoltz, et al. Kullback-Leibler upper confidence bounds for optimal sequential allocation. The Annals of Statistics, 41(3):1516–1541, 2013.

[27] Wei Chu, Lihong Li, Lev Reyzin, and Robert Schapire. Contextual bandits with linear payoff functions. In Proceedings of the Fourteenth International Conference on Artificial Intelligence and Statistics (AISTATS), pages 208–214, 2011.

[28] Yasin Abbasi-Yadkori, Dávid Pál, and Csaba Szepesvári. Improved algorithms for linear stochastic bandits. In Advances in Neural Information Processing Systems, pages 2312–2320, 2011.

[29] Paat Rusmevichientong and John N. Tsitsiklis. Linearly parameterized bandits. Mathematics of Operations Research, 35(2):395–411, 2010.

[30] Niranjan Srinivas, Andreas Krause, Sham M. Kakade, and Matthias W. Seeger. Information-theoretic regret bounds for Gaussian process optimization in the bandit setting. IEEE Transactions on Information Theory, 58(5):3250–3265, 2012.

[31] Thomas Jaksch, Ronald Ortner, and Peter Auer. Near-optimal regret bounds for reinforcement learning. Journal of Machine Learning Research, 11(Apr):1563–1600, 2010.

[32] Daniel Russo and Benjamin Van Roy. Learning to optimize via information-directed sampling. In Advances in Neural Information Processing Systems, pages 1583–1591, 2014.

[33] Olivier Chapelle and Lihong Li. An empirical evaluation of Thompson sampling. In Advances in neural information processing systems, pages 2249–2257, 2011.

[34] Steven L. Scott. A modern Bayesian look at the multi-armed bandit. Applied Stochastic Models in Business and Industry, 26(6):639–658, 2010.

[35] Shipra Agrawal and Navin Goyal. Analysis of Thompson sampling for the multi-armed bandit problem. In Conference on Learning Theory (COLT), pages 39–1, 2012.

[36] Nathaniel Korda, Emilie Kaufmann, and Remi Munos. Thompson sampling for 1-dimensional exponential family bandits. In Advances in Neural Information Processing Systems, pages 1448–1456, 2013.

[37] Emilie Kaufmann, Nathaniel Korda, and Rémi Munos. Thompson sampling: an asymptotically optimal finite-time analysis. In Proceedings of the 23rd international conference on Algorithmic Learning Theory, pages 199–213. Springer-Verlag, 2012.

[38] Che-Yu Liu and Lihong Li. On the prior sensitivity of Thompson sampling. In International Conference on Algorithmic Learning Theory (ALT), pages 321–336, 2016.

[39] Ilya O Ryzhov, Warren B. Powell, and Peter I. Frazier. The knowledge gradient algorithm for a general class of online learning problems. Operations Research, 60(1):180–195, 2012.

[40] Ilya O Ryzhov, Peter I Frazier, and Warren B Powell. On the robustness of a one-period look-ahead policy in multi-armed bandit problems. Procedia Computer Science, 1(1):1635–1644, 2010.

[41] Yingfei Wang, Chu Wang, and Warren Powell. The knowledge gradient for sequential decision making with stochastic binary feedbacks. In International Conference on Machine Learning (ICML), pages 1138–1147, 2016.
[42] Daniel Russo and Benjamin Van Roy. Learning to optimize via information-directed sampling. *Operations Research, 66*(1):230–252, 2017.

[43] Yasin Abbasi-Yadkori and Csaba Szepesvári. Regret bounds for the adaptive control of linear quadratic systems. In *Proceedings of the 24th Annual Conference on Learning Theory (COLT)*, pages 1–26, 2011.

[44] Morteza Ibrahimi, Adel Javanmard, and Benjamin V. Roy. Efficient reinforcement learning for high dimensional linear quadratic systems. In *Advances in Neural Information Processing Systems*, pages 2636–2644, 2012.

[45] Junya Honda and Akimichi Takemura. Optimality of Thompson sampling for Gaussian bandits depends on priors. In *Artificial Intelligence and Statistics*, pages 375–383, 2014.

[46] Bo-Cheng Wei. Exponential family nonlinear models. *Lecture Notes in Statistics*, 1998.
Appendix

A Proof of Lemma 1

Before proving the lemma, we first introduce the following useful property.

**Lemma 5** For any \( a \in (0, 1) \) and for any \( x > 0 \), we have

\[
a \log(1 + x) < \log(1 + ax).
\]

**(Proof of Lemma 5)** If \( x = 0 \), then \( a \log(1 + x) = 0 \) and \( \log(1 + ax) = 0 \). Otherwise, by taking derivatives with respect to \( x \) on both sides, we have

\[
\frac{d(a \log(1 + x))}{dx} = \frac{a}{1 + x}, \quad \text{and} \quad \frac{d\log(1 + ax)}{dx} = \frac{a}{1 + ax}.
\]

Since \( \frac{a}{1 + x} < \frac{a}{1 + ax} \) for all \( a \in (0, 1) \) and \( x > 0 \), the proof is complete. \( \square \)

Now, we are ready to prove Lemma 1. Recall that

\[
I(\nu, n, \alpha(t)) = (n\nu + \alpha(t)) \log(n\nu + \alpha(t)) + n \log n
- (n + \alpha(t)) \log(n + \alpha(t)) - n\nu \log(n\nu).
\]

By taking the partial derivative of \( I(\nu, n, \alpha(t)) \) with respect to \( n \), we have

\[
\frac{\partial I}{\partial n} = \left( \nu \log(n\nu + \alpha(t)) + (n\nu + \alpha(t)) \frac{\nu}{n\nu + \alpha(t)} \right) + (\log n + 1)
- (n + \alpha(t)) \log(n + \alpha(t)) - n\nu \log(n\nu).
\]

For all \( n \geq 1 \) and \( \alpha(t) > 0 \). Moreover, we can observe that \( I(\nu, n, \alpha(t)) \) is right-continuous at \( \nu = 0 \) and the function value at \( \nu = 0 \) is

\[
I(0, n, \alpha(t)) = \alpha(t) \log \alpha(t) + n \log n - (n + \alpha(t)) \log(n + \alpha(t)).
\]

Therefore, we can conclude that \( I(\nu, n, \alpha(t)) \) is strictly increasing with \( \nu \), for all \( \nu \geq 0 \). \( \square \)

B Proof of Lemma 2

We start by considering the case where \( \nu > 0 \). Recall that

\[
I(\nu, n, \alpha(t)) = (n\nu + \alpha(t)) \log(n\nu + \alpha(t)) + n \log n
- (n + \alpha(t)) \log(n + \alpha(t)) - n\nu \log(n\nu).
\]

By taking the partial derivative of \( I(\nu, n, \alpha(t)) \) with respect to \( \nu \), we have

\[
\frac{\partial I}{\partial \nu} = (n \log(n\nu + \alpha(t)) + n) + 0 - 0 - (n \log(n\nu) + n)
= n \log \frac{n\nu + \alpha(t)}{n\nu} > 0,
\]

for all \( n \geq 1 \) and \( \alpha(t) > 0 \). Moreover, we can observe that \( I(\nu, n, \alpha(t)) \) is right-continuous at \( \nu = 0 \) and the function value at \( \nu = 0 \) is

\[
I(0, n, \alpha(t)) = \alpha(t) \log \alpha(t) + n \log n - (n + \alpha(t)) \log(n + \alpha(t)).
\]

Therefore, we can conclude that \( I(\nu, n, \alpha(t)) \) is strictly increasing with \( \nu \), for all \( \nu \geq 0 \). \( \square \)
C Proof of Lemma 3

For simplicity of notation, let \( K = \frac{2}{\mu_1 - \mu_2} \). Then, we evaluate \( I(\mu_2, n_2, \alpha(t)) \) at \( n_2 = K_2 \alpha(t) \) as
\[
I(\mu_2, K_2 \alpha(t), \alpha(t)) = (\mu_2 K_2 \alpha(t) + \alpha(t)) \log (\mu_2 K_2 \alpha(t) + \alpha(t)) + K_2 \alpha(t) \log (K_2 \alpha(t))
\]
\[
= (K_2 \alpha(t) + \alpha(t)) \log (K_2 \alpha(t) + \alpha(t)) - \mu_2 K_2 \alpha(t) \log (\mu_2 K_2 \alpha(t))
\]
\[
= \alpha(t) \log (\alpha(t)) \left( \frac{\mu_2 K_2 + 1}{K_2} - (K_2 + 1) - \mu_2 K_2 \right)
\]
\[
+ \alpha(t) \left( (\mu_2 K_2 + 1) \log (\mu_2 K_2 + 1) + K_2 \log K_2 \right)
\]
\[
- (K_2 + 1) \log (K_2 + 1) - \mu_2 K_2 \log (\mu_2 K_2)
\]
\[
= \alpha(t) \left[ \left( (\mu_2 K_2 + 1) \log (\mu_2 K_2 + 1) - \mu_2 K_2 \log (\mu_2 K_2) \right) \right]
\]
\[
- ((K_2 + 1) \log (K_2 + 1) - K_2 \log K_2)
\]
\[
\geq \alpha(t) \left( 1 \cdot f'(\mu_2 K_2 + 1) - 1 \cdot f'(K_2) \right) = \alpha(t) \log \left( \frac{\mu_2 K_2 + 1}{K_2} \right).
\]

(35)

Similarly, we have
\[
I(\mu_1, K_1 \alpha(t), \alpha(t)) = \alpha(t) \log (\alpha(t)) \left( \frac{\mu_1 K_1 + 1}{K_1 + 1} \right)
\]
\[
+ \alpha(t) \left( (\mu_1 K_1 + 1) \log (\mu_1 K_1 + 1) + K_1 \log K_1 \right)
\]
\[
- (K_1 + 1) \log (K_1 + 1) - \mu_1 K_1 \log (\mu_1 K_1)
\]
\[
\geq \alpha(t) \left( 1 \cdot f'(\mu_1 K_1) - 1 \cdot f'(K_1 + 1) \right) = \alpha(t) \log \left( \frac{\mu_1 K_1}{K_1 + 1} \right).
\]

(39)

Note that \( \frac{\mu_1 K_1}{K_1 + 1} \) increases with \( K_1 \). Therefore,
\[
I(\mu_1, K_1 \alpha(t), \alpha(t)) \geq \alpha(t) \log \left( \frac{\mu_1 K_1}{K_1 + 1} \right), \forall K_1 \geq K.
\]

(40)

When \( K_1 = K \),
\[
\frac{\mu_1 K_1}{K_1 + 1} = \frac{\mu_1 \frac{2}{\mu_1 - \mu_2}}{\frac{2}{\mu_1 - \mu_2} + 1} = \frac{2 \mu_1}{2 + (\mu_1 - \mu_2)}
\]

When \( K_2 = K \),
\[
\frac{\mu_2 K_2 + 1}{K} = \frac{\mu_2 \frac{2}{\mu_1 - \mu_2} + 1}{\frac{2}{\mu_1 - \mu_2}} = \frac{\mu_1 + \mu_2}{2}
\]

Therefore, we have
\[
\frac{\mu_1 K_1}{K_1 + 1} - \frac{\mu_2 K_2 + 1}{K} = \frac{4 \mu_1 + 2(\mu_1 + \mu_2) + \mu_1^2 - \mu_2^2}{2(2 + (\mu_1 - \mu_2))} > 0.
\]

(41)

For any \( K_1 \geq K \) and \( K_2 \geq K \),
\[
I(\mu_1, K_1 \alpha(t), \alpha(t)) \geq \alpha(t) \log \frac{\mu_1 K_1}{K_1 + 1}
\]
\[
\geq \alpha(t) \log \frac{\mu_1 K}{K + 1}
\]
\[
\geq \alpha(t) \log \frac{\mu_2 K + 1}{K}
\]
\[
\geq I(\mu_2, K \alpha(t), \alpha(t))
\]
\[
\geq I(\mu_2, K_2 \alpha(t), \alpha(t))
\]
D Proof of Lemma

Similar to the proof of Lemma 3 we have

\[ I(\mu_2, K_2, \alpha(t), \alpha(t)) = \alpha(t) \log \frac{\mu_2 K_2 + 1}{K_2}. \tag{42} \]

Moreover, we know \( \frac{\mu_2 K_2 + 1}{K_2} \leq \frac{\mu_2}{1 - \frac{\mu_2}{K_2}} = \frac{\mu_2 + 1}{\mu_2}. \) Next, we evaluate \( I(\mu_1, n_1, \alpha(t)) \) at \( \mu_1 = 0 \) and \( n_1 = K_1 \alpha(t) \) as

\[ I(0, K_1 \alpha(t), \alpha(t)) = \alpha(t) \log(\alpha(t)) + (K_1 \alpha(t) - (K_1 + 1)) \log(K_1 + 1) \]

where the last inequality holds due to the fact that \( 1 - \frac{1}{x} \leq \log x \leq x - 1 \) for all \( x > 0. \) Recall that \( M^*(\mu_1, \mu_2) = \sup \{ K_1 : K_1 \log K_1 - (K_1 + 1) \geq \log \left( \frac{\mu_2 + 1}{\mu_2} \right) \}. \) We can observe that \( M^* > 0, \) since \( K_1 \log K_1 - (K_1 + 1) = 0 \) at \( K_1 = 0, \) and \( K_1 \log K_1 - (K_1 + 1) \) is decreasing with \( K_1. \) Therefore, \( I(0, n_1, \alpha(t)) > I(\mu_2, n_2, \alpha(t)), \) for all \( n_1 \leq M^*(\mu_1, \mu_2) \cdot \alpha(t) \) and \( n_2 \geq \frac{2}{\log(\mu_1 - \mu_2)} \).

E Proof of Proposition

Recall that

\[ \pi_t^{\text{BMLE}} = \arg\max_{i \in \{1, \cdots, N\}} \left\{ \max_{\mu \in [0, 1]^N} \left\{ \frac{S_i(t) + \alpha(t)}{N_i(t)} \cdot \prod_{j \neq i} \mu_j^{S_j(t)} (1 - \mu_j)^{N_j(t) - S_j(t)} \right\} \right\}. \tag{47} \]

By taking partial derivative with respect to \( \mu, \) the maximizer of the term \((*)\) in (47) is \( \mu_i = \frac{S_i(t) + \alpha(t)}{N_i(t)} \) and \( \mu_j = \frac{S_j(t)}{N_j(t)} \) for all \( j \neq i. \) Recall that for each \( i \in \{1, \cdots, N\}, \)

\[ p_i(t) := \frac{S_i(t)}{N_i(t)}, \quad \tilde{p}_i(t) := \frac{S_i(t) + \alpha(t)}{N_i(t) + \alpha(t)}. \]

We also define

\[ Z_i := \tilde{p}_i(t)^{S_i(t) + \alpha(t)} \cdot (1 - \tilde{p}_i(t))^{N_i(t) - S_i(t)} \cdot \prod_{j \neq i} p_j(t)^{S_j(t)} (1 - p_j(t))^{N_j(t) - S_j(t)}. \tag{48} \]

Note that \( Z_i(t) \) is always non-negative. For any pair \( j, k \in \{1, \cdots, N\}, \) it is easy to verify by cancelling common terms that \( Z_j(t) \geq Z_k(t) \) if and only if

\[ \frac{\tilde{p}_j(t)^{S_j(t) + \alpha(t)} \cdot (1 - \tilde{p}_j(t))^{N_j(t) - S_j(t)}}{p_j(t)^{S_j(t)} (1 - p_j(t))^{N_j(t) - S_j(t)}} \geq \frac{\tilde{p}_k(t)^{S_k(t) + \alpha(t)} \cdot (1 - \tilde{p}_k(t))^{N_k(t) - S_k(t)}}{p_k(t)^{S_k(t)} (1 - p_k(t))^{N_k(t) - S_k(t)}}. \tag{49} \]

Recall that

\[ I(\mu, n, \alpha(t)) := (n \mu + \alpha(t)) \log(n \mu + \alpha(t)) + n \log n - (n + \alpha(t)) \log(n + \alpha(t)) - n \mu \log(n \mu). \tag{50} \]

By taking logarithms on both sides of (49), we know that \( Z_j(t) \geq Z_k(t) \) if and only if \( I(p_j(t), N_j(t), \alpha(t)) \geq I(p_k(t), N_k(t), \alpha(t)). \) Therefore, we can conclude that \( \pi_t^{\text{BMLE}} = \arg\max_{i \in \{1, \cdots, N\}} I(p_i(t), N_i(t), \alpha(t)). \)
F Derivation of the Alternative BMLE Index in (11)

Recall that we define

\[ Z_i := \tilde{p}_i(t)^{S_i(t) + \alpha(t)} (1 - \tilde{p}_i(t))^{N_i(t) - S_i(t)} \cdot \prod_{j \neq i} p_j(t)^{S_j(t)(1 - p_j(t))^{N_j(t) - S_j(t)}}, \]  

where \( p_i(t) := \frac{S_i(t)}{N_i(t)} \) and \( \tilde{p}_i(t) := \frac{S_i(t) + \alpha(t)}{N_i(t) + \alpha(t)} \), for each arm \( i \). Then, for any pair of arms \( j \) and \( k \), we can calculate the following

\[ \log \frac{Z_k(t)}{Z_j(t)} = N_k(t) \left( p_k(t) \log \frac{\tilde{p}_k(t)}{p_k(t)} + (1 - p_k(t)) \log \frac{1 - \tilde{p}_k(t)}{1 - p_k(t)} \right) \]

\[ - \frac{N_j(t)}{N_k(t)} \left( p_j(t) \log \frac{\tilde{p}_j(t)}{p_j(t)} + (1 - p_j(t)) \log \frac{1 - \tilde{p}_j(t)}{1 - p_j(t)} \right) \]

\[ + \alpha(t) \log \frac{\tilde{p}_k(t)}{p_j(t)}. \]  

Given the definition that \( \tilde{I}(p_i(t), N_i(t), \alpha(t)) := \alpha(t) \log \tilde{p}_i(t) - N_i(t) \text{KL}(p_i(t)||\tilde{p}_i(t)) \), it is easy to verify that \( Z_k(t) \geq Z_j(t) \) if and only if \( \tilde{I}(p_k(t), N_k(t), \alpha(t)) \geq \tilde{I}(p_j(t), N_j(t), \alpha(t)) \). □

G Proof of Proposition[2]

Recall that the Gaussian distribution with mean \( \theta_i \) and variance \( \sigma^2 \) can be represented in the canonical exponential form with \( \eta_i = \theta_i / \sigma^2 \), \( b(\eta_i) = \sigma^2 \eta_i^2 / 2 \), \( c(x) = (x^2 / 2\sigma^2) + \log \sqrt{2\pi \sigma^2} \). Moreover, we already know that in the Gaussian case,

\[ \pi^\text{BMLE}_i = \arg \max_{\eta \in \mathbb{R}_N} \left\{ \max_{\eta \in \mathbb{R}_N} \left\{ L(\mathcal{H}_i; \eta) \cdot \exp \left( \eta_i \cdot \alpha(t) \right) \right\} \right\}. \]  

(56)

Note that if there is no bias (i.e., \( \alpha(t) = 0 \)) in the inner maximization problem of (56), the corresponding optimizer is the standard maximum likelihood estimator that can be obtained as \( \eta^\text{MLE}_i = b^{-1}(S_i(t)/N_i(t)) \), where \( b^{-1}(\cdot) \) denotes the inverse function of the first derivative of \( b(\cdot) \) (e.g. see [46]). This also implies that the maximum likelihood estimator for \( \theta_i \) is \( \hat{\theta}^\text{MLE} = S_i(t)/N_i(t) \), for all \( i \). Similarly, in the biased case, it is easy to verify that the optimizer of \( \max_{\eta \in \mathbb{R}_N} \left\{ L(\mathcal{H}_i; \eta) \cdot \exp \left( \eta_i \cdot \alpha(t) \right) \right\} \) is \( \eta^\text{BMLE}_i = b^{-1}(\alpha(t)/N_i(t)) \) and \( \hat{\theta}^\text{BMLE}_i = (S_i(t) + \alpha(t))/N_i(t) \), for all \( j \neq i \). This directly implies that \( \hat{\theta}^\text{BMLE}_j = (S_j(t) + \alpha(t))/N_j(t) \) and \( \hat{\theta}^\text{BMLE}_j = (S_j(t) + \alpha(t))/N_j(t) \), for all \( j \neq i \). For ease of notation, define \( L^*_i := \max_{\eta \in \mathbb{R}_N} \left\{ L(\mathcal{H}_i; \eta) \cdot \exp \left( \eta_i \cdot \alpha(t) \right) \right\} \). By applying \( \hat{\theta}^\text{BMLE}_i \) and \( \hat{\theta}^\text{BMLE}_j \) to \( L^*_i \) and eliminate the common terms, we have

\[ \pi^\text{BMLE}_i = \arg \max_{\eta \in \mathbb{R}_N} \left\{ \exp \left( \frac{S_i(t) + \alpha(t)}{N_i(t)} \cdot \alpha(t) \right) \cdot \prod_{i \neq j, i, s \leq t} \exp \left( \frac{S_i(t) + \alpha(t)}{N_i(t)} \cdot X_s - b \left( \frac{S_i(t) + \alpha(t)}{N_i(t)} \cdot c(X_s) \right) \right) \right\} \]

(57)

\[ = \arg \max_{\eta \in \mathbb{R}_N} \left\{ \left( \frac{S_i(t) + \alpha(t)}{N_i(t)} \cdot \alpha(t) \right) + \frac{1}{2} \sum_{i \neq j, i, s \leq t} \left[ \left( X_s - \frac{S_i(t)}{N_i(t)} \right)^2 - \left( X_s - \frac{S_i(t) + \alpha(t)}{N_i(t)} \right)^2 \right] \right\} \]

(58)

\[ = \arg \max_{\eta \in \mathbb{R}_N} \left\{ \frac{S_i(t)}{N_i(t)} + \frac{\alpha(t)}{2N_i(t)} \right\}. \]  

(59)

(60)

It is easy to check that the equality of (59)-(60) indeed hold by applying logarithmic operation. □
To begin with, for each arm \(i\), we define \(p_{i,n}\) to be the total reward collected in the first \(n\) pulls of arm \(i\). Next, for each arm \(i\), we define two types of events,

\[
G^+_i(n, t) = \left\{ p_{i,n} - \theta_i \leq \sqrt{\frac{3 \log t}{2n}} \right\},
\]

\[
G^-_i(n, t) = \left\{ \theta_i - p_{i,n} \leq \sqrt{\frac{3 \log t}{2n}} \right\}.
\]

Note that by the Hoeffding inequality, we have

\[
\mathbb{P}(G^+_i(n, t) \notin \mathbb{R}) \leq e^{-2n \frac{3 \log t}{2n}} = \frac{1}{t^3},
\]

\[
\mathbb{P}(G^-_i(n, t) \notin \mathbb{R}) \leq e^{-2n \frac{3 \log t}{2n}} = \frac{1}{t^3}.
\]

Consider the bias term \(\alpha(t) = \gamma(t) \log t\), where \(\gamma(t)\) is a real positive function that satisfies \(\lim_{t \to \infty} \gamma(t) = \infty\). Our target is to quantify the total number of trials of each sub-optimal arm. Recall that we assume arm 1 is the unique optimal arm. Without loss of generality, we can focus on characterizing \(\mathbb{E}[N_2(T)]\):

\[
\mathbb{E}[N_2(T)] \leq Q(T) + \mathbb{E} \left[ \sum_{t=Q(T)+1}^T \mathbb{I}(I(p_2(t), N_2(t), \alpha(t)) \geq I(p_1(t), N_1(t), \alpha(t), N_2(t) \geq Q(T)) \right]
\]

\[
= Q(T) + \sum_{t=Q(T)+1}^T \mathbb{P} \left( I(p_2(t), N_2(t), \alpha(t)) \geq I(p_1(t), N_1(t), \alpha(t), N_2(t) \geq Q(T) \right)
\]

\[
\leq Q(T) + \sum_{t=Q(T)+1}^T \sum_{n_1=1}^t \sum_{n_2=Q(T)} \mathbb{P} \left( I(p_{2,n_2}, n_2, \alpha(t)) \geq \min_{1 \leq n_1 \leq t} I(p_{1,n_1}, n_1, \alpha(t)) \right)
\]

\[
\leq Q(T) + \sum_{t=Q(T)+1}^T \sum_{n_1=1}^t \sum_{n_2=Q(T)} \left( \mathbb{P}(G_1^-(n_1, t) \notin \mathbb{R}) + \mathbb{P}(G_2^+(n_2, t) \notin \mathbb{R}) \right)
\]

\[
\leq Q(T) + 2 \log T + \sum_{t=Q(T)+1}^T \sum_{n_1=1}^t \sum_{n_2=Q(T)} \mathbb{P} \left( I(p_{2,n_2}, n_2, \alpha(t)) \geq I(p_{1,n_1}, n_1, \alpha(t)), G_1^-(n_1, t), G_2^+(n_2, t) \right)
\]

where the last equation follows from the fact that \(\sum_{t=Q(T)+1}^T \left( \frac{1}{t} \right) \leq \log T\). We choose \(Q(T) = \frac{32}{\gamma(T)} \alpha(T) = \frac{32}{8} \gamma(T) \log T\). Next, we need to discuss the following four cases separately.

**Case 1:** \(n_1 \geq \frac{\gamma}{8} \log t, n_1 \geq \frac{8}{\Delta} \alpha(t), n_2 \geq Q(T) = \frac{32}{8} \alpha(t) \geq \frac{8}{\Delta} \alpha(t)\)
Since $n_1 \geq \frac{32}{3\Delta^2} \log t$, we have $p_{1,n_1} \geq \theta_1 - \frac{3}{8} \Delta$ on the event $G_1^-(n_1,t)$. Similarly, as $n_2 \geq \frac{32}{3\Delta^2} \log t$, we have $p_{2,n_2} \leq \theta_2 + \frac{3}{8} \Delta$ on the event $G_2^+(n_2,t)$. Therefore, we know

$$p_{1,n_1} - p_{2,n_2} \geq \frac{\Delta}{4}. \quad (74)$$

By Lemma 3 we know $I(p_{1,n_1}, n_1, \alpha(t)) > I(p_{2,n_2}, n_2, \alpha(t))$, for any $n_1 \geq \frac{8}{3\Delta} \alpha(t)$, $n_2 \geq \frac{8}{3\Delta} \alpha(t)$. Hence, in Case 1, we always have $I(p_{1,n_1}, n_1, \alpha(t)) > I(p_{2,n_2}, n_2, \alpha(t))$.

- **Case 2**: $n_1 \geq \frac{32}{3\Delta^2} \log t$, $n_1 < \frac{8}{3\Delta} \alpha(t)$, $n_2 \geq Q(T) = \frac{32}{3\Delta^2} \alpha(t) \geq \frac{8}{3\Delta} \alpha(t)$.

Similar to Case 1, since both $n_1, n_2 \geq \frac{32}{3\Delta^2} \log t$, we have $p_{1,n_1} \geq \theta_1 - \frac{3}{8} \Delta$ on the event $G_1^-(n_1,t)$.

Similarly, as $n_2 \geq \frac{32}{3\Delta^2} \alpha(t) \geq \frac{32}{3\Delta^2} \log t$, we have $p_{2,n_2} \leq \theta_2 + \frac{3}{8} \Delta$ on the event $G_2^+(n_2,t)$. Therefore, we know $p_{1,n_1} - p_{2,n_2} \geq \frac{\Delta}{4}$. Hence we have:

$$I(p_{1,n_1}, n_1, \alpha(t)) \geq I(\theta_1 - \frac{3\Delta}{8}, n_1, \alpha(t)) \quad (75)$$

$$> I(\theta_1 - \frac{3\Delta}{8}, \frac{8}{3\Delta} \alpha(t), \alpha(t)) \quad (76)$$

$$> I(\theta_2 + \frac{3\Delta}{8}, n_2, \alpha(t)) \quad (77)$$

$$> I(p_{2,n_2}, n_2, \alpha(t)), \quad (78)$$

where (75) follows from Lemma 2, (76) follows from Lemma 1, (77) follows from Lemma 3, and (78) holds due to Lemma 2.

- **Case 3**: $n_1 < \frac{32}{3\Delta^2} \log t$, $n_1 < \frac{8}{3\Delta} \alpha(t)$, $n_2 \geq Q(T) = \frac{32}{3\Delta^2} \alpha(t) \geq \frac{8}{3\Delta} \alpha(t)$.

Recall that $\alpha(t) = \gamma(t) \log t$. Under the condition that $n_2 \geq Q(T) = \frac{32}{3\Delta^2} \alpha(t)$, we know that $t \geq Q(T)$ and hence

$$\alpha(t) \geq \gamma(Q(T)) \log t = \gamma\left(\frac{32}{3\Delta^2} \alpha(t)\right) \log t. \quad (79)$$

Recall that

$$M^*(\mu_1, \mu_2) = \sup \left\{ K_1 : K_1 \log K_1 - K_1(K_1 + 1) \geq \log\left(\frac{\mu_1 + \mu_2}{2}\right) \right\}. \quad (80)$$

Since $(K_1 \log K_1 - K_1(K_1 + 1))$ is decreasing for all $K_1 > 0$, $M^*(\mu_1, \mu_2)$ is decreasing with $\mu_1$ and $\mu_2$. Next, we substitute $p_{1,n_1}, p_{2,n_2}$ into Lemma 4. Note that there must exist a constant $T_0 > 0$ such that for any $T \geq T_0$, we have

$$\frac{32}{3\Delta^2} \leq M^*(1, \theta_1 - \frac{5}{8} \Delta) \gamma\left(\frac{32}{3\Delta^2} \alpha(t)\right), \quad (81)$$

under the condition that $\gamma(t)$ satisfies either $\lim_{t \to \infty} \gamma(t) = \infty$ or $\gamma(t) \geq \frac{32}{3\Delta^2 M^*(1, \theta_1 - \frac{5}{8} \Delta)}$, for all $T \geq T_0$. This implies that for any $T \geq T_0$, we have

$$n_1 < M^*(p_{1,n_1}, p_{2,n_2}) \alpha(t), \quad (82)$$

since $M^*(p_{1,n_1}, p_{2,n_2}) \geq M^*(1, \theta_1 - \frac{5}{8} \Delta)$ on the “good” event $G_2^+(n_2,t)$. Therefore, we further know that

$$I(p_{1,n_1}, n_1, \alpha(t)) > I(0, n_1, \alpha(t)) \quad (83)$$

$$> I(p_{2,n_2}, n_2, \alpha(t)), \quad (84)$$

where (83) follows from Lemma 2 and (84) holds due to Lemma 4.

- **Case 4**: $n_1 < \frac{32}{3\Delta^2} \log t$, $n_1 \geq \frac{8}{3\Delta} \alpha(t)$, $n_2 \geq Q(T) = \frac{32}{3\Delta^2} \alpha(t) \geq \frac{8}{3\Delta} \alpha(t)$.

Recall that $\alpha(t) = \gamma(t) \log t$. Similar to Case 3, under the condition that $n_2 \geq Q(T) = \frac{32}{3\Delta^2} \alpha(t)$, we know $t \geq Q(T)$ and

$$\alpha(t) \geq \gamma(L) \log t = \gamma\left(\frac{32}{3\Delta^2} \alpha(t)\right) \log t. \quad (85)$$
Then, there must exist a constant $T_1 > 0$ such that for any $T \geq T_1$, we have
\[ \frac{32}{\Delta^2} < \frac{8}{\Delta^2} \gamma \left( \frac{32}{\Delta^2} \alpha(t) \right), \] (86)
under the condition that $\gamma(t)$ satisfies either $\lim_{t \to \infty} \gamma(t) = \infty$ or $\gamma(t) \geq \frac{4}{5\Delta}$, for all $T \geq T_1$.
Therefore, the two events \( \{ n_1 < \frac{8}{\Delta^2} \log t \} \) and \( \{ n_1 \geq \frac{8}{\Delta^2} \alpha(t) \} \) cannot happen at the same time.

To sum up, in all the above four cases, we have
\[ \mathbb{P} \left( I(p_{2,n_2}, n_2, \alpha(t)) \geq I(p_{1,n_1}, n_1, \alpha(t)), G_1^-(n_1, t), G_2^+(n_2, t) \right) = 0, \] (87)
for any $T \geq \max\{T_0, T_1\}$. Based on the discussions in Case 3 and Case 4, we can choose a $\gamma(t)$ that satisfies either $\lim_{t \to \infty} \gamma(t) = \infty$ or $\gamma(t) = \max\{ \frac{4}{5\Delta}, \frac{32}{\Delta^2} \gamma(t), \frac{32}{5\Delta^2} \}$.
Now, we are ready to put all the pieces together.

\[
E[N_2(T)] \leq Q(T) + 2 \log T
+ \sum_{t=Q(T)+1}^{T} \sum_{n_1=1}^{t} \sum_{n_2=Q(T)}^{t} \mathbb{P} \left( I(p_{2,n_2}, n_2, \alpha(t)) \geq I(p_{1,n_1}, n_1, \alpha(t)), G_1^-(n_1, t), G_2^+(n_2, t) \right),
\] (88)
\[
\leq Q(T) + 2 \log T + \max\{T_0, T_1\}
= \frac{32}{3\Delta^2} \alpha(t) + 2 \log T + \max\{T_0, T_1\}
= \frac{32}{3\Delta^2} \gamma(T) \log T + 2 \log T + \max\{T_0, T_1\}. \] (90)

For any sub-optimal arm $i$ other than arm 2, the above results still hold by replacing $\Delta$ with $\Delta_i$. Note that by (81) and (86), we know that both $T_0$ and $T_1$ depend on parameter $\theta$ and the choice of $\gamma(t)$, but they are independent of $T$. For ease of notation, we use $C_\gamma(\theta)$ to denote $\max\{T_0, T_1\}$.

Finally, we derive regret bounds for two different types of $\gamma(t)$. Under a bias term $\gamma(t)$ with $\lim_{t \to \infty} \gamma(t) = \infty$, the total regret is upper bounded as
\[
\text{Regret}(T) \leq \sum_{i=2}^{N} \Delta_i \cdot E[N_i(T)]
= \sum_{i=2}^{N} \left( \frac{32}{3\Delta_i} \gamma(T) \log T + \Delta_i(2 \log T + \max\{T_0, T_1\}) \right)
= O \left( \frac{\gamma(T) \log T}{\Delta} \right). \] (94)

On the other hand, if a lower bound $\Delta$ for the minimum gap $\Delta$ is known, we can choose the bias term $\gamma(t) = \max\{ \frac{4}{5\Delta}, \frac{32}{\Delta^2} \gamma(t), \frac{32}{5\Delta^2} \}$ for the BMLE algorithm, and the corresponding pseudo regret is $O(\log T)$.

\[ \square \]

\section{Sample Path Bounds on Regret}

The Biased Maximum Likelihood Estimator (4) also provides high confidence sample path guarantees on regret for each choice of bias term $\alpha(\cdot)$. The sample path bounds can be tuned through the choice of $\alpha(\cdot)$. We illustrate the proof for the case where there are two Bernoulli arms.

\textbf{Proposition 5} Consider a two-armed Bernoulli bandit with $\theta_1 > \theta_2$. For any $\delta > 0$, and $c > 1$, there is a (non-random) constant $K = K(\theta_1, \theta_2, \alpha(\cdot), \delta, c)$, such that
\[ \mathbb{P} \left( \text{Regret}(t) \leq c\alpha(t) + K \text{ for all } t \right) \geq 1 - \delta. \]
Proof. First, simple algebra shows that the index of an arm can be redefined as
\[
\bar{I}_j(t) \equiv \bar{I}(S_j(t), N_j(t), \alpha(t)) = (S_j(t) + N_j(t) + \alpha(t)) \left[ H\left( \frac{S_j(t)}{S_j(t) + N_j(t) + \alpha(t)} \right) - H\left( \frac{S_j(t) + \alpha(t)}{S_j(t) + N_j(t) + \alpha(t)} \right) \right],
\]
where \( H(p) = -p \log p - (1-p) \log (1-p) \) denotes the entropy of a binary random variable (with logarithms to base \( e \)). Under the BMLE algorithm, the selected arm at each time \( t \) is
\[
\pi^\text{MLE}_t = \arg\max_{i \in \{1, \ldots, N\}} \bar{I}(S_i(t), N_i(t), \alpha(t)).
\]
With \( \beta > 1 \), and \( 0 < c' < \frac{\bar{\delta}(\beta-1)}{4}\beta \), let \( \varepsilon(n) := \sqrt{\frac{2 \log n - \log \varepsilon}{2n}}. \) As in the proof of Propositions 3 and 4, let \( \bar{p}_{i,n} \) denote the (random) total number of successes of arm \( i \) in \( n \) pulls. Define the “good” event,
\[
G := \{ |\bar{p}_{i,n} - \theta_i| \leq \varepsilon(n) \text{ for } i = 1, 2, \text{ and for all } n \}.
\]
By Hoeffding’s inequality,
\[
\mathbb{P}(G^C) \leq \sum_{n=1}^{\infty} \frac{4c'}{n^{\beta / 2}} < \delta.
\]
Note that by concavity of entropy, \( H(p + a) \leq H(p) + a H'(p) \), and so
\[
\bar{I}_2(t) - \bar{I}_1(t) \leq \alpha(t) \left[ \log \left( \frac{N_1(t) + \alpha(t)}{S_1(t)} \right) - \log \left( \frac{N_2(t) + \alpha(t)}{S_2(t) + \alpha(t)} \right) \right].
\]
Hence \( \pi^\text{MLE}_t = 1 \), i.e., arm 1 is pulled, whenever \( \frac{N_1(t) + \alpha(t)}{S_1(t)} \leq \frac{N_2(t) + \alpha(t)}{S_2(t) + \alpha(t)}. \)
Define \( \bar{\varepsilon}(n) := n \varepsilon(n) \). Then, on \( G \), for all \( t \), we have
\[
S_1(t) \geq \theta_1 N_1(t) - \bar{\varepsilon}(N_1(t)), \quad S_2(t) \leq \theta_2 N_2(t) + \bar{\varepsilon}(N_2(t)).
\]
Hence, on \( G \), using \( N_1(t) = t - N_2(t) \) yields
\[
S_1(t)N_2(t) - S_2(t)N_1(t) - S_2(t)\alpha(t) - N_1(t)\alpha(t) - \alpha^2(t) \geq t \left[ (\theta_1 - \theta_2) N_2(t) - \bar{\varepsilon}(N_2(t)) - \alpha(t) \right] - \bar{\varepsilon}(N_1(t)) N_2(t) + \alpha(t) \left[ -\theta_2 N_2(t) - \bar{\varepsilon}(N_2(t)) + N_2(t) - \alpha(t) \right] + N_2(t) \left[ -\theta_1 N_2(t) + \theta_2 N_2(t) + \bar{\varepsilon}(N_2(t)) \right], \text{ for all } t.
\]
Let \( c'' > \frac{1}{\theta_1 - \theta_2} \). We now show that \( c'' \alpha(t) \) is an upper barrier that \( N_2(t) \) cannot cross from below at any time \( t \) on \( G \). To see this, one first notes that if \( N_2(t) = c'' \alpha(t) \), and \( N_1(t) = t - c'' \alpha(t) \), then
\[
S_1(t)N_2(t) - S_2(t)N_1(t) - S_2(t)\alpha(t) - N_1(t)\alpha(t) - \alpha^2(t) \geq t \alpha(t) [c''(\theta_1 - \theta_2) - 1 + o(1)].
\]
Since \( c''(\theta_1 - \theta_2) > 1 \), there exists a constant \( K_1 \) for which
\[
S_1(t)N_2(t) - S_2(t)N_1(t) - S_2(t)\alpha(t) - N_1(t)\alpha(t) - \alpha^2(t) > 0, \text{ for all } t \geq K_1.
\]
Further, we can show by differentiation that,
\[
\frac{d}{dN_2(t)} \left( \text{RHS of } (98) \right) \geq t (\theta_1 - \theta_2 + o(1)).
\]

---

\(^6\)This explicit expression for the index is interesting in its own right. It is not the entropy \( H \left( \frac{S_j(t)}{N_j(t)} \right) \) of an arm that is involved in the terms here, since the denominator is \( S_j(t) + N_j(t) \) rather than \( N_j(t) \). What is instead involved is the consideration of the numbers of successes \textit{as well} as the total numbers of pulls, and the decision on which arm to pull depends on the difference in that entropy.
Hence, there exists a constant $K_2$ such that for all $t \geq K_2$,

$$\frac{d}{dN_2(t)} \left( \text{RHS of } (98) \right) > 0.$$  

So the inequality (99) also holds if $N_2(t)$ is increased above $c'\alpha(t)$ for $t \geq \max\{K_1, K_2\}$. Therefore the inequality (99) holds for $N_2(t) = c\alpha(t) + K$, for all $K \geq 0$, for all $t \geq \max\{K_1, K_2\}$.

Hence, $\pi_t^{\text{BMLE}} = 1$, and consequently $N_2(t + 1) = N_2(t)$ whenever $N_2(t)$ hits $c'\alpha(t) + K$ at any time $t \geq \max\{K_1, K_2\}$, on $G$. In fact, the same inequalities also hold in an open interval around $c'$. Hence, $N_2(t)$ cannot increase beyond $c'\alpha(t) + K$ from below, at any time $t \geq \max\{K_1, K_2\}$, on $G$.

Now we choose $K := \max\{K_1, K_2\}$. Clearly, $N_2(t)$ cannot exceed $c\alpha(t) + K$ for $1 \leq t \leq K$. Therefore, we see that $c'\alpha(t) + K$ is an upper barrier for $N_2(t)$ for all $t$ on $G$. The result for regret follows by multiplying by $(\theta_1 - \theta_2)$.

**Remark 8** It should be noted that such high confidence sample path bounds can also be obtained for fixed sampling schemes, which alternately choose arms 1 and 2 along a fixed sequence of times $t_1, t_2, t_3, \cdots$, and choose the empirically best arm at all other times $t \neq t_j$ for any $j$. However, such non-adaptive schemes yield poor performance.

### J Additional Empirical Results

#### J.1 Study of Computation Times for Policies

In this subsection, we present the computation times required to compute decisions in BMLE and other baseline policies. The computation times are measured on a Linux server with (i) an Intel Xeon E5-2697A v4 processor\(^3\) operating at a base clock rate 2.60 GHz and (ii) a total of 450 GB memory. Throughout this section, we measure the average computation time per pull for each policy over 20 simulation trials and a time horizon of 1000 for each trial.

Figure 3 shows the joint performance of both metrics of interest: Computation time per decision as well as Regret. BMLE is seen to provide best performance, with orders of magnitude less computation time per decision. Especially compared with V-IDS and IDS, BMLE achieves similar or slightly better regret performance with much smaller time per decision. For Bernoulli bandits and Gaussian bandits, Figure 2 and Figure 3 separately show the average computation time per decision for the cases of 10, 30, 50, and 70 arms. In each trial, the true value of parameter for each arm is drawn randomly from interval $(0, 1)$ through a uniform distribution. The computation time per decision is computed through counting the total time spent in each trial and then divide it by $20 \times 1000$. The numerical integral for IDS is calculated through 1000 equally spaced points. The rest hyperparameters of the algorithms have the same values as used in Section 5. We observe that the computation times of BMLE and other policies that enjoy a simple closed-form expression (e.g. UCB, and MOSS) are about three orders of magnitude smaller than other policies that require sampling or finding an approximated solution for some optimization problem, such as IDS and V-IDS.

#### J.2 Additional Simulation Results on Regret Performance

In this subsection, we present additional simulation results to demonstrate the efficacy of the proposed BMLE algorithm. Recall that Figure 2 plots the mean regret performance of BMLE and other baseline methods for Gaussian bandits. Tables 2 and 3 provide detailed statistics, including not just the mean but also the standard error and quantiles of the final regrets, with the row-wise smallest values highlighted in boldface.

Similar to the Bernoulli case, we observe that BMLE has the smallest value of regret at medium to high quantiles, and close to smallest value at other lower quantiles. Together with the presented statistic of standard error, they suggest that the performance variation of BMLE is smaller across different trials, and hence BMLE’s performance is more robust.

\(^3\)While there are 16 cores in the processor, we force the program to run on just one core for a fair comparison.
Figure 3: Comparison of computation time and regret for Bernoulli and Gaussian bandits: (a) \( \{ \theta_i \}_{i=1}^{10} = \{ 0.455, 0.46, 0.465, 0.47, 0.475, 0.48, 0.485, 0.49, 0.495, 0.5 \} \) and \( T = 3 \times 10^4 \). (b) \( \{ \mu_i \}_{i=1}^{10} = \{ 0.42, 0.44, 0.46, 0.48, 0.5, 0.52, 0.54, 0.56, 0.58, 0.6 \} \), \( \sigma = 0.8 \), and \( T = 3 \times 10^5 \). (We use TUCB and BUCB as the shorthand of UCB-Tuned and BayesUCB, respectively).

Table 2: Distribution statistics of final regret for Gaussian bandits over 100 trials with 5 arms: \( \{ \mu_i \}_{i=1}^{5} = \{ 0.48, 0.49, 0.5, 0.51, 0.52 \} \), \( \sigma = 0.8 \), and \( T = 3 \times 10^5 \).

| Algorithm | BMLE | UCB | TUCB | TS | BUCB | GPUCB | TGPUCB | KG* | V-IDS |
|-----------|------|-----|------|----|------|-------|--------|-----|------|
| Mean Regret | 302.6 | 1888.6 | 561.3 | 863.7 | 1294.7 | 2399.4 | 819.0 | 1348.4 | 646.8 |
| Standard Error | 72.6 | 299.4 | 262.9 | 452.3 | 381.2 | 295.3 | 427.1 | 316.6 | 1014.7 |
| Quantile .10 | 191.7 | 1454.4 | 342.7 | 377.6 | 939.1 | 2019.1 | 504.9 | 923.1 | 42.7 |
| Quantile .25 | 254.5 | 1725.7 | 435.7 | 519.7 | 1003.9 | 2191.1 | 561.0 | 1161.7 | 113.3 |
| Quantile .50 | 309.1 | 1879.7 | 582.8 | 782.8 | 2135.3 | 5526.5 | 766.6 | 1407.5 | 244.6 |
| Quantile .75 | 349.5 | 2112.8 | 573.3 | 1100.8 | 1473.9 | 2655.6 | 981.9 | 1628.3 | 421.7 |
| Quantile .90 | 340.4 | 2406.8 | 1238.0 | 1569.7 | 2185.2 | 2851.9 | 1269.4 | 1714.2 | 3021.8 |
| Quantile .95 | 343.0 | 2406.8 | 1238.0 | 1569.7 | 2185.2 | 2851.9 | 1269.4 | 1714.2 | 3021.8 |

Table 3: Distribution statistics of final regret for Gaussian bandits over 100 trials with 5 arms: \( \{ \mu_i \}_{i=1}^{5} = \{ 0.49, 0.495, 0.5, 0.505, 0.51 \} \), \( \sigma = 0.8 \), and \( T = 3 \times 10^5 \).

| Algorithm | BMLE | UCB | TUCB | TS | BUCB | GPUCB | TGPUCB | KG* | V-IDS |
|-----------|------|-----|------|----|------|-------|--------|-----|------|
| Mean Regret | 633.4 | 1751.1 | 946.6 | 1017.8 | 1254.2 | 1873.4 | 1007.8 | 1377.2 | 1235.2 |
| Standard Error | 629.1 | 291.4 | 496.4 | 479.9 | 257.2 | 219.2 | 604.8 | 329.8 | 1405.2 |
| Quantile .10 | 189.4 | 1441.8 | 440.2 | 562.1 | 1011.2 | 1621.3 | 487.7 | 1034.0 | 104.7 |
| Quantile .25 | 245.3 | 1565.3 | 590.1 | 678.3 | 1119.5 | 1737.1 | 572.2 | 1117.2 | 226.6 |
| Quantile .50 | 342.5 | 1718.1 | 829.8 | 987.2 | 1255.0 | 1841.8 | 903.0 | 1357.7 | 595.7 |
| Quantile .75 | 615.8 | 1914.0 | 1192.1 | 1114.5 | 1411.4 | 2040.0 | 1124.7 | 1530.0 | 1779.9 |
| Quantile .90 | 1706.6 | 2121.4 | 1652.9 | 1561.4 | 1541.5 | 2134.0 | 1749.7 | 1781.1 | 2856.3 |
| Quantile .95 | 1852.0 | 2230.5 | 1938.0 | 1852.0 | 1679.2 | 2155.1 | 2105.4 | 1911.0 | 3139.1 |
Figure 4: Average computation time per decision, for Bernoulli bandits over 20 trials with time horizon 1000.
Figure 5: Average computation time per decision, for Gaussian bandits over 20 trials with time horizon 1000.