Abstract

Bayesian bandit algorithms with approximate inference have been widely used in practice with superior performance. Yet, few studies regarding the fundamental understanding of their performances are available. In this paper, we propose a Bayesian bandit algorithm, which we call Generalized Bayesian Upper Confidence Bound (GBUCB), for bandit problems in the presence of approximate inference. Our theoretical analysis demonstrates that in Bernoulli multi-armed bandit, GBUCB can achieve $O(\sqrt{T\log T})$ frequentist regret if the inference error measured by symmetrized Kullback-Leibler divergence is controllable. This analysis relies on a novel sensitivity analysis for quantile shifts with respect to inference errors. To our best knowledge, our work provides the first theoretical regret bound that is better than $o(T)$ in the setting of approximate inference. Our experimental evaluations on multiple approximate inference settings corroborate our theory, showing that our GBUCB is consistently superior to BUCB and Thompson sampling.

1. Introduction

The stochastic bandit problem, dated back to Robbins (1952), is an important sequential decision making problem that is widely used in real-world applications. It aims to find optimal adaptive strategies that maximize cumulative reward. At each time step, the learning agent chooses an action (arm) among all possible actions and observes its corresponding reward (but not others), which requires balancing exploration and exploitation. Thompson sampling (Thompson, 1933) and its extension provide an elegant and efficient approach to tackle this exploration-exploitation dilemma. With exact posterior computation, Thompson sampling can achieve nearly optimal performance in terms of both frequentist regret (Agrawal & Goyal, 2012; 2013a; Kaufmann et al., 2012b) and Bayesian regret (Russo & Van Roy, 2014). However, in complex models such as neural networks, maintaining exact posterior distributions tends to be intractable (Riquelme et al., 2018) and thus, approximate Bayesian inference methods are widely employed, such as variational inference (Blei et al., 2017) and Markov chain Monte Carlo (Andrieu et al., 2003).

Few theoretical studies have been developed around Bayesian bandit approaches with approximate inference, despite its superior performance in practice (Riquelme et al., 2018; Snoek et al., 2015; Osband et al., 2016; Urteaga & Wiggins, 2018; Guo et al., 2020; Zhang et al., 2021). Lu & Van Roy (2017) gave a theoretical analysis of an approximate sampling method called Ensemble Sampling, which possessed a constant KL divergence error from the exact posterior and indicated a linear regret. Phan et al. (2019) showed that even with a small but constant inference error (in terms of $\alpha$-divergence), Thompson sampling with general approximate inference could have a linear regret in the worst case. Their work also showed that Thompson sampling combined with a small amount of forced exploration could achieve an $o(T)$ regret upper bound. This improvement, however, was mostly credited to the forced exploration other than the intrinsic property of Thompson sampling. It remains a mystery why approximate Bayesian sampling methods can work well empirically but fails theoretically (Phan et al., 2019), and a study regarding the fundamental understanding of their performance is necessary. Nevertheless, this question is not well investigated even in basic multi-armed bandits. In this work, we bridge this gap by providing a novel theoretical framework and pointing out that, minimizing KL divergence is insufficient to guarantee a sub-linear regret and meanwhile reducing the symmetrized KL divergence can contribute to the improvement of model performance.

In this paper, we propose a Bayesian bandit algorithm that can efficiently accommodate approximate inference, which we call the Generalized Bayesian Upper Confidence Bound (GBUCB). Under constant inference error, GBUCB can achieve $O(\sqrt{T\log T})$ frequentist regret, which to our
knowledge is the first theoretical regret bound that is better than $o(T)$. Bayesian Upper Confidence Bound (BUCB) was introduced by Kaufmann et al. (2012a); Kaufmann (2018) as a powerful Bayesian approach for multi-armed bandits, and also has its versions in contextual bandits (Srinivas et al., 2009; Guo et al., 2020). We provide the first study to extend the work of BUCB to the setting of approximate inference. In particular, we redesign the quantile choice in the algorithm to address the challenge of approximate inference: The original choice of $t^{-1}$ provides the best regret bound without approximate inference, but in the presence of approximate inference, it leads to an undesirable quantile shift which degrades the performance. With a careful adjustment of this quantile choice, we theoretically demonstrate that a sub-linear regret upper bound is achievable, if the inference error, which is measured by symmetrized Kullback-Leibler (KL) divergences (equivalently, sum of two $\alpha$-divergences with $\alpha = 0, 1$), is bounded. Moreover, we also show a negative answer in the other direction: Instead of symmetrized KL, controlling a KL divergence alone is not sufficient to guarantee a sub-linear regret for both Thompson sampling and GBUCB. This therefore suggests that naive approximate inference method that only minimizes KL divergence could perform poorly, and that it is critical to design approaches that reduce symmetrized divergences.

Our main contributions are summarized as follows:
1) We propose a general Bayesian bandit algorithm GBUCB to address the challenge of approximate inference. Our theoretical study shows that GBUCB can achieve a $O(\sqrt{T} (\log T)^c)$ regret upper bound when symmetrized KL divergence is controllable. This provides the first theoretical regret upper bound that is better than $o(T)$ in a general setting of approximate inference to the best of our knowledge.
2) We develop a novel sensitivity analysis of quantile shift with respect to inference error. This provides a fundamental tool to analyze Bayesian quantiles in the presence of approximate inference, which has potential for broader applications, e.g., when the inference error is time-dependent.
3) We demonstrate that a controllable KL divergence of one direction alone is insufficient to guarantee a sub-linear regret. Worst-case examples are constructed and illustrated where TS/BUCB/GBUCB has $\Omega(T)$ regret if KL divergence of one direction alone is controllable. Hence, special consideration on reducing the symmetrized KL divergence is necessary for real-world applications.
4) Our experimental evaluations corroborate well our theory, showing that our GBUCB is consistently superior to BUCB and Thompson sampling on multiple approximate inference settings.

## 1.1. Related Work

The theoretical optimality of bandit algorithms has been extensively studied over decades (Li et al., 2019; Bubeck & Cesa-Bianchi, 2012). The seminal paper Lai & Robbins (1985) (and subsequently Burnetas & Katehakis (1996)) established the first problem-dependent frequentist regret lower bound, showing that without any prior knowledge on the distributions, a regret of order $\log T$ is unavoidable. Thompson sampling (Agrawal & Goyal, 2012; Kaufmann et al., 2012b; Gopalan et al., 2014) and BUCB (Kaufmann et al., 2012a; Kaufmann, 2018) had been shown to match this lower bound, which indicated the theoretical optimality of those algorithms. Beyond basic multi-armed bandit problems, Bayesian approaches also exhibited powerful strength in the contextual bandit problems (Srinivas et al., 2009; Agrawal & Goyal, 2013b; Russo & Van Roy, 2014). Agrawal & Goyal (2013b) showed that linTS (a version of Thompson sampling in the linear contextual problems) could achieve a regret bound of $O(d^{3/2}\sqrt{T})$. Russo & Van Roy (2014) demonstrated that the Bayesian regret of LinTS was bounded above by $O(d\sqrt{T})$ which matched the minimax lower bound (Dani et al., 2008). All of those studies are in the setting of exact posterior computation. However, beyond Gaussian processes and linear models, exact computation of the posterior distribution is generally intractable and thus, approximate inference is necessary.

Since Thompson sampling had been shown to exhibit linear regret in the worst-case scenario of approximate inference as mentioned (Lu & Van Roy, 2017; Phan et al., 2019), some recent work focused on designing specialized methods to construct Bayesian indices. Mazumdar et al. (2020) constructed Langevin algorithms to generate approximate samples and showed an optimal problem-dependent frequentist regret. O’Donoghue & Lattimore (2021) proposed variational Bayesian optimistic sampling, suggesting to solve a convex optimization problem over the simplex at every time step. Unlike these, our study presents general results that rely only on the approximate inference error level, but not on the specific method of approximate inference.

Beyond Bayesian, another mainstream of bandit algorithms to address the exploration-exploitation tradeoff is upper confidence bound (UCB)-type algorithms (Auer, 2002; Auer et al., 2002a;b; Dani et al., 2008; Gopalan & Cappé, 2011; Seldin et al., 2013; Zhou et al., 2020). Chapelle & Li (2011) revealed that Thompson sampling empirically outperformed UCB algorithm in practice, partly because UCB was typically conservative as its configuration was data-independent which led to over-exploration (Hao et al., 2019). BUCB (Kaufmann et al., 2012a) could be viewed as a mid-ground between TS and UCB. On the other hand, empirical studies (Kaufmann, 2018) showed that Thompson sampling and BUCB performed similarly well in general.
2. Thompson Sampling, BUCB, and GBUCB

The stochastic multi-armed bandit problem consists of a set of \( K \) actions (arms), each with a stochastic scalar reward following a probability distribution \( \nu_i \) \((i = 1, \ldots, K)\). At each time step \( t = 1, \ldots, T \) where \( T \) is the time horizon, the agent chooses an action \( A_t \in \{K\} \) and in return observes an independent reward \( X_t \) drawn from the associated probability distribution \( \nu_{A_t} \). The goal is to devise a strategy \( A = (A_t)_{t \in [T]} \) to maximize the accumulated rewards through the observations from historic interaction.

In general, a wise strategy should be sequential, in the sense that the upcoming actions are determined and adjusted by the past observations: letting \( F_t = \sigma(A_1, X_1, \ldots, A_t, X_t) \) be the \( \sigma \)-field generated by the observations up to time \( t \), \( A_t \) is \( \sigma(F_t, U_t) \)-measurable, where \( U_t \) is a uniform random variable independent from \( F_{t-1} \) (as algorithms may be randomized). More precisely, let \( \mu_1 , \ldots, \mu_K \) denote the mean rewards of the actions \( \nu_1, \ldots, \nu_K \), and without loss of generality, we assume that \( \mu_1 = \max_{j \in [K]} \mu_j \). Then maximizing the rewards is equivalent to minimizing the (frequentist) regret, which is defined as the expected difference between the reward accumulated by an “ideal” strategy (a strategy that always playing the best action), and the reward accumulated by a strategy \( A \):

\[
R(T, A) := \mathbb{E} \left[ T \mu_1 - \sum_{t=1}^{T} X_t \right] = \mathbb{E} \left[ \sum_{t=1}^{T} (\mu_1 - \mu_{A_t}) \right].
\]  

(1)

The expectation is taken with respect to both the randomness in the sequence of successive rewards from each action \( j \), denoted by \( (Y_{j,s})_{s \in \mathbb{N}} \), and the possible randomization of the algorithm. \((U_t)_{t \in [T)} \). Let \( N_j(t) = \sum_{s=1}^{t} \mathbb{1}(A_s = j) \) denote the number of draws from action \( j \) up to time \( t \), so that \( X_t = Y_{A_t, N_{A_t}(t)} \). Moreover, let \( \hat{\mu}_{j,s} = \sum_{k=1}^{s} Y_{j,k} \) be the empirical mean of the first \( s \) rewards from action \( j \) and let \( \hat{\mu}_j(t) \) be the empirical mean of action \( j \) after \( t \) rounds of the bandit algorithm. Therefore \( \hat{\mu}_j(t) = 0 \) if \( N_j(t) = 0 \), \( \hat{\mu}_j(t) = \hat{\mu}_{j,N_j(t)} \) otherwise.

Note that the true mean rewards \( \mu = (\mu_1, \ldots, \mu_K) \) are fixed and unknown to the agent. In order to perform Thompson sampling, or more generally, Bayesian approaches, we artifically define a prior distribution \( \Pi_0 \) on \( \mu \). Let \( \Pi_t \) be the exact posterior distribution of \( \mu \mid F_{t-1} \) with density function \( \pi_t \) with marginal distributions \( \pi_{t,1}, \ldots, \pi_{t,K} \) for actions \( 1, \ldots, K \). Specifically, if at time step \( t \), the agent chooses action \( A_t = j \) and consequently observes \( X_t = Y_{A_t, N_{A_t}(t)} \), the Bayesian update for action \( j \) is

\[
\pi_{t,j} (x_j) \propto \nu_j(X_t) \pi_{t-1,j} (x_j),
\]  

(2)

whereas for \( i \neq j \), \( \pi_{t,i} = \pi_{t-1,i} \).

In each time step \( t \), we assume that the exact posterior computation in (2) cannot be obtained explicitly and an approximate inference method is able to give us an approximate distribution \( Q_t \) (instead of \( \Pi_t \)). We use \( q_t \) to denote the density function of \( Q_t \).

First, we consider a standard case where the exact posterior is accessible. In Thompson sampling (Agrawal & Goyal, 2012), we obtain a sample \( \tilde{m} \) from the posterior distribution \( \Pi_{t-1} \) and then select action \( A_t \) using the following strategy: \( A_t = i \) if \( \tilde{m}_i = \max_{j \in [K]} \tilde{m}_j \). In Bayesian Upper Confidence Bound (BUCB) (Kaufmann et al., 2012a), we obtain the quantile of the posterior distribution

\[
q_j(t) = Qu(1 - \frac{1}{t} (\log T)^c, \Pi_{t-1,j})
\]

for each action \( j \) where \( Qu(t, \rho) \) is the quantile function associated to the distribution \( \rho \), such that \( P_{\rho}(X \leq Qu(t, \rho)) = t \). Then we select action \( A_t \) as follows: \( A_t = i \) if \( q_i(t) = \max_{j \in [K]} q_j(t) \).

Next, we move to a more concrete example, Bernoulli multi-armed bandit problems (Agrawal & Goyal, 2012; 2013a; Kaufmann et al., 2012a; Kaufmann, 2018). In these problems, each (stochastic) reward follows a Bernoulli distribution \( \nu_t \sim \text{Bernoulli}(\mu_t) \) and these distributions are independent of each other. The prior \( \Pi_{0,j} \) is (usually) chosen to be the independent and identically distributed (i.i.d.) Beta(1, 1), or the uniform distribution for every action \( j \). Then the posterior distribution for action \( j \) is a Beta distribution \( \Pi_{t,j} = \text{Beta}(1 + S_j(t), 1 + N_j(t) - S_j(t)) \), where \( S_j(t) = \sum_{s=1}^{t} \mathbb{1}(A_s = j) X_s \) is the empirical cumulative reward from action \( j \) up to time \( t \). Then, Thompson sampling/BUCB chooses the samples/quantiles of the posterior \( \Pi_{t,j} = \text{Beta}(1 + S_j(t), 1 + N_j(t) - S_j(t)) \) respectively at each time step.

In the presence of approximate inference, Thompson sampling draws the sample \( \tilde{m} \) from \( Q_{t-1} \), as the exact \( \Pi_{t-1} \) is not accessible. Correspondingly, we modify the specific sequence of quantiles chosen by the BUCB algorithm with a general sequence of \( \{\gamma_t\} \)-quantiles, which we call a Generalized Bayesian Upper Confidence Bound (GBUCB) algorithm. The detailed algorithm of GBUCB is described in Algorithm 1. For Bernoulli multi-armed bandit problems, we suggest to choose the following quantiles

\[
q_j(t) = Qu(1 - \frac{1}{\sqrt{t} (\log T)^c}, Q_{t-1,j}).
\]  

(3)

where \( \gamma_t = 1 - \frac{1}{\sqrt{t} (\log T)^c} \). This \( \frac{1}{\sqrt{t}} \) instead of the original \( \frac{1}{t} \) in \( \gamma_t \) is a delicate choice to address the tradeoff between the optimal regret and the presence of inference error; see Remark 3.11 in Section 3.

As discussed in Kaufmann et al. (2012a), the horizon-dependent term \( (\log T)^c \) is only an artifact of the theoretical analysis to obtain a finite-time regret upper bound (for...
Algorithm 1 Generalized Bayesian Upper Confidence Bound (GBUCB) with Approximate Inference

Input: $T$ (time horizon), $\Pi_0 = Q_0$ (initial prior on $\mu$), $c$ (parameters of the quantile), a real-value increasing sequence $\{\gamma_t\}$ such that $\gamma_t \rightarrow 1$ as $t \rightarrow \infty$

for $t = 1$ to $T$ do
  for each action $j = 1, \ldots, K$ do
    compute $q_j(t) = Qu(\gamma_t, Q_{t-1,j})$.
  end for
  draw action $A_t = \arg \max_{j=1,\ldots,K} q_j(t)$
  get reward $X_t = Y_{A_t, N_{A_t}(t)}$
  define the exact posterior distribution $\Pi_t$ according to (2) but only obtain an approximate distribution $Q_t$
end for

$c \geq 5$). In practice, the model with choice $c = 0$ (i.e., without the horizon-dependent term) already achieves superior performance. This is confirmed by our experiments in Section 4 and a similar observation in BUCB was indicated in Kaufmann et al. (2012a).

3. Theoretical Analysis

In this section, we present a theoretical analysis of GBUCB. In section 3.1, we provide the necessary background of KL divergence on approximate inference error measurement. Then in Section 3.2, we develop a novel sensitivity analysis of quantile shift with respect to inference error. This provides a fundamental tool to analyze Bayesian quantiles in the presence of approximate inference. The general results therein will be used for our derivation for the regret upper bound of GBUCB in Section 3.3, and are also potentially useful for broad applications, e.g., when the inference error is time-dependent. Lastly, in Section 3.4, we provide examples where Thompson sampling/BUCB/GBUCB has a linear regret with arbitrarily small inference error measured by KL divergence alone. All proofs are given in Appendix.

3.1. KL Divergence for Inference Error Measurement

KL divergence is widely used in variational inference (Blei et al., 2017; Kingma & Welling, 2013) which is one of the most popular approaches in Bayesian approximate inference. It was also adopted in previous study on Thompson sampling with approximate inference (Phan et al., 2019; Lu & Van Roy, 2017). The KL divergence between two distributions $P_1$ and $P_2$ with density functions $p_1(x)$ and $p_2(x)$ is defined as:

$$KL(P_1, P_2) = \int p_1(x) \log \left(\frac{p_1(x)}{p_2(x)}\right) dx.$$ 

When using the approximate Bayesian inference methods, the exact posterior distribution $\Pi_t$ and the approximate distribution $Q_t$ may differ from each other. To provide a general analysis of approximate sampling methods, we use the KL divergence as the measurement of inference error (statistical distance) between $\Pi_t$ and $Q_t$. Our starting point is the following.

Assumption 3.1.

$$KL(Q_{t,j}, P_{t,j}) \leq \epsilon, \forall t \in [T], j \in [K]$$

In other words, the symmetrized KL divergence between $Q_{t,j}$ and $\Pi_{t,j}$ is controllable. To enhance credibility on this assumption, we remark that some recent papers (Ruiz & Titsias, 2019; Brekelmans et al., 2020) consider the symmetrized KL divergence in variational inference. This assumption states that while we only have access to the approximate distribution $Q_{t,j}$, the inference error (measured by symmetrized KL divergence) between the exact $\Pi_{t,j}$ and $Q_{t,j}$ only differs from a constant $\epsilon$ (at most) at each time step $t$. We note that our assumption (as well as our subsequent results) is general in the sense that it does not assume any specific methods of approximate inference.

Remark 3.2. In multi-armed bandit problem, the most practical (and probably natural) way to define the prior distribution $\Pi_0$ is to assume independence among each action $\Pi_{0,1}, \ldots, \Pi_{0,K}$ and thus the posterior distribution is also independently updated among each action (Agrawal & Goyal, 2012; Kaufmann et al., 2012a). Therefore we focus on the inference error for the distribution of each action in (4), which appears more realistic than the inference error for the joint distribution of all actions assumed in Phan et al. (2019).

If the inference error measured by symmetrized KL divergences (equivalently, two $\alpha$-divergences with $\alpha = 0, 1$) is controllable, then we can show that a low regret bound is indeed achievable. This does not contradict the results in Phan et al. (2019). To quote them, “we do not mean to imply that low regret is impossible but simply that making an $\alpha$-divergence a small constant alone is not sufficient.”

3.2. Quantile Shift with Inference Error

We put the following basic assumption:

Assumption 3.3. $p_1(x)$ and $p_2(x)$ have the same support.

This assumption is to guarantee that the KL divergence in (4) is well-defined. We rigorously state our theorem as follows:

Theorem 3.4. Let $R_i$ denote the quantile function of the distribution $P_i$, i.e., $R_i(p) := Qu(p, P_i)$ ($i = 1, 2$). Suppose Assumption 3.3 holds. Let $\gamma > \frac{1}{2}$. Let $\delta_{\gamma, \epsilon}$ satisfy that

$$R_1(\gamma) = R_2(\gamma + \delta_{\gamma, \epsilon})$$
a) If $KL(P_1, P_2) \leq \epsilon$, then
   \[
   \delta_{\gamma, \epsilon} < (1 - \gamma) \left(1 - \exp(-\frac{\epsilon + \log(2)}{1 - \gamma})\right).
   \]

b) If $KL(P_2, P_1) \leq \epsilon$, then
   \[
   \delta_{\gamma, \epsilon} \geq (1 - \gamma)(M_{\epsilon} - 1)
   \]
   where $M_{\epsilon} > 1$ is the (unique) solution of $M_{\epsilon} \log(M_{\epsilon}) = 2(\epsilon + e^{-1})$. Note that $M_{\epsilon}$ only depends on $\epsilon$.

We only consider the quantile $\gamma > \frac{1}{2}$ in the theorem since the quantile chosen by the GBUCB algorithm is greater than $\frac{1}{2}$ when $t$ is large (since $\gamma_t \to 1$). This theorem states that with $\epsilon$ inference error, the $\gamma$-quantile of the distribution $P_1$ is the $(\gamma + \delta_{\gamma, \epsilon})$-quantile of the distribution $P_2$ where the shift $\delta_{\gamma, \epsilon}$ is close to 0. This theorem is distribution-free, in the sense that the bound of $\delta_{\gamma, \epsilon}$ does not depend on any specific distributions (noting that distribution changes as $t$ evolves in bandit problems). For instance, we have $\delta_{\gamma, \epsilon} \geq -O_{\epsilon}(1 - \gamma)$ where the hidden constant in $O_{\epsilon}$ only depends on $\epsilon$, independent of $\gamma$ or distributions (in other words, independent of $t$). This observation is important in the robustness of using quantiles in the GBUCB.

The proof of Theorem 4.1 relies on the following lemma, which provides a quantile-based representation of KL divergence.

**Lemma 3.5.** Under the same condition in Theorem 3.4, we have that
\[
KL(P_1, P_2) = -\int_0^1 \log\left(\frac{d}{du} R_2^{-1}(R_1(u))\right) du.
\]

### 3.3. Regret Bound for GBUCB

In this section, we rigorously derive the upper bound of the problem-dependent frequentist regret for GBUCB in Bernoulli multi-armed bandit problems.

Note that by definition (1), we can express the regret as
\[
R(T, A) := E\left[\sum_{t=1}^T (\mu_1 - \mu_{A_t})\right] = \sum_{j=1}^K (\mu_1 - \mu_j) E[N_j(t)].
\]

Therefore, in order to bound the problem-dependent regret $R(T, A)$, it is sufficient to consider $E[N_j(t)]$.

For $(p, q) \in [0, 1]^2$, we denote the Bernoulli Kullback-Leibler divergence between two points by
\[
d(p, q) = p \log\left(\frac{p}{q}\right) + (1-p) \log\left(\frac{1-p}{1-q}\right),
\]
with, by convention, $0 \log 0 = 0 \log(0/0) = 0$ and $\infty \log(x/0) = +\infty$ for $x > 0$. We also denote that $d^+(p, q) = d(p, q) \mathbb{I}\{p < q\}$ for convenience.

We adopt the Assumption 3.3 in this setting.

**Assumption 3.6.** $q_{t, j}(x)$ has the support $(0, 1)$ for any $t \in [T], j \in [K]$.

Note that $\pi_{t, j}(x)$ is the pdf of Beta$(1 + S_j(t), 1 + N_j(t) - S_j(t))$ so its support is $(0, 1)$.

The following is our main theorem: a finite-time regret bounds for our GBUCB algorithm. Without loss of generality, we assume action 1 is optimal.

**Theorem 3.7.** Suppose Assumption 3.1, 3.6 hold. For any $\xi > 0$, choosing the parameter $c \geq 5$ in the GBUCB algorithm and setting $\gamma_t = 1 - \frac{1}{t \log(t)} (0 < \zeta < 1)$, the number of draws of any sub-optimal action $j \geq 2$ is upper-bounded by
\[
E[N_j(T)] \leq \frac{(1 + \xi) K_c}{d(\mu_1, \mu_1)} \max\{T^{\xi}, (1 - \zeta) T^{\xi}, \frac{c T^{1-\zeta}}{1 - \zeta}\} + o_{\xi, c, \epsilon}\left(\max\{T^{\xi}, (1 - \zeta) T^{\xi}, \frac{c T^{1-\zeta}}{1 - \zeta}\}\right),
\]
where $K_c$ is a constant only depending on the inference error $\epsilon$. More specifically, these exists an absolute constant $C_0$, such that
\[
K_c \leq C_0 max\{M_{\epsilon}, \epsilon + (\log(2))\}.
\]

It is easy to see that to minimize the regret upper bound, we may choose $\xi = \frac{1}{2}$ in Theorem 3.7.

**Corollary 3.8.** Suppose Assumption 3.1, 3.6 hold. For any $\xi > 0$, choosing the parameter $c \geq 5$ in the GBUCB algorithm and setting $\gamma_t = 1 - \frac{1}{t \log(t)} (0 < \zeta < 1)$, (See (3)), the number of draws of any sub-optimal action $j \geq 2$ is upper-bounded by
\[
E[N_j(T)] \leq \frac{(1 + \xi) K_c}{d(\mu_1, \mu_1)} \sqrt{T}(\log T)^{\xi} + o_{\xi, c, \epsilon}(\sqrt{T}(\log T)^{\xi}).
\]

This result states that with $\epsilon$ inference error, the regret of the GBUCB algorithm is bounded above by $\sqrt{T}(\log T)^{\xi}$, which is the first algorithm providing the theoretical regret bound that is better than $o(T)$ to the best of our knowledge.

**Remark 3.9.** It appears a little surprising at first glance that the result in Corollary 3.13 indicates a $\sqrt{T}(\log T)^{\xi}$ regret upper bound regardless of how large $\epsilon$ is (except that it influences the constant $K_c$), since we may expect that a large $\epsilon$ allows the “fully swap” of the posterior of the optimal action and a suboptimal action, making any Bayesian index approaches not able to distinguish them. However, as time goes by, the exact posterior will be more and more “concentrated” on the true mean with little variability, making the symmetrized KL divergence between two actions larger and larger. That means for a fixed $\epsilon$ (no matter how large it is), the symmetrized KL divergence between the exact posteriors of two actions will be sufficiently large when $t$ is sufficiently large so the “fully swap” cannot happen.
Remark 3.10. Kaufmann et al. (2012a) have shown that in the absence of approximate inference, \( \mathbb{E}[N_j(T)] = O(\log T) \) which matches the problem-dependent regret lower bound in Lai & Robbins (1985). Yet, it is conjectured that this bound is no longer available due to the approximate inference.

Remark 3.11. The \( \frac{1}{\sqrt{T}} \) in the choice of the quantiles in GBUCB, instead of the original \( \frac{1}{T} \) in BUCB, is a delicate choice to address the tradeoff between making the regret optimal without approximate inference and the presence of inference error. On a technical level, a larger power \( \zeta \) in \( t^\zeta \) improves the regret bound without the presence of approximate inference but simultaneously leads to high-level quantile shift caused by approximate inference. Choosing \( \zeta = \frac{1}{2} \) is a subtle balance of those two.

The analysis of Theorem 3.7 relies on the bounds on the quantiles of the exact posterior distributions (Theorem 3.4). More specifically, we have the following lemma:

**Lemma 3.12.** Under the same condition in Theorem 3.7, the quantiles of the approximate distributions \( q_j(t) \) chosen by the GBUCB algorithm satisfy the following bound:

\[
\underline{q}_j(t) \leq q_j(t) \leq \overline{q}_j(t)
\]

where

\[
\underline{q}_j(t) = \arg\max_{x > \frac{s_j(t)}{N_j(t) + 1}} \left\{ d\left( \frac{S_j(t)}{N_j(t) + 1}, x \right) \leq \frac{\zeta \log(t) + c \log(\log T) - \log(M_j) - \log(N_j(t) + 2)}{N_j(t) + 1} \right\},
\]

\[
\overline{q}_j(t) = \arg\max_{x < \frac{s_j(t)}{N_j(t)}} \left\{ d\left( \frac{S_j(t)}{N_j(t)}, x \right) \leq \frac{\zeta \log(t) + c \log(\log T) + (\epsilon + \log(2))t^\zeta(\log T)^c}{N_j(t)} \right\}.
\]

Based on Lemma 3.12, we can obtain a UCB-type decomposition of the number of draws of any sub-optimal action \( j \geq 2 \), which is the first step to prove Theorem 3.7:

**Lemma 3.13.** Under the same condition in Theorem 3.7, we have that for any constant \( \beta_T \),

\[
N_2(T) \leq \sum_{t=1}^{T} \mathbb{1}\{\mu_1 - \beta_T > \underline{u}_1(t)\} + \sum_{t=1}^{T} \mathbb{1}\{\mu_1 - \beta_T \leq \overline{u}_2(t)\} \cap (A_t = 2).
\] (5)

Finally, to obtain Theorem 3.7, it is sufficient to analyze the two terms in Lemma 3.13.

### 3.4. KL Divergence of One Direction

We show that a controllable KL divergence of one direction alone cannot guarantee a sub-linear regret. We provide two worst-case examples, one where Thompson sampling has a linear regret, the other where BUCB/GBUCB has a linear regret, even when KL divergence of one direction is arbitrarily small. A similar study on Thompson sampling has been conducted in Phan et al. (2019) where they focus on the inference error for the joint distribution of entire actions. In this work, nevertheless, we focus on a more realistic setting where the inference error for the distribution of each action is assumed; see Remark 3.2. Therefore, their examples cannot be directly applied in our setting. Moreover, our second example shows that BUCB/GBUCB could have a linear regret if only KL divergence of one direction is considered, which is brand new.

**Assumption 3.14.**

\[
KL(P_{t,j}, Q_{t,j}) \leq \epsilon, \forall t \in [T], j \in [K]
\] (6)

We establish the following theorem for Thompson sampling:

**Theorem 3.15.** Consider a Bernoulli multi-armed bandit problem where the number of actions is \( K = 2 \) and \( \mu_1 > \mu_2 \). The prior \( \Pi_{0,j} \) is chosen to be the i.i.d. Beta(1, 1), or the uniform distribution for every action \( j = 1, 2 \). For any error threshold \( \epsilon > 0 \), there exists a sequence of distributions \( Q_t \) such that for all \( t \geq 1 \):

1. The probability of sampling from \( Q_{t-1} \) choosing action 2 is greater than a positive constant.
2. \( Q_{t-1} \) satisfies Assumption 3.1, 3.14.

Therefore Thompson sampling from the approximate distribution \( Q_{t-1} \) will cause a finite-time linear frequentist regret:

\[
R(T, A) = O(T).
\]

In fact, we can explicitly construct such a distribution \( Q_t \) as follows:

\[
q_{t,1}(x_1) = \begin{cases} \frac{1}{2} \Pi_{t,1}(x_1) & \text{if } 0 < x_1 < b_t \\ \frac{1}{2} \Pi_{t,1}(x_1) & \text{if } b_t < x_1 < 1 \end{cases}
\]

\[
q_{t,2}(x_2) = \Pi_{t,2}(x_2)
\]

(7)

where \( \Pi_{t,1} \) is the cdf of \( \Pi_{t,1} \) and \( r > 1, b_t \in (0, 1) \) will be specified in the proof.

This theorem shows that making KL divergence of one direction a small constant alone, even for each action \( j \), is not enough to guarantee a sub-linear regret of Thompson sampling. Note that Theorem 3.15 is an enhancement of the
results in Phan et al. (2019) as the $Q_t$ constructed by our theorem satisfies more restrictive assumptions (Assumption 3.1, 3.14). We can derive a similar observation for the BUCB/GBUCB algorithm as follows:

**Theorem 3.16.** Consider a Bernoulli multi-armed bandit problem where the number of actions is $K = 2$ and $\mu_1 > \mu_2$. The prior $\Pi_{t,j}$ is chosen to be the i.i.d. $\text{Beta}(1, 1)$, or the uniform distribution for every action $j = 1, 2$. Consider the general GBUCB algorithm described in Algorithm 1. For any error threshold $\epsilon > 0$, there exists a constant $T_0$ only depending on the sequence $\{\gamma_t\}$ and a sequence of distributions $Q_{t-1}$ such that for all $t \geq 1$:

1. The GBUCB algorithm always chooses action 2 when $t \geq T_0$.
2. $Q_{t-1}$ satisfies Assumption 3.1, 3.14.

Therefore the GBUCB algorithm from the approximate distribution $Q_{t-1}$ will cause a finite-time linear frequentist regret:

$$R(T, A) = \Omega(T).$$

Again, we can explicitly construct such a distribution $Q_t$ as follows:

$$q_{t,1}(x_1) = \pi_{t,1}(x_1)$$

$$q_{t,2}(x_2) = \begin{cases} \frac{1}{1-F_{t,2}(b_t)} \pi_{t,2}(x_2) & \text{if } 0 < x_1 < b_t \\ \frac{1}{1-F_{t,2}(b_t)} \pi_{t,2}(x_2) & \text{if } b_t < x_1 < 1 \end{cases}$$

(8)

where $F_{t,2}$ is the cdf of $\Pi_{t,2}$ and $r > 1$, $b_t \in (0, 1)$ will be specified in the proof.

This theorem shows that making KL divergence of one direction a small constant alone, even for each action $j$, is not enough to guarantee a sub-linear regret of BUCB/GBUCB.

We emphasize that the examples in Theorems 3.15 and 3.16 are in the worst-case sense. In other words, there exist worst-case examples where Thompson sampling/GBUCB exhibits a linear regret if only one KL divergence is controllable. This does not imply that GBUCB and Thompson sampling fail on average in the presence of approximate inference. In fact, Theorem 3.7 shows that a sub-linear regret can be achieved in any case as long as the inference error measured by symmetrized KL divergence is controllable.

4. **Experiments**

In this section, we conduct numerical experiments to show the correctness of our theory. In Section 4.1, we compare the performance of GBUCB with the following baselines: BUCB and Thompson sampling. In Section 4.2, we construct worst-case examples showing that both GBUCB and Thompson sampling can degenerate to linear regret, if only assuming KL divergence of one direction. Our code will be publicly available to facilitate other researchers.

We consider the Bernoulli multi-armed bandit problem which has 2 actions with mean reward $[0.7, 0.3]$ and use $\text{Beta}(1, 1)$ as the prior distribution of mean reward for each action. At each time step $t$, the exact posterior distribution for each action is $\text{Beta}(1 + S_j(t), 1 + N_j(t) - S_j(t))$, where $S_j(t)$ is the empirical cumulative reward from action $j$ up to time $t$ and $N_j(t)$ is the number of draws from action $j$ up to time $t$.

4.1. **Generally Misspecified Posteriors**

Suppose the posterior distributions are misspecified to the following distributions:

$$(P1) : (1 - w) * \text{Beta}(1 + S_j(t), 1 + N_j(t) - S_j(t)) + w * \text{Beta}(\frac{1 + S_j(t)}{2}, 1 + N_j(t) - S_j(t))$$

$$(P2) : (1 - w) * \text{Beta}(1 + S_j(t), 1 + N_j(t) - S_j(t)) + w * \text{Beta}(2(1 + S_j(t)), 2(1 + N_j(t) - S_j(t)))$$

where $w = 0.9, 0.8, 0.7$. Note that the first problem setting $(P1)$ mimics the situation where the approximation covers the posterior’s entire support ($\alpha$ in $\alpha$-divergence inference error is large), while the second problem setting $(P2)$ mimics the situation where the approximation fits the posterior’s dominant mode ($\alpha$ in $\alpha$-divergence inference error is small); See Minka et al. (2005) for the implication of $\alpha$-divergence.

Figure 1 presents the results of GBUCB and the baselines. Those results demonstrate that:

1) Overall, GBUCB achieves consistently superior performance than the baselines and it outperforms BUCB with considerable improvements. These results confirms the effectiveness of GBUCB across multiple settings.
2) GBUCB performs well without the horizon-dependent term (i.e., $c = 0$ in Equation (3)). This brings GBUCB with practical advantages in real-world applications since it does not require advanced knowledge of the horizon (i.e., anytime). A similar observation of BUCB was also noticed in Kaufmann et al. (2012a).

4.2. **Worst-Case Misspecified Posteriors**

We consider the worst-case examples, Equations (7) and (8), presented in Section 3.4, where the posterior distributions are misspecified using KL divergence of one direction.

The results of Thompson sampling, BUCB, and GBUCB are displayed in Figure 2. From these worst-case examples, we observe that:

1) Thompson sampling exhibits a linear regret after $t \geq 1$. As we have shown in Theorem 3.15, the linear coefficient (i.e., the slope) of the regret depends on $r$, the level of inference error. Larger $r$ implies larger slope of the regret, which has been illustrated in both Figure 2 and the proof of Theorem 3.15.
2) BUCB/GBUCB exhibits a linear regret with constant slope $\mu_1 - \mu_2$ after $t \geq T_0$ (where $T_0$ is introduced in Theorem 3.16). The artificial choice of $r$ is to make $T_0 = 100, 200, 333$ where $\gamma T_0 = \frac{1}{r}$; please refer to the proof of Theorem 3.16 for details.

In summary, our experiments evidently demonstrate the superior performance of our proposed GBUCB on multi-armed bandit problems with generally misspecified posteriors. Our results also align closely with our theory that simply making KL divergence a small constant alone is insufficient to guarantee a sub-linear regret of Thompson sampling/BUCB/GBUCB. Hence, a controllable symmetrized KL divergence is necessary for the sub-linear regret upper bound.

5. Conclusions and Future Work

In this paper, we propose a general Bayesian bandit algorithm, which we call Generalized Bayesian Upper Confidence Bound (GBUCB), that achieves superior performance for multi-armed bandit problems with approximate inference. We prove that, with controllable symmetrized KL divergence, GBUCB can achieve $O(\sqrt{T \log T})$ frequentist regret. In comparison with the baselines, we empirically demonstrate the effectiveness of GBUCB among various problem settings. In addition, we construct worse-case examples to show the necessity of symmetrized KL divergence, which is further verified by the observations in our experiments. Future work will extend the idea of GBUCB to contextual bandit problems with approximate inference.
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We provide further results and discussions in this appendix. Section A presents the missing proofs for results in Section 3.2 in the main paper. Section B presents the missing proofs for results in Section 3.3. Section C presents the missing proofs for results in Section 3.4.

A. Proofs of Results in Section 3.2

Proof of Theorem 3.4. Note that $R_1(\gamma) = R_2(\gamma + \delta_{\gamma,\epsilon})$ implies $R_2^{-1}(R_1(\gamma)) = \gamma + \delta_{\gamma,\epsilon}$ and $R_1^{-1}(R_2(\gamma + \delta_{\gamma,\epsilon})) = \gamma$. Obviously $R_2^{-1}(R_1(0)) = 0$ and $R_2^{-1}(R_1(1)) = 1$. On a high level, our proof technique is to split the $KL(P_1, P_2)$ into two parts using the quantile-based representation of KL divergence in Lemma 3.5, and then use Jensen’s inequality (since $- \log$ is a convex function) to bound $\delta_{\gamma,\epsilon}$.

a) 

\[
KL(P_1, P_2) = -\int_0^1 \log \left( \frac{d}{du} R_2^{-1}(R_1(u)) \right) du \\
= -\int_0^\gamma \log \left( \frac{d}{du} R_2^{-1}(R_1(u)) \right) du - \int_\gamma^1 \log \left( \frac{d}{du} R_2^{-1}(R_1(u)) \right) du \\
\leq -\gamma \log \left( \frac{1}{\gamma} \int_0^\gamma \frac{d}{du} R_2^{-1}(R_1(u)) du \right) - (1 - \gamma) \log \left( \frac{1}{1 - \gamma} \int_\gamma^1 \frac{d}{du} R_2^{-1}(R_1(u)) du \right) \\
= -\gamma \log \left( \frac{R_2^{-1}(R_1(\gamma)) - R_2^{-1}(R_1(0))}{\gamma} \right) - (1 - \gamma) \log \left( \frac{R_2^{-1}(R_1(1)) - R_2^{-1}(R_1(\gamma))}{1 - \gamma} \right) \\
= -\gamma \log \left( \frac{\gamma + \delta_{\gamma,\epsilon}}{\gamma} \right) - (1 - \gamma) \log \left( \frac{1 - (\gamma + \delta_{\gamma,\epsilon})}{1 - \gamma} \right).
\]

Let 

\[g(\delta) = -\gamma \log \left( \frac{\gamma + \delta}{\gamma} \right) - (1 - \gamma) \log \left( \frac{1 - (\gamma + \delta)}{1 - \gamma} \right).\]

Taking the derivative of $g(\delta)$ with respect to $\delta$, we obtain 

\[g'(\delta) = -\frac{1}{1 + \frac{\delta}{\gamma}} + \frac{1}{1 - \frac{\delta}{1 - \gamma}}.\]

It is easy to see that $g(\delta)$ is strictly decreasing when $\delta \in (-\gamma, 0)$ and strictly increasing when $\delta \in (0, 1 - \gamma)$ with minimum $g(0) = 0$. This fact shows that $\epsilon \geq g(\delta)$ is equivalent to $\delta$ in an interval around 0, i.e., $\delta \in [\delta, \delta] \subset (-\gamma, 1 - \gamma)$. More explicitly, we can obtain an explicit but loose bound for $\delta, \delta$.

When $\delta_{\gamma,\epsilon} > 0$, we have 

\[-\gamma \log \left( \frac{\gamma + \delta_{\gamma,\epsilon}}{\gamma} \right) \geq -1 \cdot \log \left( \frac{1 - (\gamma + \delta_{\gamma,\epsilon})}{1 - \gamma} \right) = \log(\gamma),\]

as and $\delta_{\gamma,\epsilon} < 1 - \gamma$. Therefore $\epsilon \geq KL(P_1, P_2)$ implies that 

\[-(1 - \gamma) \log \left( \frac{1 - (\gamma + \delta_{\gamma,\epsilon})}{1 - \gamma} \right) \leq \epsilon - \log(\gamma)\]

which is equivalent to 

\[\delta_{\gamma,\epsilon} \leq (1 - \gamma) \left( 1 - \exp\left( -\frac{\epsilon - \log(\gamma)}{1 - \gamma} \right) \right) \leq (1 - \gamma) \left( 1 - \exp\left( -\frac{\epsilon + \log(2)}{1 - \gamma} \right) \right),\]

as $\gamma \geq \frac{1}{2}$. 

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b) 

\[ KL(P_2, P_1) \]

\[ = - \int_0^1 \log \left( \frac{d}{du} R_1^{-1}(R_1(u)) \right) du \]

\[ = - \int_{\gamma + \delta, e}^{\gamma + \delta, e} \log \left( \frac{d}{du} R_1^{-1}(R_1(u)) \right) du - \int_1^{\gamma + \delta, e} \log \left( \frac{d}{du} R_1^{-1}(R_1(u)) \right) du \]

\[ \geq - (\gamma + \delta, e) \log \left( \frac{1}{\gamma + \delta, e} \right) \int_{\gamma + \delta, e}^{\gamma + \delta, e} \frac{d}{du} R_1^{-1}(R_1(u)) du \]

\[ - (1 - \gamma - \delta, e) \log \left( \frac{1}{1 - \gamma - \delta, e} \right) \int_{\gamma + \delta, e}^{\gamma + \delta, e} \frac{d}{du} R_1^{-1}(R_1(u)) du \]

\[ = - (\gamma + \delta, e) \log \left( \frac{\gamma}{\gamma + \delta, e} \right) - (1 - \gamma - \delta, e) \log \left( \frac{1 - \gamma}{1 - \gamma - \delta, e} \right). \]

Let \( h(x) = x \log(x) \). Taking the derivative of \( h(x) \) with respect to \( x \), we obtain

\[ h'(x) = \log(x) + 1. \]

Therefore \( h(x) \) is strictly decreasing when \( x \in (0, e^{-1}) \) and strictly increasing when \( x \in (e^{-1}, +\infty) \) with minimum \( h(e^{-1}) = -e^{-1} \).

When \( \delta, e < 0 \), we have

\[ -(\gamma + \delta, e) \log \left( \frac{\gamma}{\gamma + \delta, e} \right) = \gamma \frac{\gamma}{\gamma + \delta, e} \log \left( \frac{\gamma + \delta, e}{\gamma} \right) \geq -\gamma e^{-1} \]

as \( h(x) \geq -e^{-1} \). Therefore \( \epsilon \geq KL(P_2, P_1) \) implies that

\[ -(1 - \gamma - \delta, e) \log \left( \frac{1 - \gamma}{1 - \gamma - \delta, e} \right) \leq \epsilon + \gamma e^{-1} \]

Let \( M_{\gamma, e} := \frac{-\delta, e}{1 - \gamma} + 1 \geq 1 \) since \( \delta, e < 0 \). Then the above inequality is equivalent to

\[ (1 - \gamma)M_{\gamma, e} \log(M_{\gamma, e}) \leq \epsilon + \gamma e^{-1}. \]

Therefore we obtain

\[ M_{\gamma, e} \log(M_{\gamma, e}) \leq 2(\epsilon + e^{-1}) \]

as \( \frac{1}{2} \leq r \leq 1 \). Since \( h(x) \) is strictly increasing when \( x > 1 \), it follows that \( M_{\epsilon} \) is unique and

\[ 1 \leq M_{\gamma, e} \leq M_{\epsilon}. \]

Therefore, we obtain that \( KL(P_2, P_1) \leq \epsilon \) implies that

\[ \delta, e \geq -(1 - \gamma)(M_{\epsilon} - 1). \]

Proof of Lemma 3.5. Let \( F_1 \) and \( F_2 \) be the cumulative distribution function of \( P_1 \) and \( P_2 \) respectively. Since \( F_1 \) and \( F_2 \) are absolute continuous and strictly increasing (as they have positive densities), we have that \( F_i(R_i(u)) = u \) for \( 0 \leq u \leq 1 \). Taking the derivative with respect to both sides of \( F_i(R_i(u)) = u \), we obtain

\[ R'_i(u) p_i(R_i(u)) = 1 \]  \hspace{1cm} (9)
where \( R'_1(u) := \frac{dR_1(u)}{du} \). Using integration by substitution, we obtain that

\[
KL(P_1, P_2) = \int_0^1 \log \left( \frac{p_1(R_1(u))}{p_2(R_1(u))} \right) p_1(R_1(u)) dR_1(u)
= \int_0^1 \log \left( \frac{R'_1(u)p_1(R_1(u))}{R'_1(u)p_2(R_1(u))} \right) p_1(R_1(u)) R'_1(u) du
= - \int_0^1 \log (R'_1(u)p_2(R_1(u))) du
= - \int_0^1 \log \left( \frac{d}{du} R_2^{-1}(R_1(u)) \right) du
\]

where the last equation follows from the following observation:

\[
\frac{d}{du} R_2^{-1}(R_1(u)) = R'_1(u) \frac{d}{dv} R_2^{-1}(v) \bigg|_{v=R_1(u)}
= R'_1(u) \frac{1}{R'_2(R_2^{-1}(v))} \bigg|_{v=R_1(u)}
= R'_1(u)p_2(R_2^{-1}(v))) \bigg|_{v=R_1(u)} \text{ by equation (9)}
\]

Hence we conclude that

\[
KL(P_1, P_2) = - \int_0^1 \log \left( \frac{d}{du} R_2^{-1}(R_1(u)) \right) du.
\]

**B. Proofs of Results in Section 3.3**

**Proof of Theorem 3.7.** Without loss of generality, we let \( j = 2 \). (Note that we have assumed the action 1 is optimal.) By Lemma 3.13, we only need to bound the two following two terms:

\[
D_1 := \sum_{i=1}^T \mathbb{1}\{ \mu_1 - \beta_T > \tilde{u}_1(t) \}, \quad D_2 := \sum_{i=1}^T \mathbb{1}\{ (\mu_1 - \beta_T \leq \tilde{u}_2(t)) \cap (A_t = 2) \}
\]

Let \( \beta_T = \sqrt{\frac{1}{\log T}} \). We further split \( D_1 \) into two parts:

\[
D_{1,1} := \sum_{i=1}^T \mathbb{1}\{ \mu_1 - \beta_T > \tilde{u}_1(t), N_1(t) + 2 \leq (\log T)^2 \}, \quad D_{1,2} := \sum_{i=1}^T \mathbb{1}\{ \mu_1 - \beta_T > \tilde{u}_1(t), N_1(t) + 2 \geq (\log T)^2 \}
\]

**Step 1:** Consider \( D_{1,1} \).

Note that

\[
\frac{\zeta \log(t) + c \log(\log T) - \log(M_1) - \log(N_1(t) + 2)}{N_1(t) + 1} \geq \frac{\zeta \log(t) + (c - 2) \log(\log T) - \log(M_2)}{N_1(t) + 1}
\]

in \( \tilde{u}_1(t) \) when \( N_1(t) + 2 \leq (\log T)^2 \). Hence we have that

\[
\tilde{u}_1(t) \geq \arg \max_{x > \frac{S_1(t)}{N_1(t) + 1}} \left\{ d \left( \frac{S_1(t)}{N_1(t) + 1}, x \right) \leq \frac{\zeta \log(t) + (c - 2) \log(\log T) - \log(M_2)}{N_1(t) + 1} \right\} := \tilde{u}_1(t)
\]

when \( N_1(t) + 2 \leq (\log T)^2 \). This shows that

\[
D_{1,1} \leq \sum_{i=1}^T \mathbb{1}\{ \mu_1 > \tilde{u}_1(t) \}
\]
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Similarly as the proof in Kaufmann et al. (2012a), with a straightforward adaptation of the proof of theorem 10 in Garivier & Cappé (2011), we obtain the following self-normalized inequality

**Lemma B.1.**

$$P(\mu_1 > \tilde{u}_1(t)) \leq (\bar{\delta} \log(t) + 1) \exp(-\bar{\delta} + 1)$$

where

$$\bar{\delta} = \zeta \log(t) + (c - 2) \log(\log(T)) - \log(M_\epsilon).$$

Lemma B.1 leads to the following upper bound of $D_{1,1}$:

$$\mathbb{E}[D_{1,1}] \leq \sum_{t=1}^{T} P(\mu_1 > \tilde{u}_1(t))$$

$$\leq 1 + \sum_{t=2}^{T} \left( (\zeta \log(t) + (c - 2) \log(\log(T)) - \log(M_\epsilon)) \log(t) + 1 \right) \frac{M_\epsilon}{t^c (\log(T))^{c-2}}$$

$$\leq 1 + \sum_{t=2}^{T} \left( 1 + (c - 2) \log(\log(T)) - \log(M_\epsilon) + 1 \right) \frac{M_\epsilon}{t^c (\log(T))^{c-4}}$$

$$\leq 1 + \sum_{t=2}^{T} \left( 2 + (c - 2) \log(\log(T)) \right) \frac{M_\epsilon}{t^c (\log(T))^{c-4}}$$

$$\leq 1 + \left( 2 + (c - 2) \log(\log(T)) \right) \frac{M_\epsilon}{(\log(T))^{c-4}} \sum_{t=1}^{T} \frac{1}{x^\xi} dx$$

$$\leq 1 + \left( 2 + (c - 2) \log(\log(T)) \right) \frac{M_\epsilon}{(\log(T))^{c-4}} \int_{1}^{T} \frac{1}{x^\xi} dx$$

$$\leq 1 + \left( 2 + (c - 2) \log(\log(T)) \right) \frac{M_\epsilon}{(\log(T))^{c-4}} \frac{T^{1-\zeta} - 1}{1 - \zeta}$$

$$\leq 1 + \frac{cM_\epsilon T^{1-\zeta}}{1 - \zeta}$$

for $c \geq 5$ and $T \geq e^c$.

**Step 2:** Consider $D_{1,2}$. Note that in this term, the optimal action 1 has been sufficiently drawn to be well estimated, so we can use a loose bound

$$\mathbb{E}[D_{1,1}] \leq \sum_{t=1}^{T} \mathbb{I} \{ \mu_1 - \beta_T > S_1(t) N_1(t) + 1, N_1(t) + 2 \geq (\log(T))^2 \}$$

This right-hand side has been studied in Theorem 1 in Kaufmann et al. (2012a), so we apply their results:

$$\mathbb{E}[D_{1,2}] \leq \frac{1}{T - 1}.$$

**Step 3:** Consider $D_2$. Using the same technique as in lemma 7 in Garivier & Cappé (2011), $D_2$ is bounded by

$$D_2 := \sum_{s=1}^{T} \mathbb{I} \{ s d^+(\hat{m}_2(t), \mu_1 - \beta_T) \leq \zeta \log(T) + c \log(\log(T)) + (\epsilon + \log(2)) T^\xi (\log(T))^{\xi} \}$$

For $\xi > 0$, we let

$$K_{T, \xi} = \frac{(1 + \xi) (\zeta \log(T) + c \log(\log(T)) + (\epsilon + \log(2)) T^\xi (\log(T))^{\xi})}{d(\mu_2, \mu_1)}.$$
Step 4: Combing the above results, we obtain that

\[
E[N_2(T)] \leq E[D_{1,1}] + E[D_{1,2}] + E[D_2] \\
\leq 1 + \frac{cM_\epsilon T^{1-\zeta}}{1 - \zeta} + \frac{1}{T - 1} + \frac{(1 + \xi)(\zeta \log(T) + c \log(\log(T)) + (\epsilon + \log(2))T^\zeta \log(T)\epsilon)}{d(\mu_2, \mu_1)} \\
+ \frac{(1 + \xi/2)^2}{\xi^2(\min\{\mu_2(1 - \mu_2), \mu_1(1 - \mu_1)\})^2} \\
\leq \frac{(1 + \xi)K_\epsilon}{d(\mu_2, \mu_1)} \max\{T^\zeta \log(T)\epsilon, cT^{1-\zeta} \frac{1}{1 - \zeta}\} + o_{\xi, c, \epsilon}(\max\{T^\zeta \log(T)\epsilon, cT^{1-\zeta} \frac{1}{1 - \zeta}\}).
\]

Proof of Lemma 3.12. We first notice that by Theorem 3.4 part b) (where \(P_1\) corresponds to \(Q_{t,j}\), we have

\[
g_j(t) = Qu(1 - \frac{1}{t^s(\log T)^c}, Q_{t-1,j}) \\
= Qu(1 - \frac{1}{t^s(\log T)^c} + \delta_{1-s} - \frac{1}{t^s(\log T)^c} \epsilon, \Pi_{t-1,j}) \\
\leq Qu(1 - \frac{1}{t^s(\log T)^c} - \frac{1}{t^s(\log T)^c} (M_\epsilon - 1), \Pi_{t-1,j}) \\
= Qu(1 - \frac{M_\epsilon}{t^s(\log T)^c}, \Pi_{t-1,j})
\]

since \(KL(\Pi_{t,j}, Q_{t,j}) \leq \epsilon\) and we have use the fact that \(Qu\) is non-decreasing. Now we apply the proof of Lemma 1 in
Kaufmann et al. (2012a), the tight bounds of the quantiles of the Beta distributions, to obtain

\[
Qu(1 - \frac{M_t}{\log T}^\epsilon, \Pi_{t-1,j}) \\
\geq \arg \max_{x > \frac{S_j(t)}{N_j(t) + 1}} \left\{ d \left( \frac{S_j(t)}{N_j(t) + 1}, x \right) \leq \log \left( \frac{1}{\frac{M_t}{\log T}^\epsilon (N_j(t)+2)} \right) N_j(t) + 1 \right\} \\
\geq \arg \max_{x > \frac{S_j(t)}{N_j(t) + 1}} \left\{ d \left( \frac{S_j(t)}{N_j(t) + 1}, x \right) \leq \zeta \log(t) + c \log(\log T) - \log(M_t) - \log(N_j(t)+2) \right\} N_j(t) + 1 \\
= u_j(t)
\]

Similarly, by Theorem 3.4 part a) (where \( P_t \) corresponds to \( Q_{t,j} \)), we have

\[
q_j(t) = Qu(1 - \frac{1}{\kappa(\log T)^\epsilon}, Q_{t-1,j}) \\
= Qu(1 - \frac{1}{\kappa(\log T)^\epsilon} + \delta_t - \frac{1}{\kappa(\log T)^\epsilon}, \Pi_{t-1,j}) \\
\leq Qu(1 - \frac{1}{\kappa(\log T)^\epsilon} + \frac{1}{\kappa(\log T)^\epsilon} \left( 1 - \exp(-\frac{\epsilon + \log(2)}{\kappa(\log T)^\epsilon}) \right), \Pi_{t-1,j}) \\
= Qu(1 - \frac{\exp(-\epsilon + \log(2))t^\epsilon(\log T)^\epsilon}{\kappa(\log T)^\epsilon}, \Pi_{t-1,j})
\]

since \( KL(Q_{t,j}, \Pi_{t,j}) \leq \epsilon \) and we have use the fact that \( Qu \) is non-decreasing. Now we apply the proof of Lemma 1 in Kaufmann et al. (2012a), the tight bounds of the quantiles of the Beta distributions, to obtain

\[
Qu(1 - \frac{1}{\kappa(\log T)^\epsilon} (1 - \exp(-\epsilon + \log(2))t^\epsilon(\log T)^\epsilon)) \\
\leq \arg \max_{x > \frac{S_j(t)}{N_j(t)+1}} \left\{ d \left( \frac{S_j(t)}{N_j(t) + 1}, x \right) \leq \log \left( \frac{1}{\frac{1}{\kappa(\log T)^\epsilon} (N_j(t)+1)^2} \right) N_j(t) \right\} \\
\leq \arg \max_{x > \frac{S_j(t)}{N_j(t)+1}} \left\{ d \left( \frac{S_j(t)}{N_j(t) + 1}, x \right) \leq \frac{\zeta \log(t) + c \log(\log T) + (\epsilon + \log(2))t^\epsilon(\log T)^\epsilon}{N_j(t)} \right\} N_j(t) \]

Therefore, we conclude that

\[
u_j(t) \leq q_j(t) \leq \nu_j(t).
\]
Proof of Lemma 3.13. We have that by definition,

\[ N_2(T) = \sum_{t=1}^{T} \mathbb{1}\{A_t = 2\} \]

\[ = \sum_{t=1}^{T} \mathbb{1}\{(\mu_1 - \beta_T > q_1(t)) \cap (A_t = 2)\} + \sum_{t=1}^{T} \mathbb{1}\{(\mu_1 - \beta_T \leq q_1(t)) \cap (A_t = 2)\} \]

\[ \leq \sum_{t=1}^{T} \mathbb{1}\{(\mu_1 - \beta_T > q_1(t))\} + \sum_{t=1}^{T} \mathbb{1}\{(\mu_1 - \beta_T \leq q_1(t)) \cap (A_t = 2)\} \]

\[ \leq \sum_{t=1}^{T} \mathbb{1}\{(\mu_1 - \beta_T > q_1(t))\} + \sum_{t=1}^{T} \mathbb{1}\{(\mu_1 - \beta_T \leq \bar{q}_2(t)) \cap (A_t = 2)\} \]

where the last inequality follows from the fact that \( q_1(t) \geq q_1(t) \) and when \( A_t = 2, q_1(t) \leq q_2(t) \leq \bar{q}_2(t) \).

\[ \square \]

C. Proofs of Results in Section 3.4

Proof of Theorem 3.15. First, we set

\[ q_{t,2} = \pi_{t,2} \]

Then we have \( KL(\Pi_{t,2}, Q_{t,2}) = 0 \) and \( q_{t,2} = \pi_{t,2} \) has the same support \((0, 1)\), satisfying Assumptions 3.1, 3.14 on action \( j = 2 \).

We set \( b_t = Q u(\frac{1}{2}, \Pi_{t,2}) \in (0, 1) \), the \( \frac{1}{2} \)-quantile of the distribution \( \Pi_{t,2} \) (or equivalently, \( Q_{t,2} \)). Let \( F_{t,1} \) be the cdf of \( \Pi_{t,1} \). We have \( F_{t,1}(b_t) \in (0, 1) \). For \( r > 1 \), we set

\[ q_{t,1}(x_1) = \begin{cases} 1 - \frac{1}{r}(1 - F_{t,1}(b_t)) \pi_{t,1}(x_1) & \text{if } 0 < x_1 < b_t \\ \frac{1}{r} \pi_{t,1}(x_1) & \text{if } b_t < x_1 \leq 1 \end{cases} \]

Step 1: We show that \( q_{t,1}(x_1) \) is indeed a density satisfying Assumption 3.6 on action \( j = 1 \). First of all, it is obvious that \( q_{t,1} > 0 \) on \((0, 1)\) as \( \pi_{t,1} > 0 \) on \((0, 1)\). Moreover

\[ \int_0^1 q_{t,1}(x_1) dx_1 = \int_0^{b_t} q_{t,1}(x_1) dx_1 + \int_{b_t}^1 q_{t,1}(x_1) dx_1 \]

\[ = \int_0^{b_t} \left( 1 - \frac{1}{r}(1 - F_{t,1}(b_t)) \right) \pi_{t,1}(x_1) dx_1 + \int_{b_t}^1 \frac{1}{r} \pi_{t,1}(x_1) dx_1 \]

\[ = \left( 1 - \frac{1}{r}(1 - F_{t,1}(b_t)) \right) F_{t,1}(b_t) + \frac{1}{r} \left( 1 - F_{t,1}(b_t) \right) \]

\[ = 1. \]

Step 2: We show that there exists a \( r > 1 \) (independent of \( t \)) such that \( q_{t,1} \) satisfies Assumption 3.14 on action \( j = 1 \).

We have that

\[ KL(\Pi_{t,1}, Q_{t,1}) = \int_0^{b_t} \pi_{t,1}(x_1) \log \left( \frac{\pi_{t,1}(x_1)}{q_{t,1}(x_1)} \right) dx_1 + \int_{b_t}^1 \pi_{t,1}(x_1) \log \left( \frac{\pi_{t,1}(x_1)}{q_{t,1}(x_1)} \right) dx_1 \]

\[ = \int_0^{b_t} \pi_{t,1}(x_1) \log \left( \frac{F_{t,1}(b_t)}{1 - \frac{1}{r}(1 - F_{t,1}(b_t))} \right) dx_1 + \int_{b_t}^1 \pi_{t,1}(x_1) \log (r) dx_1 \]

\[ = \log \left( \frac{F_{t,1}(b_t)}{1 - \frac{1}{r}(1 - F_{t,1}(b_t))} \right) F_{t,1}(b_t) + \log (r) \left( 1 - F_{t,1}(b_t) \right) \]

We note that

\[ \frac{F_{t,1}(b_t)}{1 - \frac{1}{r}(1 - F_{t,1}(b_t))} \leq \frac{r - 1 + F_{t,1}(b_t)}{1 - \frac{1}{r}(1 - F_{t,1}(b_t))} = r \]
as \( r > 1 \). Hence we have
\[
KL(\Pi_{t,1}, Q_{t,1}) \leq \log (r) F_{t,1}(b_t) + \log (r) (1 - F_{t,1}(b_t)) = \log (r).
\]

Then for \( 1 < r < e^\epsilon \), we have that
\[
KL(\Pi_{t,1}, Q_{t,1}) \leq \log (r) \leq \log (e^\epsilon) = \epsilon.
\]

Step 3: We show that the probability of sampling from \( Q_{t-1} \) choosing action 2 is greater than a positive constant \( \frac{1}{2} (1 - \frac{1}{r}) \), which thus leads to a linear regret.

In fact, the probability of sampling from \( Q_{t-1} \) choosing action 2 is given by \( \mathbb{P}_{Q_{t-1}}(x_2 \geq x_1) \). Therefore we have that
\[
\mathbb{P}_{Q_{t-1}}(x_2 \geq x_1) \geq \mathbb{P}_{Q_{t-1}}(x_2 \geq b_{t-1} \geq x_1) = \mathbb{P}_{Q_{t-1}}(x_2 \geq b_{t-1}) \mathbb{P}_{Q_{t-1}}(x_1 \leq b_{t-1})
\]

since \( Q_{t-1,1} \) and \( Q_{t-1,2} \) are independent.
\[
\mathbb{P}_{Q_{t-1,2}}(x_2 \geq b_{t-1}) = \frac{1}{2}
\]

since \( b_t \) is the \( \frac{1}{2} \)-quantile of the distribution \( \Pi_{t,2} \) and \( p_{t,2} > 0 \) on \( (0,1) \).

\[
\mathbb{P}_{Q_{t-1,1}}(x_1 \leq b_{t-1}) = 1 - \mathbb{P}_{Q_{t-1,1}}(x_1 > b_{t-1}) = 1 - \frac{1}{r} (1 - F_{t-1,1}(b_{t-1})) \geq 1 - \frac{1}{r}
\]

by our construction of \( Q_{t-1,1} \). Therefore we have that
\[
\mathbb{P}_{Q_{t-1}}(x_2 \geq x_1) \geq \frac{1}{2}(1 - \frac{1}{r}) > 0
\]

We conclude that the lower bound of the average expected regret is given by
\[
R(T, \mathcal{A}) = \sum_{j=1}^{2} (\mu_1 - \mu_j) \mathbb{E} [N_j(t)] \geq (\mu_1 - \mu_2) \frac{T}{2} (1 - \frac{1}{r}) = \Omega(T)
\]

leading to a linear regret. \( \square \)

Proof of Theorem 3.16. First, we set
\[
q_{t,1} = \pi_{t,1}.
\]

Then we have \( KL(\Pi_{t,1}, Q_{t,1}) = 0 \) and \( q_{t,1} = \pi_{t,1} \) has the same support \( (0,1) \), satisfying Assumptions 3.1, 3.14 on action \( j = 1 \).

We set \( b_t = Q\mu(\gamma_t, \Pi_{t,1}) \in (0,1) \), the \( \gamma_t \)-quantile of the distribution \( \Pi_{t,1} \) (or equivalently, \( Q_{t,1} \)). Let \( F_{t,2} \) be the cdf of \( \Pi_{t,2} \). We have \( F_{t,2}(b_t) \in (0,1) \). For \( r > 1 \), we set
\[
q_{t,2}(x_2) = \begin{cases} 
\frac{1}{r} \pi_{t,2}(x_2) & \text{if } 0 < x_1 < b_t \\
1 - \frac{1 - \frac{1}{r} F_{t,2}(b_t)}{1 - F_{t,2}(b_t)} \pi_{t,2}(x_2) & \text{if } b_t \leq x_1 < 1
\end{cases}
\]

Step 1: We show that \( q_{t,2}(x_2) \) is indeed a density satisfying Assumption 3.6 on action \( j = 2 \). First of all, it is obvious that \( q_{t,2} > 0 \) on \( (0,1) \) as \( \pi_{t,2} > 0 \) on \( (0,1) \). Moreover
\[
\int_0^{b_t} q_{t,2}(x_2) dx_2 = \int_0^{b_t} \frac{1}{r} \pi_{t,2}(x_2) dx_2 + \int_{b_t}^{1} 1 - \frac{1}{r} F_{t,2}(b_t) \pi_{t,2}(x_2) dx_2
\]
\[
= \int_0^{b_t} \frac{1}{r} \pi_{t,2}(x_2) dx_2 + \int_{b_t}^{1} 1 - \frac{1}{r} F_{t,2}(b_t) \pi_{t,2}(x_2) dx_2
\]
\[
= \frac{1}{r} F_{t,2}(b_t) + \frac{1 - \frac{1}{r} F_{t,2}(b_t)}{1 - F_{t,2}(b_t)} (1 - F_{t,2}(b_t))
\]
\[
= 1.
\]
Step 2: We show that when \( r = e^\epsilon \) (independent of \( t \)), then \( q_{t,2} \) satisfies Assumption 3.14 on action \( j = 2 \).

We have that
\[
KL(\Pi_{t,2}, Q_{t,2}) = \int_0^{b_2} \pi_{t,2}(x_2) \log \left( \frac{\pi_{t,2}(x_2)}{q_{t,2}(x_2)} \right) dx_2 + \int_{b_2}^1 \pi_{t,2}(x_2) \log \left( \frac{\pi_{t,2}(x_2)}{q_{t,2}(x_2)} \right) dx_2
\]
\[
= \int_0^{b_2} \pi_{t,2}(x_2) \log (r) dx_2 + \int_{b_2}^1 \pi_{t,2}(x_2) \log \left( \frac{1 - F_{t,2}(b_1)}{1 - F_{t,2}(b_1)} \right) dx_2
\]
\[
= \log (r) F_{t,2}(b_1) + \log \left( \frac{1 - F_{t,2}(b_1)}{1 - F_{t,2}(b_1)} \right) (1 - F_{t,2}(b_1))
\]

We note that
\[
\frac{1 - F_{t,2}(b_1)}{1 - F_{t,2}(b_1)} \leq \frac{r - F_{t,2}(b_1)}{1 - F_{t,2}(b_1)} = r
\]
as \( r > 1 \). Hence we have
\[
KL(\Pi_{t,2}, Q_{t,2}) \leq \log (r) F_{t,2}(b_1) + \log (r) (1 - F_{t,2}(b_1)) = \log (r).
\]

Then for \( r = e^\epsilon \), we have that
\[
KL(\Pi_{t,2}, Q_{t,2}) \leq \log (e^\epsilon) = \epsilon.
\]

Since \( \gamma_t \to 1 \) as \( t \to +\infty \), there exists a \( T_0 > 0 \) such that for any \( t \geq T_0 + 1 \), we have that \( \gamma_t > e^{-\epsilon} \).

Step 3: We show that the GBUCB algorithm always chooses action 2 when \( t \geq T_0 \), which thus leads to a linear regret.

We note that when \( t - 1 \geq T_0 - 1 \), by definition,
\[
P_{Q_{t-1,1}}(x_1 \leq b_{t-1}) = P_{\Pi_{t-1,1}}(x_1 \leq b_{t-1}) = \gamma_{t-1},
\]
\[
P_{Q_{t-1,2}}(x_2 \leq b_{t-1}) = \frac{1}{r} F_{t-2}(b_{t-1}) \leq \frac{1}{r} = e^{-\epsilon} < \gamma_{t-1},
\]
which implies that
\[
Q_{u}(\gamma_{t-1}, Q_{t-1,1}) = b_{t-1} < Q_{u}(\gamma_{t-1}, Q_{t-1,2})
\]
Therefore after time step \( t \geq T_0 \), the GBUCB algorithm will always choose the action 2. We conclude that the lower bound of the average expected regret is given by
\[
R(T, \mathcal{A}) = \sum_{j=1}^{2} (\mu_1 - \mu_j) \mathbb{E} [N_j(t)] \geq (\mu_1 - \mu_2)(T - T_0) = \Omega(T)
\]
leading to a linear regret.