Thompson Sampling with Approximate Inference

My Phan

College of Information and Computer Science University of Massachusetts Amherst, MA myphan@cs.umass.edu

Yasin Abbasi-Yadkori

VinAI Hanoi, Vietnam yasin.abbasi@gmail.com

Justin Domke

College of Information and Computer Science University of Massachusetts Amherst, MA domke@cs.umass.edu

Abstract

We study the effects of approximate inference on the performance of Thompson sampling in the k-armed bandit problems. Thompson sampling is a successful algorithm for online decision-making but requires posterior inference, which often must be approximated in practice. We show that even small constant inference error (in α -divergence) can lead to poor performance (linear regret) due to underexploration (for $\alpha<1$) or over-exploration (for $\alpha>0$) by the approximation. While for $\alpha>0$ this is unavoidable, for $\alpha\leq0$ the regret can be improved by adding a small amount of forced exploration even when the inference error is a large constant.

1 Introduction

The stochastic k-armed bandit problem is a sequential decision making problem where at each time-step t, a learning agent chooses an action (arm) among k possible actions and observes a random reward. Thompson sampling (Russo et al., 2018) is a popular approach in bandit problems based on sampling from a posterior in each round. It has been shown to have good performance both in term of frequentist regret and Bayesian regret for the k-armed bandit problem under certain conditions.

This paper investigates Thompson sampling when only an *approximate* posterior is available. This is motivated by the fact that in complex models, approximate inference methods such as Markov Chain Monte Carlo or Variational Inference must be used. Along this line, <u>Lu & Van Roy</u> (2017) propose a novel inference method – Ensemble sampling – and analyze its regret for linear contextual bandits. To the best of our knowledge this is the most closely related theoretical analysis of Thompson sampling with approximate inference.

This paper analyzes the regret of Thompson sampling with approximate inference. Rather than considering a particular inference algorithm, we parameterize the error using the α -divergence, a typical measure of inference accuracy. Our contributions are as follows:

• Even small inference errors can lead to linear regret with naive Thompson sampling. Given any error threshold $\epsilon > 0$ and any α we show that approximate posteriors with error at most ϵ in α -divergence at all times can result in linear regret (both frequentist and Bayesian). For $\alpha > 0$ and for any reasonable prior, we show linear regret due to over-exploration by the approximation (Theorem Γ , Corrolary Γ). For $\alpha < 1$ and for priors satisfying certain

conditions, we show linear regret due to under-exploration by the approximation, which prevents the posterior from concentrating (Theorem 2, Corrolary 2).

Forced exploration can restore sub-linear regret. For α ≤ 0 we show that adding forced exploration to Thompson sampling can make the posterior concentrate and restore sub-linear regret (Theorem 3) even when the error threshold is a very large constant. We illustrate this effect by showing that the performances of Ensemble sampling (Lu & Van Roy) 2017) and mean-field Variation Inference (Blei et al., 2017) can be improved in this way either theoretically (Section 5.1) or in simulations (Section 6).

2 Background and Notations.

2.1 The k-armed Bandit Problem.

We consider the k-armed bandit problem parameterized by the mean reward vector $m=(m_1,...,m_k)\in \mathcal{R}^k$, where m_i^* denotes the mean reward of arm (action) i. At each round t, the learner chooses an action A_t and observes the outcome Y_t which, conditioned on A_t , is independent of the history up to and not including time t, $H_{t-1}=(A_1,Y_1,...,A_{t-1},Y_{t-1})$. For a time horizon T, the goal of the algorithm π is to maximize the expected cumulative reward up to time T.

Let $\Omega \subseteq \mathcal{R}^k$ be the domain of the mean and $\Omega_i \subseteq \Omega$ denote the region where the *i*th arm has the largest mean. Let the function $A^*: \Omega \to \{a_1, ..., a_k\}$ denoting the best action be defined as: $A^*(m) = i$ if $m \in \Omega_i$.

In the frequentist setting we assume that there exists a true mean m^* which is fixed and unknown to the learner. Therefore, a policy π^* that always chooses $A^*(m^*)$ will get the highest reward. The performance of policy π is measured by its expected regret compared to an optimal policy π^* , which is defined as:

Regret
$$(T, \pi, m^*) = Tm^*_{A^*(m^*)} - \mathbb{E} \sum_{t=1}^{T} m^*_{A_t}$$
 (1)

On the other hand, in the Bayesian setting, an agent expresses her beliefs about the mean vector in terms of a prior Π_0 , and therefore, the mean is treated as a random variable $M=(M_1,...,M_k)$ distributed according to the prior Π_0 . The Bayesian regret is the expectation of the regret under the prior of parameter M:

BayesRegret
$$(T, \pi) = \mathbb{E}_{\Pi_0}$$
Regret (T, π, M) . (2)

2.2 Thompson Sampling with Approximate Inference

In the frequentist setting, in order to perform Thompson sampling we define a prior which is only used in the algorithm. On the other hand, in the Bayesian setting the prior is given.

Let Π_t be the posterior distribution of $M|H_{t-1}$ with density function $\pi_t(m)$. Thompson sampling obtains a sample \widehat{m} from Π_t and then selects arm A_t as follow: $A_t = i$ if $\widehat{m} \in \Omega_i$. In each round, we assume an approximate sampling method is available that generates sample from an approximate distribution Q_t . We use q_t to denote the density function of Q_t .

Popular approximate sampling methods include Markov Chain Monte Carlo (MCMC) (Andrieu et al., 2003), Sequential Monte Carlo (Doucet & Johansen, 2009) and Variational Inference (VI) (Blei et al., 2017). There are packages that conveniently implement VI and MCMC methods, such as Stan (Carpenter et al., 2017), Edward (Tran et al., 2016), PyMC (Salvatier et al., 2016) and infer.NET (Minka et al., 2018).

To provide a general analysis of approximate sampling methods, we will use the α -divergence (Section 2.3) to quantify the distance between the posterior Π_t and the approximation Q_t .

2.3 The Alpha Divergence

The α -divergence between two distributions P and Q with density functions p(x) and q(x) is defined as:

$$D_{\alpha}(P,Q) = \frac{1 - \int p(x)^{\alpha} q(x)^{1-\alpha} dx}{\alpha (1-\alpha)}.$$
 (3)

 α -divergence generalizes many divergences, including KL(Q,P) ($\alpha \to 0$), KL(P,Q) ($\alpha \to 1$), Hellinger distance ($\alpha = 0.5$) and χ^2 divergence ($\alpha = 2$) and is a common way to measure errors in inference methods. MCMC errors are measured by the Total Variation distance, which can be upper bounded by the KL divergence using Pinsker's inequality ($\alpha = 0$ or $\alpha = 1$). Variational Inference tries to minimize the reverse KL divergence (information projection) between the target distribution and the approximation ($\alpha = 0$). Ensemble sampling (Lu & Van Roy), [2017) provides error guarantees using reverse KL divergence ($\alpha = 0$). Expectation Propagation tries to minimize the KL divergence ($\alpha = 1$) and χ^2 Variational Inference tries to minimize the χ^2 divergence ($\alpha = 2$).

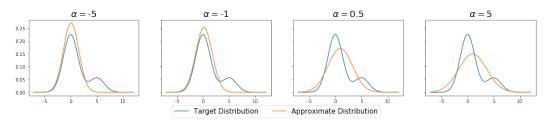


Figure 1: The Gaussian Q which minimizes $D_{\alpha}(P,Q)$ for different values of α where the target distribution P is a mixture of two Gaussians. Based on Figure 1 from (Minka, 2005)

When α is small, the approximation fits the posterior's dominant mode. When α is large, the approximation covers the posterior's entire support (Minka) 2005) as illustrated in Figure 1. Therefore changing α will affect the exploration-exploitation trade-off in bandit problems.

2.4 Problem Statement.

Problem Statement. For the k-armed bandit problem, given α and $\epsilon > 0$, if at all time-steps t we sample from an approximate distribution Q_t such that $D_{\alpha}(\Pi_t, Q_t) < \epsilon$, will the regret be sub-linear in t?

3 Motivating Example

In this section we present a simple example to show the effects of inference errors on the frequentist regret.

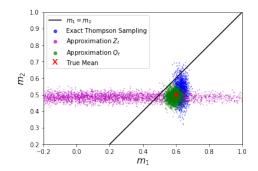
Example. Consider a 2-armed bandit problem where the reward distributions are Norm $(0.6, 0.2^2)$ and Norm $(0.5, 0.2^2)$ for arm 1 and 2 respectively. The prior Π_0 is Norm $(\mu_0^T, 0.5^2I)$ where $\mu_0 = [0.1, 0.9]$ is the vector of prior means of arm 1 and 2 respectively, and I denotes the identity matrix.

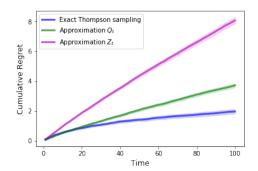
Let $\Pi_t = \operatorname{Norm}(\mu_t, \Sigma_t)$ be the posterior at time t. Approximations Q_t and Z_t are calculated such that $\operatorname{KL}(\Pi_t, Q_t) = 2$ and $\operatorname{KL}(Z_t, \Pi_t) = 1.5$ by multiplying the covariance Σ_t by a constant: $Q_t = \operatorname{Norm}(\mu_t, 4.5^2\Sigma_t)$ and $Z_t = \operatorname{Norm}(\mu_t, 0.3^2\Sigma_t)$. The KL divergence between two Gaussian distributions is provided in Appendix F

We perform the following simulations 1000 times and plot the mean cumulative regret up to time T = 100 in Figure 2b using three different policies:

- 1. (Exact Thompson Sampling) At each time-step t, sample from the true posterior Π_t .
- 2. (Approximation Q_t) At each time-step t, compute Q_t from Π_t and sample from Q_t .
- 3. (**Approximation** Z_t) At each time-step t, compute Z_t from Π_t and sample from Z_t .

The regrets of sampling from the approximations Q_t and Z_t are in both cases larger than that of exact Thompson sampling. Intuitively, the regret of Q_t is larger because Q_t explores more than the true





(a) Over-dispersed (approximation Q_t) and under-dispersed sampling (approximation Z_t) yield different posteriors after T=100 time-steps. m_1 and m_2 are the means of arms 1 and 2. Q_t picks arm 2 more often than exact Thompson sampling and Z_t mostly picks arm 2. The posteriors of exact Thompson sampling and Q_t concentrate mostly in the region where $m_1>m_2$ while Z_t 's spans both regions.

(b) The regret of sampling from the approximations Q_t and Z_t are both larger than that of exact Thompson sampling from the true posterior Π_t . Shaded regions show 95% confidence intervals.

Figure 2: Approximation Q_t (with high variance) and approximation Z_t (with small variance) are defined in Section 3 where $D_1(\Pi_t, Q_t) = 2$ and $D_0(\Pi_t, Z_t) = 1.5$. Arm 1 is the true best arm.

posterior (Figure 2a). In Section 4 we show that when $\alpha>0$ the approximation can incur this type of error, leading to linear regret. On the other hand, the regret of Z_t is larger because Z_t explores less than the exact Thompson sampling algorithm and therefore commits to the sub-optimal arm (Figure 2a). In Section 5 we show that when $\alpha<1$ the approximation can change the posterior concentration rate, leading to linear regret. We also show that adding a uniform sampling step can help the posterior to concentrate when $\alpha\leq0$, and make the regret sub-linear.

4 Regret Analysis When $\alpha > 0$

In this section we analyze the regret when $\alpha > 0$. Our result shows that the approximate method might pick the sub-optimal arm with constant probability in every time-step, leading to linear regret.

Theorem 1 (Frequentist Regret). Let $\alpha > 0$, the number of arms be k = 2 and $m_1^* > m_2^*$. Let Π_0 be a prior where $\mathbb{P}_{\Pi_0}(M_2 > M_1) > 0$. For any error threshold $\epsilon > 0$, there is a deterministic mapping $f(\Pi)$ such that for all $t \geq 0$:

- 1. Sampling from $Q_t = f(\Pi_t)$ chooses arm 2 with a constant probability.
- 2. $D_{\alpha}(\Pi_t, Q_t) < \epsilon$.

Therefore sampling from Q_t for T/10 time-steps and using any policy for the remaining time-steps will cause linear frequentist regret.

Typically, approximate inference methods minimize divergences. Broadly speaking, this theorem shows that making a divergence a small constant, alone, is not enough to guarantee sub-linear regret. We do not mean to imply that low regret is *impossible* but simply that making an α -divergence a small constant alone is not sufficient.

At every time-step, the mapping f constructs the approximation Q_t from the posterior Π_t by moving probability mass from the region Ω_1 where $m_1 > m_2$ to the region Ω_2 where $m_2 > m_1$. Then Q_t will choose arm 2 with a constant probability at every time-step. The constant average regret per time-step is discussed in Appendix A.

Therefore, if we sample from $Q_t = f(\Pi_t)$ for 0.1T time steps and use any policy in the remaining 0.9T time steps, we will still incur linear regret from the 0.1T time-steps. On the other hand, when $\alpha \leq 0$, we show in Section [5.1] that sampling an arm uniformly at random for $\log T$ time-steps and sampling from an approximate distribution that satisfies the divergence constraint for $T - \log T$ time-steps will result in sub-linear regret.

Agrawal & Goyal (2013) show that the frequentist regret of exact Thompson sampling is $O(\sqrt{T})$ with Gaussian or Beta priors and bounded rewards. Theorem [1] implies that when the assumptions in (Agrawal & Goyal, 2013) are satisfied but there is a small constant inference error at every time-step, the regret is no longer guaranteed to be sub-linear.

If the assumption $m_1^* > m_2^*$ in Theorem 1 is satisfied with a non-zero probability $(\mathbb{P}_{\Pi_0}(M_1 > M_2) > 0)$, the Bayesian regret will also be linear:

Corollary 1 (Bayesian Regret). Let $\alpha > 0$ and the number of arms be k = 2. Let Π_0 be a prior where $\mathbb{P}_{\Pi_0}(M_1 > M_2) > 0$ and $\mathbb{P}_{\Pi_0}(M_2 > M_1) > 0$. Then for any error threshold $\epsilon > 0$, there is a deterministic mapping $f(\Pi)$ such that for all $t \geq 0$ the two statements in Theorem |I| hold.

Therefore sampling from Q_t for T/10 time-steps and using any policy for the remaining time-steps will cause linear Bayesian regret.

Russo & Roy (2016) prove that the Bayesian regret of Thompson sampling for k-armed bandits with sub-Gaussian rewards is $O(\sqrt{T})$. Corollary 1 implies that even when the assumptions in Russo & Roy (2016) are satisfied, under certain conditions and with approximation errors, the regret is no longer guaranteed to be sub-linear.

5 Regret Analysis When $\alpha < 1$

In this section we analyze the regret when $\alpha < 1$. Our result shows that for any error threshold, if the posterior Π_t places too much probability mass on the wrong arm then the approximation Q_t is allowed to avoid the optimal arm. If the sub-optimal arms do not provide information about the arms' ranking, the posterior Π_{t+1} does not concentrate. Therefore Q_{t+1} is also allowed to be close in α -divergence while avoiding the optimal arm, leading to linear regret in the long term.

Theorem 2 (Frequentist Regret). Let $\alpha < 1$, the number of arms be k = 2 and $m_1^* > m_2^*$. Let Π_0 be a prior where M_2 and $M_1 - M_2$ are independent. There is a deterministic mapping $f(\Pi)$ such that for all t > 0:

- 1. Sampling from $Q_t = f(\Pi_t)$ chooses arm 2 with probability 1.
- 2. For any $\epsilon > 0$, there exists $0 < z \le 1$ such that if $\mathbb{P}_{\Pi_0}(M_2 > M_1) = z$ and arm 2 is chosen at all times before t then $D_{\alpha}(\Pi_t, Q_t) < \epsilon$. For any $0 < z \le 1$, there exists $\epsilon > 0$ such that if $\mathbb{P}_{\Pi_0}(M_2 > M_1) = z$ and arm 2 is chosen at all times before t then $D_{\alpha}(\Pi_t, Q_t) < \epsilon$.

Therefore sampling from Q_t at all time-steps results in linear frequentist regret.

We discuss why the above results are not immediately obvious. When $\alpha \to 0$, the α -divergence becomes $\mathrm{KL}(Q_t,\Pi_t)$. We might believe that the regret should be sub-linear in this case because the posterior Π_t becomes more concentrated, and so the total variation between Q_t and Π_t must decrease. For example, Ordentlich & Weinberger (2004) show the distribution-dependent Pinsker's inequality between $\mathrm{KL}(Q,P)$ and the total variation $\mathrm{TV}(P,Q)$ for discrete distributions P and Q as follows:

$$KL(Q, P) > \phi(P) \cdot TV(P, Q)^2$$
 (4)

Here, $\phi(P)$ is a quantity that will increase to infinity if P becomes more concentrated. However, the algorithm in Theorem 2 constructs an approximation distribution that never picks the optimal arm, so the posterior Π_t can not concentrate and the regret is linear. The error threshold ϵ causing linear frequentist regret is correlated with the probability mass the prior places on the true best arm (Appendix B.4).

With some assumptions on the rewards, Gopalan et al. (2014) show that the problem-dependent frequentist regret is $O(\log T)$ for finitely-supported, correlated priors with $\pi_0(m^*)>0$. Liu & Li (2016) study the prior-dependent frequentist regret of 2-armed-and-2-models bandits, and show that with some smoothness assumptions on the reward likelihoods, the regret is $O(\sqrt{T/\mathbb{P}_{\Pi_0}(M_2>M_1)})$ if arm 1 is the better arm. Theorem 2 implies that when the assumptions in (Gopalan et al.) 2014) or (Liu & Li) (2016) are satisfied, if M_2 and M_1-M_2 are independent and there are approximation errors, the regret is no longer guaranteed to be sub-linear.

If the assumption $m_1^* > m_2^*$ in Theorem 2 is satisfied with a non-zero probability $(\mathbb{P}_{\Pi_0}(M_1 > M_2) > 0)$, the Bayesian regret wil also be linear:

Corollary 2 (Bayesian Regret). Let $\alpha < 1$ and the number of arms be k = 2. Let Π_0 be a prior where $\mathbb{P}_{\Pi_0}(M_1 > M_2) > 0$ and M_2 and $M_1 - M_2$ are independent. There is a deterministic mapping $f(\Pi)$ such that for all $t \geq 0$ the 2 statements in Theorem 2 hold.

Therefore sampling from Q_t at all time-steps results in linear Bayesian regret.

Russo & Roy (2016) prove that the Bayesian regret of Thompson sampling for k-armed bandits with sub-Gaussian rewards is $O(\sqrt{T})$. Corollary 2 implies that even when the assumptions in Russo & Roy (2016) are satisfied, under certain conditions and with approximation errors, the regret is no longer guaranteed to be sub-linear.

We note that, unlike the case when $\alpha > 0$, if we use another policy in o(T) time-steps to make the posterior concentrate and sample from Q_t for the remaining time-steps, the regret can be sub-linear. We provide a concrete algorithm in Section [5.1] for the case when $\alpha \leq 0$.

5.1 Algorithms with Sub-linear Regret for $\alpha \leq 0$

In the previous section, we see that when $\alpha < 1$, the approximation has linear regret because the posterior does not concentrate. In this section we show that when $\alpha \leq 0$, it is possible to achieve sub-linear regret even when ϵ is a very large constant by adding a simple exploration step to force the posterior to concentrate (the case of $\alpha > 0$ cannot be improved according to Theorem 1). We first look at the necessary and sufficient condition that will make the posterior concentrate, and then provide an algorithm that satisfies it. Russo (2016) and Qin et al. (2017) both show the following result under different assumptions:

Lemma 1 (Lemma 14 from Russo (2016)). Let $m^* \in \mathcal{R}^k$ be the true parameter and let $a^* = A^*(m^*)$ be the true best arm. If for all arms i, $\sum_{t=1}^{\infty} P(A_t = i | H_{t-1}) = \infty$, then

$$\lim_{t \to \infty} P(A^*(M) = a^* | H_{t-1}) = 1 \text{ with probability } 1.$$
 (5)

If there exists arm i such that $\sum_{t=1}^{\infty} P(A_t = i|H_{t-1}) < \infty$, then $\liminf_{t\to\infty} P(A^*(M) = i|H_{t-1}) > 0$ with probability 1.

Russo (2016) make the following assumptions, which allow correlated priors:

Assumption 1. Let the reward distributions be in the canonical one dimensional exponential family with the density: $p(y|m) = b(y) \exp(mT(y) - A(m))$ where b, T and A are known function and A(m) is assumed to be twice differentiable. The parameter space $\Omega = (\overline{m}, \underline{m})$ is a bounded open hyper-rectangle, the prior density is uniformly bounded with $0 < \inf_{m \in \Omega} \pi_0(m) < \sup_{m \in \Omega} \pi_0(m) < \infty$ and the log-partition function has bounded first derivative with $\sup_{\theta \in [\overline{m}, \underline{m}]} |A'(m)| < \infty$.

Qin et al. (2017) make the following assumptions:

Assumption 2. Let the prior be an uncorrelated multivariate Gaussian. Let the reward distribution of arm i be $Norm(m_i, \sigma^2)$ with a common known variance σ^2 but unknown mean m_i .

Even though we consider the error in sampling from the posterior distribution, the regret is a result of choosing the wrong arm. We define $\overline{\Pi}_t$ as the posterior distribution of the best arm and \overline{Q}_t as the approximation of $\overline{\Pi}_t$ with the density functions

$$\overline{\pi}_t(i) = P(A^* = i | H_{t-1}) \text{ and } \overline{q}_t(i) = P(A_t = i | H_{t-1}).$$

We now define an algorithm where each arm will be chosen infinitely often, satisfying the condition of Lemma []

Theorem 3 (Bayesian and Frequentist Regret). Consider the case when Assumption $\boxed{1}$ or $\boxed{2}$ is satisfied. Let $\alpha \leq 0$ and $p_t = o(1)$ be such that $\sum_{t=1}^{\infty} p_t = \infty$. For any number of arms k, any prior Π_0 and any error threshold $\epsilon > 0$, the following algorithm has o(T) frequentist regret: at every time-step t,

- with probability $1-p_t$, sample from an approximate posterior Q_t such that $D_{\alpha}(\overline{\Pi}_t, \overline{Q}_t) < \epsilon$,
- with probability p_t , sample an arm uniformly at random.

Since the Bayesian regret is the expectation of the frequentist regret over the prior, for any prior if the frequentist regret is sub-linear at all points the Bayesian regret will be sub-linear.

The following lemma shows that the error in choosing the arms is upper bounded by the error in choosing the parameters. Therefore whenever the condition $D_{\alpha}(\Pi_t, Q_t) < \epsilon$ is satisfied, the condition $D_{\alpha}(\overline{\Pi}_t, \overline{Q}_t) < \epsilon$ will be satisfied and Theorem 3 is applicable.

Lemma 2.

$$D_{\alpha}(\overline{\Pi}_t, \overline{Q}_t) \leq D_{\alpha}(\Pi_t, Q_t)$$
.

We also note that we can achieve sub-linear regret even when ϵ is a very large constant. We revisit Eq. $\boxed{4}$ to provide the intuition: $\mathrm{KL}(Q,P) \geq \phi(P) \cdot \mathrm{TV}(P,Q)^2$. Here, $\phi(P)$ is a quatity that will increase to infinity if P becomes more concentrated. Hence, if $KL(\overline{Q}_t,\overline{\Pi}_t) < \epsilon$ for any constant ϵ and $\overline{\Pi}_t$ becomes concentrated, the total variation $\mathrm{TV}(\overline{Q}_t,\overline{\Pi}_t)$ will decrease. Therefore, \overline{Q}_t will become concentrated, resulting in sub-linear regret.

Application. Lu & Van Roy (2017) propose an approximate sampling method called Ensemble sampling where they maintain a set of $\mathcal M$ models to approximate the posterior and analyze its regret for the linear contextual bandits when $\mathcal M$ is $\Omega(\log(T))$. For the k-armed bandit problem and when $\mathcal M$ is $\Theta(\log(T))$, Ensemble sampling satisfies the condition $\mathrm{KL}(\overline{Q}_t,\overline{\Pi}_t)<\epsilon$ in Theorem 3 with high probability. In this case, Lu & Van Roy (2017) show a regret bound that scales linearly with T. We discuss in Appendix E how to apply Theorem 3 to get sub-linear regret with Ensemble sampling when $\mathcal M$ is $\Theta(\log(T))$.

6 Simulations

For each approximation method we repeat the following simulations for 1000 times and plot the mean cumulative regret, using five different policies.

- 1. (**Exact Thompson sampling**) Use exact posterior sampling to choose an action and update the posterior (for reference).
- 2. (**Approximation method**) Use the approximation method to choose an action and update the posterior. We use the approximation naively without any modification.
- 3. (**Forced Exploration**) With a probability (the exploration rate), choose an action uniformly at random and update the posterior. Otherwise, use the approximation method to choose an action and update the posterior. This is the method suggested by Thm. 3.
- 4. (**Approximate Sample**) Use the approximation method to choose an action. Use exact posterior sampling to update the posterior.
- (Approximate Update) Use exact posterior sampling to choose an action. Use the approximate method to update the posterior.

The last two policies are performed to understand how the approximation affects the posterior (discussed in Section 6.3). We update the posterior using the closed-form formula when both the prior and reward distribution are Gaussian in Appendix 6.

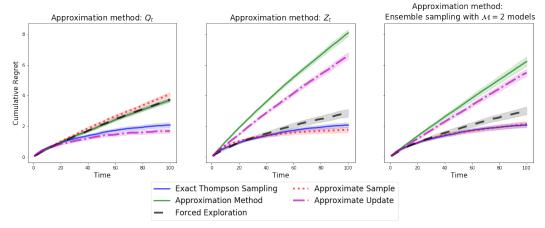
6.1 Adding Forced Exploration to the Motivating Example

In this section we revisit the example in Section 3. We apply Q_t, Z_t and Ensemble sampling with $\mathcal{M}=2$ models to the bandit problem described in the example. We set the exploration rate at time t to be 1/t, T=100 and show the results in Figure 3a and discuss them in Section 6.3.

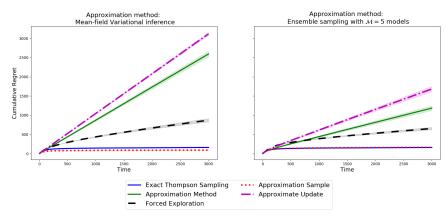
6.2 Simulations of Ensemble Sampling and Variational Inference for 50-armed bandits

Now we add forced exploration to mean-field Variational Inference (VI) and Ensemble Sampling with $\mathcal{M}=5$ models for a 50-armed bandit instance. We generate the prior and the reward distribution as follows: the prior is $\mathrm{Norm}(\mathbf{0},\Sigma_0)$. To generate a positive semi-definite matrix Σ_0 , we generate a random matrix A of size (k,k) where entries are uniformly sampled from [0,1) and set $\Sigma_0=A^TA/k$. The true mean m^* is sampled from the prior. The reward distribution of arm i is $\mathrm{Norm}(m_i^*,1)$.

Mean-field VI approximates the posterior by finding an uncorrelated multivariate Gaussian distribution Q_t that minimizes $KL(\Pi_t,Q_t)$. If the posterior is $\Pi_t=\operatorname{Norm}(\mu_t,\Sigma_t)$ then Q_t has the closed-form solution $Q_t=\operatorname{Norm}(\mu_t,\operatorname{Diag}(\Sigma_t^{-1})^{-1})$, which we used to perform the simulations. We set the exploration rate at time t to be 50/t, T=3000, show the results in Figure $3\overline{b}$ and discuss them in Section 6.3



(a) Applying approximations Q_t, Z_t and Ensemble Sampling to the motivating example (Section 6.1).



(b) Applying mean-field Variational Inference (VI) and Ensemble sampling on a 50-armed bandit (Section 6.2).

Figure 3: Updating the posterior by exact Thompson sampling or adding forced exploration does not help the over-explored approximation Q_t , but lowers the regrets of the under-explored approximations Z_t , Ensemble sampling and mean-field VI. Shaded regions show 95% confidence intervals.

6.3 Discussion

We observe in Figure 3a that the regret of Q_t calculated from the posterior updated by exact Thompson sampling does not change significantly. Moreover, exact posterior sampling with the posterior updated by Q_t has the same regret as exact Thompson sampling. These two observations imply that Q_t has the same effect on the posterior as exact Thompson sampling. Therefore adding forced exploration is not helpful.

On the other hand, in Figures 3a and 3b the regrets of Z_t , Ensemble sampling and mean-field VI calculated from the posterior updated by exact Thompson sampling decrease significantly. Moreover, exact posterior sampling with the posterior updated by the approximations has similar regret to using the approximations. This behaviour is likely because the approximation causes the posterior to concentrate in the wrong region I In combination, these two observations suggest that these methods do not explore enough for the posterior to concentrate. Therefore adding forced exploration is helpful, which is compatible with the result in Theorem 3

¹Note that in the case where there are 2 arms (Figure 3a), exact posterior sampling with the posterior updated by the approximate method has slightly lower regret than naively using the approximate method. This is only because there are only 2 regions, so exact posterior sampling explores more than the approximation in the other region, which happens to be the correct one.

7 Related Work

There have been many works on sub-linear Bayesian and frequentist regrets for exact Thompson sampling. We discussed relevant works in detail in Section 4 and Section 5.

Ensemble sampling (Lu & Van Roy) 2017) gives a theoretical analysis of Thompson sampling with one particular approximate inference method. Lu & Van Roy (2017) maintain a set of $\mathcal M$ models to approximate the posterior, and analyzed its regret for linear contextual bandits when $\mathcal M$ is $\Omega(\log(T))$. For the k-armed bandit problem and when $\mathcal M$ is $\Theta(\log(T))$, Ensemble sampling satisfies the condition $\mathrm{KL}(\overline{Q}_t,\overline{\Pi}_t)<\epsilon$ in Theorem 3 with high probability. In this case, the regret of Ensemble sampling scales linearly with T.

We show in Theorem 2 that when the constraint $\mathrm{KL}(Q_t,\Pi_t)<\epsilon$ is satisfied, which implies by Lemma 2 that $\mathrm{KL}(\overline{Q}_t,\Pi_t)<\epsilon$ is satisfied, there can exist approximation algorithms that have linear regret in T. This result provides a linear lower bound, which is complementary with the linear regret upper bound of Ensemble Sampling in ($\mathbb{L}u$ & $\mathbb{V}u$ Roy), $\mathbb{Z}u$ Moreover, we show in Appendix $\mathbb{E}u$ that we can apply Theorem $\mathbb{Z}u$ to get sub-linear regret with Ensemble sampling with $\Theta(\log(T))$ models.

In reinforcement learning, there is a notion that certain approximations are "stochastically optimistic" and that this has implications for regret (Osband et al., 2016). This is similar in spirit to our analysis in terms of α -divergence, in that the characteristics of inference errors are important.

There has been a number of empirical works using approximate methods to perform Thompson sampling. Riquelme et al. (2018) implement variational inference, MCMC, Gaussian processes and other methods on synthetic and real world data sets and measure the regret. Urteaga & Wiggins (2018) derive a variational method for contextual bandits. Kawale et al. (2015) use particle filtering to implement Thompson sampling for matrix factorization.

Finally, if exact inference is not possible, it remains an open question if it is better to use Thompson sampling with approximate inference, or to use a different bandit method that does not require inference with respect to the posterior. For example Kveton et al. (2019) propose an algorithm based on the bootstrap.

8 Conclusion

In this paper we analyzed the performance of approximate Thompson sampling when at each timestep t, the algorithm obtains a sample from an approximate distribution Q_t such that the α -divergence between the true posterior and Q_t remains at most a constant ϵ at all time-steps.

Our results have the following implications. To achieve a sub-linear regret, we can only use $\alpha > 0$ for o(T) time-steps. Therefore we should use $\alpha \leq 0$ with forced exploration to make the posterior concentrate. This method theoretically guarantees a sub-linear regret even when ϵ is a large constant.

Acknowledgments

We thank Huy Le for providing the proof of Lemma 9.

References

Agrawal, S. and Goyal, N. Further optimal regret bounds for Thompson sampling. In *Proceedings of the Sixteenth International Conference on Artificial Intelligence and Statistics (AISTATS 2013)*, volume 31 of *Proceedings of Machine Learning Research*, pp. 99–107. PMLR, 2013.

Andrieu, C., de Freitas, N., Doucet, A., and Jordan, M. I. An introduction to MCMC for machine learning. *Machine Learning*, 50(1):5–43, 2003. ISSN 1573-0565. doi: 10.1023/A:1020281327116.

Blei, D. M., Kucukelbir, A., and McAuliffe, J. D. Variational inference: A review for statisticians. *Journal of the American Statistical Association*, 112(518):859–877, 2017. doi: 10.1080/01621459. 2017.1285773.

Carpenter, B., Gelman, A., Hoffman, M., Lee, D., Goodrich, B., Betancourt, M., Brubaker, M., Guo, J., Li, P., and Riddell, A. Stan: A probabilistic programming language. *Journal of Statistical Software*, 76(1), 2017.

- Cichocki, A. and Amari, S. Families of alpha- beta- and gamma- divergences: Flexible and robust measures of similarities. *Entropy*, 12:1532–1568, 2010.
- Doucet, A. and Johansen, A. A tutorial on particle filtering and smoothing: Fifteen years later. *Handbook of Nonlinear Filtering*, 12:656–704, 2009.
- Gopalan, A., Mannor, S., and Mansour, Y. Thompson sampling for complex online problems. In *Proceedings of the 31st International Conference on Machine Learning*, volume 32 of *Proceedings of Machine Learning Research*, pp. 100–108, Bejing, China, 22–24 Jun 2014. PMLR.
- Kawale, J., Bui, H. H., Kveton, B., Tran-Thanh, L., and Chawla, S. Efficient Thompson sampling for online matrix-factorization recommendation. In *Advances in Neural Information Processing Systems* 28 (NIPS 2015), pp. 1297–1305. Curran Associates, Inc., 2015.
- Kveton, B., Szepesvari, C., Vaswani, S., Wen, Z., Lattimore, T., and Ghavamzadeh, M. Garbage in, reward out: Bootstrapping exploration in multi-armed bandits. In *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pp. 3601–3610, Long Beach, California, USA, 09–15 Jun 2019. PMLR.
- Liu, C.-Y. and Li, L. On the prior sensitivity of thompson sampling. In *Algorithmic Learning Theory*, pp. 321–336, Cham, 2016. Springer International Publishing. ISBN 978-3-319-46379-7.
- Lu, X. and Van Roy, B. Ensemble sampling. In *Advances in Neural Information Processing Systems* 30 (NIPS 2017), pp. 3260–3268. Curran Associates, Inc., 2017.
- Minka, T. Divergence measures and message passing. Technical Report MSR-TR-2005-173, January 2005.
- Minka, T., Winn, J., Guiver, J., Zaykov, Y., Fabian, D., and Bronskill, J. /Infer.NET 0.3, 2018. Microsoft Research Cambridge. http://dotnet.github.io/infer.
- Ordentlich, E. and Weinberger, M. J. A distribution dependent refinement of Pinsker's inequality. *International Symposium on Information Theory*, 2004. *ISIT* 2004. *Proceedings*., pp. 29–, 2004.
- Osband, I., Van Roy, B., and Wen, Z. Generalization and exploration via randomized value functions. In Proceedings of the 33rd International Conference on International Conference on Machine Learning - Volume 48, ICML'16, pp. 2377–2386. JMLR.org, 2016.
- Qin, C., Klabjan, D., and Russo, D. Improving the expected improvement algorithm. In *Advances in Neural Information Processing Systems 30*, pp. 5381–5391. Curran Associates, Inc., 2017.
- Riquelme, C., Tucker, G., and Snoek, J. Deep Bayesian bandits showdown: An empirical comparison of bayesian deep networks for thompson sampling. In *International Conference on Learning Representations (ICLR 2018)*, 2018.
- Russo, D. Simple Bayesian algorithms for best arm identification. In 29th Annual Conference on Learning Theory (COLT 2016), volume 49 of Proceedings of Machine Learning Research, pp. 1417–1418. PMLR, 2016.
- Russo, D. and Roy, B. V. An information-theoretic analysis of Thompson sampling. *Journal of Machine Learning Research*, 17(68):1–30, 2016.
- Russo, D. J., Roy, B. V., Kazerouni, A., Osband, I., and Wen, Z. A tutorial on Thompson sampling. *Foundations and Trends*® *in Machine Learning*, 11(1):1–96, 2018. ISSN 1935-8237. doi: 10.1561/2200000070.
- Salvatier, J., Wiecki, T. V., and Fonnesbeck, C. Probabilistic programming in Python using PyMC3. *PeerJ Computer Science*, 2:e55, 2016.
- Tran, D., Kucukelbir, A., Dieng, A. B., Rudolph, M., Liang, D., and Blei, D. M. Edward: A library for probabilistic modeling, inference, and criticism. *arXiv preprint arXiv:1610.09787*, 2016.
- Urteaga, I. and Wiggins, C. Variational inference for the multi-armed contextual bandit. In *Proceedings of the Twenty-First International Conference on Artificial Intelligence and Statistics (AISTATS 2018)*, volume 84 of *Proceedings of Machine Learning Research*, pp. 698–706. PMLR, 2018.