Thompson Sampling via Local Uncertainty

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Abstract

Thompson sampling is an efficient algorithm for sequential decision making, which exploits the posterior uncertainty to solve the exploration-exploitation dilemma. There has been significant recent interest in integrating Bayesian neural networks into Thompson sampling. Most of these methods rely on global variable uncertainty for exploration. In this paper, we propose a new probabilistic modeling framework for Thompson sampling, where local latent variable uncertainty is used to sample the mean reward. Variational inference is used to approximate the posterior of the local variable, and semi-implicit structure is further introduced to enhance its expressiveness. Our experimental results on eight contextual bandits benchmark datasets show that Thompson sampling guided by local uncertainty achieves state-of-the-art performance while having low computational complexity.

1 Introduction

There has been significant recent interest in employing deep neural networks to better solve sequential decision-making problems, such as these in reinforcement learning (Mnih et al., 2013, 2015, 2016; Arulkumaran et al., 2017; François-Lavet et al., 2018) and contextual bandits (Riquelme et al., 2018; Russo et al., 2018). In a typical setting, by sequentially interacting with the environment, the agent or algorithm needs to learn how to take a sequence of decisions in order to maximize the expected cumulative reward. Using a deep neural network

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as a powerful function approximator, whose task is to learn the mapping from an observed contextual feature vector to the hidden reward distributions, has become a common practice. Since the model training and data collection usually happen at the same time, the model needs to not only accurately approximate the distribution of the observed data, but also gain enough flexibility to predict that of the future data.

Addressing the exploration-exploitation dilemma has always been a vital part of sequential decision making. More specifically, to maximize the expected cumulative reward, the agent needs to balance its effort in exploration, which chooses actions that may potentially increase its understanding of the environment, and its effort in exploitation, which takes the action that is expected to be the best given existing information. Typically, under-exploitation will possibly trap the agent at a bad local optimal solution, while over-exploitation could lead to a significant exploration cost. Various strategies have been proposed to tackle the exploration-exploitation dilemma, such as ε-greedy (Sutton & Barto, 1998), upper-confidence bound (Auer, 2002), Boltzmann exploration (Cesa-Bianchi et al., 2017; Sutton & Barto, 1998), and Thompson sampling (Thompson, 1933). More recently, carefully adding random noise to model parameters (Plappert et al., 2017; Fortunato et al., 2017; Gal & Ghahramani, 2016) or bootstrap sampling (Osband et al., 2016) before decision making also provide effective ways to encourage exploration.

Thompson sampling (TS) (Thompson, 1933), an elegant and widely used exploration strategy, is known for both its simplicity and good practical performance (Chapelle & Li, 2011; Agrawal & Goyal, 2012, 2013; Russo et al., 2018). TS will keep updating the posteriors of the parameters of the hidden reward distributions, and take actions according to the posterior predictive distributions of the rewards. Relying on posterior uncertainty to do exploration is the promising point of TS. Unfortunately, the exact posteriors are tractable for only a few models with limited representation power. Therefore, significant effort has been dedicated to posterior approximation. A recent development along this direction is empowering TS with Bayesian neural networks (Hinton & Van Camp, 1993; Bishop, 2006; Graves, 2011; Neal, 2012; Hernández-Lobato & Adams, 2015), and relying on the posteriors of the neural network weights to perform exploration under the TS framework (Riquelme et al., 2018).

Various inference methods have been employed to capture the uncertainty of the neural network weights, including Bayes by backprop (BBB) (Blundell et al., 2015), stochastic gradient Markov chain Monte Carlo (MCMC) (Welling & Teh, 2011; Li et al., 2016; Mandt et al., 2016), point estimate combined with random sampling (Riquelme et al., 2018), and interactive particles based approximation (Zhang et al., 2019). All these methods are focused on modeling the uncertainty of the global variables (i.e., weights of the deep neural network).
to maintain flexible approximation to the posterior predictive distributions.

In this paper, differing from all aforementioned methods, we propose to sample from a local latent variable distribution to model the uncertainty of the mean rewards of actions given the contextual input. More specifically, our framework uses a latent variable model to model the reward distribution given a contextual input, and encodes this input to approximate the posterior distribution of the local latent variable given both the context, which has already been observed, and reward, which is yet to be observed. To further improve the expressiveness of the latent distribution, we introduce a semi-implicit variational distribution structure into the framework. We test our framework on contextual bandits, a classical task in sequential decision making, to verify its effectiveness. Experimental results show that the proposed local uncertainty guided TS algorithms achieve state-of-the-art performance, while having low computational complexity.

2 Preliminaries

Below we briefly review contextual bandits and TS.

2.1 Contextual Bandits

In a contextual bandit problem, we denote $x \in \mathbb{R}^d$ as the $d$ dimensional context (state) given by the environment, $a \in A = \{1, \ldots, C\}$ as the action in a finite discrete space of size $C$, and $r \in \mathbb{R}$ as the scalar reward. Commonly, the agent will interact with the environment sequentially for $T$ times. At each time $t = 1, \ldots, T$, the agent observes a new context $x_t$, chooses action $a_t \in A$ based on the information provided by $x_t$, and receives reward $r_t$ provided by the environment. The reward $r_t$ can be a deterministic mapping $r_t = f(x_t, a_t)$ or a more complicated stochastic mapping $r_t = f(x_t, a_t, \epsilon_t)$, where $\epsilon_t$ represents random noise. The interactions $(x_t, a_t, r_t)$ at different times are independent from each other. The objective of the agent is to maximize the expected cumulative reward $\mathbb{E}[\sum_{t=1}^{T} r_t]$, or equivalently to minimize the expected cumulative regret as

$$\text{CR}(T) = \sum_{t=1}^{T} \mathbb{E} \left[ \max_{a_t \in A} \mathbb{E}[r(x_t, a_t)] - r_t \right].$$  \hspace{1cm} (1)

Since $x_t$ is randomly drawn from the environment, the optimal cumulative reward as $\sum_{t=1}^{T} \mathbb{E}[\max_{a_t \in A} \mathbb{E}[r(x_t, a_t)]]$ will also be random. The cumulative regret $\text{CR}(T)$, which can be used to measure the distance from the current cumulative reward to the optimal one, is often more appropriate for performance comparison.
2.2 Thompson Sampling

TS is a widely-used classical algorithm that has been shown to be effective for bandit problems both in practice (Chapelle & Li, 2011) and theory (Agrawal & Goyal, 2012). Unlike the $\epsilon$-greedy algorithm that use parameter $\epsilon$ to control exploration and upper-confidence bound (UCB) that uses variance approximation to encourage exploration (Sutton & Barto, 1998), TS uses the uncertainty from the posterior samples of the model parameters for solving exploration-exploitation dilemma. If the model is not confident about its parameters, there will be large variations among the posterior samples, which will force the model to explore more to help better approximate the true underlying distribution.

For a contextual bandit problem, vanilla TS maintains a posterior distribution $p_t(\theta)$ for global model parameter $\theta$. For $t = 1, \ldots, T$, it samples $\theta$ from its current posterior $p_{t-1}(\theta)$ and uses the sampled $\theta$ to transform the context-action pairs $(x_t, a)$ to estimate the mean rewards with $\hat{r}(a) = f(x_t, a; \theta)$; after that, it greedily chooses the best action $a_t = \arg\max_{a \in A} \hat{r}(a)$, receives reward $r_t$ from the environment, and uses the observed data to update its posterior on $\theta$ via Bayes’ rule. Vanilla TS faces the difficulty of balancing the complexity of the mapping function $f$ and the tractability of posterior inference for $\theta$, as discussed below.

3 TS via Global Uncertainty

In this section, we describe representative TS based algorithms for contextual bandits, which all share the same strategy of relying on the uncertainty of the global parameters (e.g., neural network weights) that are shared across all observations to perform exploration. They differ from each other on how complex the mapping function $f$ is and how the posterior inference on $\theta$ is implemented.

**Linear Method:** This method uses Bayesian linear regression with closed-form Gibbs sampling update equations, which relies on the posterior distributions of regression coefficients for TS updates and maintains computational efficiency due to the use of conjugate priors. This method assumes that at time $t$, the reward $y_t$ of an action given contextual input $x_t$ is generated as $y_t = x_t^T \beta + \epsilon_t$, where $\beta$ is the vector of regression coefficients and $\epsilon_t \sim \mathcal{N}(0, \sigma^2)$ is the noise. Note to avoid cluttered notation, we omit the action index. This method places a normal prior on $\beta$ and inverse gamma prior on $\sigma^2$. At time $t$, given $x_t$ and the current random sample of $\beta$, it takes the best action under TS and receives reward $y_t$; with $x_{1:t}$ and $y_{1:t}$, it samples $\sigma^2$ from its inverse gamma distributed conditional posterior, and then samples $\beta$ from its Gaussian distributed conditional posterior; it proceeds to the next time
and repeats the same update scheme under TS.

While this linear method accurately captures the posterior uncertainty of the global parameters $\beta$ and $\sigma^2$, its representation power is limited by both the linear mean and Gaussian distribution assumptions on reward $y$ given context $x$. In practice, the linear method often provides surprisingly competitive results, thanks to its ability to provide accurate uncertainty estimation. However, when its assumptions do not hold well in practice, such as when there are complex nonlinear dependencies between the rewards and contextual vectors, the linear method, even though with accurate posterior estimation, may not be able to converge to a good local optimal solution. Following [Riquelme et al.](2018), we refer to this linear method as “LinFullPost” in what follows.

**Neural Linear:** To enhance the representation power of LinFullPost while maintaining closed-form posterior sampling, [Riquelme et al.](2018) propose the “Neural Linear” method, which feeds the representation of the last layer of a neural network as the covariates of a Bayesian linear regression model. It models the reward distribution of an action conditioning on $x$ as $y \sim N(\beta^T z_x, \sigma^2)$, where $z_x$ is the output of the neural network given $x$ as the input. It separates representation learning and uncertainty estimation into two parts. The neural network part is responsible for finding a good representation of $x$, while the Bayesian linear regression part is responsible for obtaining uncertainty estimation on the regression coefficient vector $\beta$, and making the decision on which action to choose under TS. The training for the two parts can be performed at different time-scales. It is reasonable to update the Bayesian linear regression part as soon as a new data arrives, while to update the neural network part only after collecting a number of new data points.

As Neural Linear transforms context $x$ into latent space $z$ via a deterministic neural network, the model uncertainty still all comes from sampling the global parameters $\beta$ and $\sigma$ from their posteriors under the Bayesian linear regression part. Hence, it also relies on the uncertainty of global model parameters to perform TS.

**Bayesian By Backprop (BBB):** This method uses variational inference to perform uncertainty estimation on the neural network weights ([Blundell et al.](2015)). In order to exploit the reparameterization trick for tractable variational inference ([Kingma & Welling](2013)), it models the neural network weights with independent Gaussian distributions, whose means and variances become the network parameters to be optimized. However, the fully factorized mean-field variational inference used by BBB is well-known to have the tendency to underestimate posterior uncertainty ([Jordan et al.](1999), [Blei et al.](2017a)). Moreover, it is also questionable whether the weight uncertainty can be effectively translated into reward uncertainty given context $x$ ([Bishop](2006), [Sun et al.](2019)), especially considering that BBB makes both the independent and Gaussian assumptions on its network weights. For TS,
underestimating uncertainty often leads to under exploration. As the neural network weights are shared across all observations, BBB also relies on the uncertainty of global parameters to perform TS.

**Particle-Interactive TS via Discrete Gradient Flow (π-TS-DGF):** The π-TS-DGF method of [Zhang et al. (2019)](Zhang_etal_2019) casts posterior approximation as a distribution optimization problem under the Wasserstein-gradient-flow framework. In this setting, posterior sampling in TS can be considered as a convex optimization problem on the space of probability measures. For tractability, it maintains a set of particles that interact with each other and evolve over time to approximate the posterior. For the contextual bandit problem, each particle corresponds to a set of neural network weights, and the algorithm uniformly at random chooses one particle at each time and uses it as a posterior sample of the neural network weights. A benefit of π-TS-DGF is that it imposes no explicit parametric assumption on the posterior distribution. However, it faces an uneasy choice of setting the number of particles. Maintaining a large number of particles means training many sets of neural network weights at the same time, which is considerably expensive in computation, while a small number of particles might lead to bad uncertainty estimation due to inaccurate posterior approximation. The computational cost prevents π-TS-DGF from using large-size neural networks. Similar to BBB, π-TS-DGF also relies on the uncertainty of global parameters to perform exploration.

### 4 TS via Local Uncertainty

Vanilla TS has several limitations. Its performance is sensitive to the accuracy of the mapping function $f(x, a; \theta)$ and maintaining the exact posteriors for all model parameters is often computationally infeasible. Utilizing global parameter uncertainty to capture the posterior uncertainty of the mean rewards is challenging: first, the number of global parameters is often large, making it difficult to model their uncertainty under limited data without imposing strong assumptions; second, the model size is often constrained by the computational cost and training stability; third, the uncertainty on the global parameters may not be well translated into the uncertainty of the mean rewards by the mapping function.

To overcome these aforementioned limitations of vanilla TS, we propose TS via local uncertainty (LU). Rather than following the convention to impose uncertainty on global parameter $\theta$ to model the mean reward uncertainty, we apply uncertainty on local latent variables to balance exploration and exploitation under TS. We first construct a neural network powered latent variable model to model the mean reward distribution, and then introduce a contextual variational distribution to model the pre-posterior uncertainty on the mean rewards, which is used to guide the selection of actions. We first consider a contextual
variational distribution using a diagonal Gaussian construction, and then another one using a semi-implicit construction.

4.1 Local Latent Variable based Mean Reward Estimation

In a contextual bandit problem, the agent needs to continuously update its estimate of the unknown mean reward distributions through its interactions with the environment. In this case, given context $\mathbf{x}$, taking different actions $a$ will heavily impact the accumulated data for rewards, which predominantly influences the approximation of the mean reward distribution. TS via global uncertainty relies on the posterior sample of the global parameter to capture the uncertainty of the mean reward of an action at time $t$ as

$$\mathbb{E}[r_t | x_t, a_t, \beta], \quad \beta \sim p(\beta | x_{1:t-1}, a_{1:t-1}, r_{1:t-1}).$$

(2)

It chooses the action whose mean reward given $x_t$ and $\beta$ is the largest, receives reward from the environment, and then updates the posterior of the global parameter $\beta$ before taking another contextual vector.

By contrast, denoting $r_t \in \mathbb{R}^|A|$ as the rewards of all actions in $A$, we use a latent variable model to approximate the distribution of $r_t$ given $x_t$ as

$$r_t \sim p(r_t | x_t, z_t), \quad z_t \sim p(z).$$

This provides a flexible marginal distribution, whose density is often intractable, to model $r_t$ given $x_t$ as

$$p(r_t | x_t) = \mathbb{E}_{z_t \sim p(z)}[p(r_t | x_t, z_t)].$$

To maximize the likelihood of this intractable marginal, we resort to variational inference (Jordan et al., 1999; Bishop & Tipping, 2000; Blei et al., 2017b; Kingma & Welling, 2013). We introduce contextual variational distribution $q(z_t | x_t)$ to approximate the posterior $p(z_t | x_t, r_t)$ by minimizing the Kullback–Leiber (KL) divergence as $\text{KL}(q(z_t | x_t)p(z_t | x_t, r_t))$. Since one may show that $\log p(r_t | x_t) = \text{ELBO} + \text{KL}(q(z_t | x_t)p(z_t | x_t, r_t))$ and the KL divergence is non-negative, where the evidence lower bound (ELBO) is expressed as

$$\mathcal{L}_t = \mathbb{E}_{z_t \sim q(\cdot | x_t)} \left[ \log p(r_t | x_t, z_t) + \log \frac{p(z_t)}{q(z_t | x_t)} \right],$$

(3)

minimizing $\text{KL}(q(z_t | x_t)p(z_t | x_t, r_t))$ becomes the same as maximizing the ELBO.

Note for TS via LU, since the algorithm needs to decide which action to choose before receiving the real reward $r_t$, the contextual variational distribution $q(z_t | x_t)$ can not further
depend on $r_t$. At time $t$, before optimizing the ELBO, we need to first sample from the mean reward distribution using

$$
E[r_t | x_t, a_t, z_t], \quad z_t \sim q(z_t | x_t),
$$

where $E[r_t | x, a_t, z_t] = \int r_t \cdot p(r_t | x, a_t, z_t)dr_t$; we then choose the action whose mean reward given $z_t$ and $x_t$ is the largest, observe the true reward $r_t$ returned by the environment, and optimize the parameters of $p$ and $q$ to maximize the ELBO in (3).

Note a key difference between TS via LU and TS via global uncertainty is that to estimate the mean rewards of all actions, a random sample from the contextual variational distribution of the local variable $z_t$, as shown in (4), has replaced the role of a random sample from the posterior distribution of the global variable $\beta$, as shown in (2). In other words, rather than approximating the posterior of global parameters, our model estimates the posterior of local latent variable $z_t$, and utilizes its uncertainty to perform exploration under TS. We use a neural network to define the deterministic mapping from $x_t$ and $z_t$ to the mean rewards of all actions, and train the network parameter according to the ELBO in (3). We describe two different versions of TS via LU, as will be discussed in detail, in Algorithms 2 and 3, respectively.

The change from relying on global uncertainty to replying on local uncertainty brings several benefits. First, the neural network that maps $x_t$ and $z_t$ to the mean rewards can be made as complex as needed, without the need to worry about the tractability of posterior inference on the global parameters, the number of which is often so large that uncertainty estimation on them becomes possible only under strong distribution assumptions. Second, the uncertainty comes from the input feature space, e.g., $x_t$ can be concatenated with $z_t$, rather than from the weight space, leading to more direct influence on the uncertainty of the mean rewards. Third, $z_t$ often has a much lower dimension than $\beta$, making it much more computationally efficient when the dimension of $\beta$ is high.

4.2 Local Uncertainty Modeling with Gaussian Variational Posterior

We model both the rewards conditioning on $x_t$ and $z_t$ and the prior using diagonal Gaussian distributions as

$$
p(r_t | x_t, z_t) = N(\mu_{r_t}, \Sigma_r), \quad \mu_{r_t} = \mathcal{T}_\theta([x_t, z_t]),
\quad p(z_t) = N(0, \Sigma_z),
$$

8
where $T_\theta$ is a neural networks parameterized by $\theta$ that maps the $[x_t, z_t]$ concatenation to the mean rewards of all actions as $\mu_r \in \mathbb{R}^{|A|}$; both $\Sigma_r \in \mathbb{R}^{|A| \times |A|}$ and $\Sigma_z \in \mathbb{R}^{|z| \times |z|}$ are diagonal covariance matrix. Under this construction, the estimated mean rewards of all actions can be expressed as

$$E[r_t | x_t, z_t] = T_\theta([x_t, z_t]).$$  \hfill (6)

We define the contextual variational distribution as a diagonal Gaussian distribution as

$$q(z_t | x_t) = \mathcal{N}(\mu_{z_t}, \Sigma_{z_t}),$$
$$\mu_{z_t} = T_{\phi_1}(h), \quad \Sigma_{z_t} = T_{\phi_2}(h), \quad h = T_{\phi_0}(x_t),$$  \hfill (7)

where $\phi_0, \phi_1, \phi_2$ are neural network parameters. Then, we use Algorithm 2 for contextual bandit problems. A limitation of this algorithm is that $q(z_t | x_t)$ is restricted to be a Gaussian distribution, which might not be flexible enough to well model the true posterior that may exhibit multi-modality, skewness, and heavy tails. To improve its expressiveness, below we leverage semi-implicit variational inference (SIVI) of [Yin & Zhou 2018] that mixes a distribution, which is simple to sample from but not required to be explicit, with an explicit and reparameterizable distribution to make the resulted hierarchical distribution more flexible, while maintaining tractable inference.

### 4.3 Local Uncertainty Modeling with Semi-Implicit Variational Posterior

Keeping likelihood $p(r_t | x_t, z_t)$ and prior $p(z_t)$ the same as in [5], we model the contextual variational distribution using a semi-implicit construction as

$$q(z_t | x_t) = \int q(z_t | \psi_t, x_t)q(\psi_t | x_t)d\psi_t$$  \hfill (8)

where the first-layer explicit distribution is defined as

$$q(z_t | \psi_t, x_t) = \mathcal{N}(\psi_t, \Sigma_{z_t}), \quad \Sigma_{z_t} = T_{\phi_2}(x_t),$$  \hfill (9)

and the mean $\psi_t$ is drawn from an implicit distribution, which generates its random samples by nonlinearly transforming random noise $\epsilon_t \sim p(\epsilon)$ as

$$\psi_t = T_{\phi_1}([x_t, \epsilon_t]), \quad \epsilon_t \sim p(\epsilon).$$  \hfill (10)
We choose \( p(\epsilon) = \mathcal{N}(0, 4\mathbf{I}) \) in this paper. Note while the probability density function of \( p(\epsilon) \) is analytic, that of \( \psi_t \) is implicit if the transformation \( T_{\phi_t} \) is not invertible.

While given \( \epsilon_t \) and \( x_t \), the local latent variable \( z_t \) follows a diagonal Gaussian distribution, the marginal distribution \( q(z_t | x_t) \), obtained by integrating out the random noise \( \epsilon_t \), becomes an implicit distribution that is no longer restricted to follow a diagonal Gaussian as in Section 4.2. Thus, given the same mean reward mapping function as in (6), we can better capture the uncertainty on the mean rewards by sampling the local latent variable \( z_t \) from a more flexible contextual variational distribution \( q(z_t | x_t) \) as in (8).

While the original ELBO becomes intractable given an implicit contextual variational distribution, as in Yin & Zhou (2018); Molchanov et al. (2019), we can optimize an asymptotic lower bound of the ELBO that is amenable to direct optimization via stochastic gradient descent. More specifically, we follow semi-implicit variational inference (SIVI) of Yin & Zhou (2018) to sample \( K + 1 \) \( \psi_t \)'s, use only one of them to sample \( z_t \) from the conditional distribution \( q(z_t | \psi_t, x_t) \), and combine them for computing an asymptotic lower bound of the ELBO as

\[
\mathcal{L}_{K,t} = \mathbb{E}_{\epsilon_t^{(0)}, \ldots, \epsilon_t^{(K)} \sim p(\epsilon)} \mathbb{E}_{z_t \sim q(z_t | \psi_t^{(0)}, x_t)} \left[ \ln p(r_t | x_t, z_t) + \ln \frac{p(z_t)}{\frac{1}{K+1} \sum_{k=0}^{K} q(z_t | \psi_t^{(k)}, x_t)} \right],
\]

where \( \psi_t^{(k)} := T_{\phi_t}([x_t, \epsilon_t^{(k)}]) \). Note different from related works (Ranganath et al., 2016; Maaløe et al., 2016) that also employ a hierarchical variational distribution, SIVI allows \( q_{\phi}(\psi) \) to follow an implicit distribution (Huszár, 2017; Tran et al., 2017) and directly optimizes a surrogate ELBO.

We describe TS guided by semi-implicit LU in Algorithm 3. The hyperparameter \( K \) is related to how close \( \mathcal{L}_{K,t} \) is to the exact ELBO. A moderate value as \( K = 50 \) is found to be sufficient for neural network training, which does not bring much extra computational cost. Benefiting from the expressiveness improvement of using the semi-implicit structure, the distribution of \( \mathbb{E}[r_t | x_t, z_t] \) under \( q(z_t | x_t) \) becomes more flexible and can fit more complicated mean reward distributions. While this added flexibility may slightly degrade the performance for problems with simple reward distributions, overall, semi-implicit local uncertainty works very well over all our tested datasets, especially for data with complex reward distributions.

5 Experiments

We evaluate Gaussian variational LU guided TS, referred to as LU-Gauss, and semi-implicit variational LU guided TS, referred to as LU-SIVI, on the contextual bandits benchmark.
used in Riquelme et al. (2018). We evaluate our models on eight different datasets from this benchmark, including Mushroom, Financial, Statlog, Jester, Wheel, Covertype, Adult, and Census, which exhibit a wide range of statistical properties. Details on these datasets are provided in Table 2. For both LU-Gauss and LU-SIVI, we choose the Adam optimizer with the learning rate set as $10^{-3}$.

We compare the proposed LU-Gauss and LU-SIVI to LinFullPost, BBB, and Neural Linear implemented in Riquelme et al. (2018), and $\pi$-TS-DGF of Zhang et al. (2019). The details on the neural network structures are provided in the Appendix. Since each experiment involves randomly sampling a subset of contextual vectors from the full dataset, all results are averaged over 50 independent random trials. In each random trial, we rerun the code of LinFullPost, BBB, and Neural Linear provided by Riquelme et al. (2018) and the code of $\pi$-TS-DGF provided by Zhang et al. (2019). For the proposed LU-Gauss and LU-SIVI TS algorithms, Python code using TensorFlow 1.14 is available. To ensure a fair comparison, these 50 random sequences for each dataset are made to be the same across all the aforementioned algorithms. Note we have also considered making comparison with functional variational Bayesian neural networks (FBNNs) of Sun et al. (2019). However, as the code for FBNNs is too computationally expensive for us to run, we defer the details on comparison with FBNNs to the Appendix.

5.1 Exploratory Analysis

To analyze how the performance is impacted by the expressiveness of the variational distribution $q(z_t | x_t)$ that is used to model the local uncertainty, we choose the Mushroom dataset as an example, in which the stochastic rewards exhibit multi-modality. The Mushroom dataset has two distinct classes: poisonous and safe, and the agent has two possible actions: Eat or Not Eat. Eating a safe mushroom will be awarded +5, while eating a poisonous mushroom will be awarded either +5 or −35, which are equally likely to occur. If the agent chooses to not eat the mushroom, it will receive 0 reward. Thus, given a poisonous mushroom, the true reward distribution of Action Not Eat has a single mode at zero, while that of Action Eat has two modes, +5 and −35, with mean −15. For this reason, given a poisonous mushroom, a variational distribution that is not flexible enough will face the risk of concentrating the high density region of its mean reward distribution of Action Eat around +5, which is a local mode, leading to the wrong action; by contrast, a sufficiently flexible variational distribution could escape the local mode at +5 even if it initially concentrates its mean reward distribution around it, leading to better exploration.

\[^1\]https://drive.google.com/file/d/1aRZkRDZEv66J22TmpIJCbFtN8M-vUCR/view?usp=sharing
Running both LU-Gauss and LU-SIVI on the same random sequence of contextual vectors selected from the Mushroom dataset, we perform two different exploratory analyses: 1) We pick one poisonous mushroom, whose contextual feature vector $x_p$ is being regarded as edible at the beginning of training by both LU-Gauss and LU-SIVI, and visualize how the histogram of the sampled mean rewards of $x_p$ at each time step changes as the training progresses; 2) We visualize how the histogram of the sampled mean rewards of all poisonous mushroom at each step changes as the training progresses.

More specifically, for the first analysis, we use (7) to sample $z_{t,p}^{(s)} | x_p \sim q(z_{t,p} | x_p)$ for LU-Gaussian, or use (9) and (10) to sample $z_t^{(s)} | x_p \sim q(z_t | \psi_t^{(s)}, x_p)$, $\psi_t^{(s)} | x_p \sim q(\psi_t | x_p)$ for LU-SIVI, and then use (6) to compute a mean reward given $x_p$ and $z_{t,p}^{(s)}$ as $E[r_{t,p}^{(s)} | x_p, z_{t,p}^{(s)}] = T_\theta([x_p, z_{t,p}^{(s)}])$. We draw $S = 2000$ mean reward samples as $r_{t,p}^{(1)}, \ldots, r_{t,p}^{(S)}$ for each $t$ to form a histogram for that training step, and visualize these histograms over training steps as a heatmap, as shown in Fig. 1.

For Action Not Eat, as shown in Figs. 1(a) and (c), the empirical distribution of the sampled mean rewards for this poisonous mushroom becomes more and more concentrated around zero for both LU-Gauss and LU-SIVI. For Action Eat, as shown in Figs. 1(b) and (d), while both LU-Gauss and LU-SIVI initially consider this poisonous mushroom $x_p$ as edible with a positive reward, their mean reward distributions given $x_p$ become more and more different as the training progresses. In particular, LU-Gauss first becomes less certain and then more certain, with its high density region of the mean reward empirical distribution first shifting below zero, then moving back above zero, and eventually concentrating around +5, which means it mistakenly treats this poisonous mushroom as edible at many training steps.
steps. By contrast, LU-SIVI gradually increases its uncertainty and then maintains it around the same level, with its high density region of the mean reward empirical distribution quickly shifting below zero and remaining below zero at most of the training steps, which means it correctly identifies this poisonous mushroom most of the time.

For the second analysis, we take a single random sample of the mean reward for each mushroom at $t$, use the sampled mean rewards over all poisonous mushrooms as $\{r_{t,p}\}_p$ to form a histogram, and visualize the histograms over time as a heatmap, as shown in Fig. 2. For Action Not Eat, as shown in Figs. 2(a) and (c), both LU-Gauss and LU-SIVI quickly capture the underlying reward distribution, concentrating the histograms around zero. For Action Eat, as shown in Figure 2(b), under LU-Gauss, the sampled mean rewards of all poisonous mushrooms gradually concentrate around two density modes, with one clearly below zero and the other clearly above zero, suggesting that LU-Gauss will make a large number of mistakes in treating poisonous mushrooms as edible. By contrast, as shown in Figure 2(d), under LU-SIVI, the sampled mean rewards of all poisonous mushrooms quickly move down their high density region below zero and then maintain a single density mode around $-30$, suggesting that LU-SIVI will correctly identify poisonous mushrooms most of the time.

These analyses suggest that for the Mushroom dataset, whose true reward distribution of eating a poisonous mushroom exhibits two density modes, the variational distribution of LU-Gauss shown in (7) underperforms that of LU-SIVI shown in (8) in exploration and faces a greater risk to concentrate its mean reward distribution around the undesired local mode, leading to poorer performance. LU-SIVI, which introduces a more flexible variational distribution that is also amenable to optimization via stochastic gradient descent, achieves a better balance between exploration and exploitation.

5.2 Comparison of Experimental Results

Following the same experimental settings of the contextual bandits benchmark in [Riquelme et al. (2018)], we evaluate the proposed LU-Gaussian and LU-SIVI and compare them to representative TS algorithms relying on global uncertainty. Neither LU-Gaussian nor LU-SIVI include noise injection to the global parameters, dropout layer, and bootstrapping techniques discussed in [Riquelme et al. (2018)]. These techniques, designed to better capture global uncertainty to guide TS, can potentially be combined with LU-Gaussian and LU-SIVI to further improve their performance. We leave that for future study.

In Fig. 3 for each algorithm on a dataset, we plot the mean (a colored line) and standard deviation (line shade) of its accumulative regret against the training step over 50 random
trials. In Figure 4 we present the boxplots of normalized cumulative regrets. In Table 1 we show the normalized accumulative regrets with respect to the performance of the Uniform algorithm that uniformly at random chooses its actions from $A$. 

![Figure 3: Comparison of Cumulative Regret on eight different datasets.](image)

| Algorithms | Mean Rank | Mean Value | Mushroom | Financial | Statlog | Jester | Wheel | CoverType | Adult | Census |
|------------|-----------|------------|----------|-----------|---------|--------|-------|-----------|-------|--------|
| Uniform    | 7         | 100.00     | 100.00 ± 5.47 | 100.00 ± 9.44 | 100.00 ± 0.92 | 100.00 ± 8.08 | 100.00 ± 8.08 | 100.00 ± 0.47 | 100.00 ± 0.71 |
| BBB        | 4.75      | 57.77      | 27.15 ± 7.67 | 36.64 ± 0.90 | 25.15 ± 4.95 | 75.62 ± 4.86 | 78.75 ± 27.04 | 60.25 ± 3.60 | 95.79 ± 1.40 | 63.44 ± 1.39 |
| Neural Linear | 4.75      | 52.69      | 15.73 ± 5.66 | 17.55 ± 1.75 | 13.84 ± 1.72 | 81.83 ± 4.32 | 51.07 ± 11.11 | 65.30 ± 2.56 | 96.82 ± 0.75 | 79.38 ± 1.66 |
| LinFullPost | 3.75      | 51.78      | 14.90 ± 4.97 | 10.49 ± 0.59 | 18.76 ± 1.01 | 77.85 ± 4.18 | 42.20 ± 16.42 | 59.07 ± 1.60 | 96.19 ± 0.19 | 94.82 ± 0.65 |
| π-TS-DGF   | 2.5       | 47.42      | 15.65 ± 2.65 | 8.19 ± 2.93 | 5.53 ± 1.42 | 76.32 ± 4.23 | 85.78 ± 20.36 | 47.01 ± 1.86 | 91.23 ± 2.40 | 49.64 ± 1.78 |
| LU-Gauss   | 2.5       | 44.69      | 15.19 ± 2.38 | 8.83 ± 2.96 | 6.99 ± 1.34 | 72.35 ± 5.10 | 57.74 ± 20.22 | 49.83 ± 2.07 | 90.39 ± 1.55 | 56.20 ± 1.51 |

![Table 1: Normalized Cumulative Regret.](image)
We first examine the performance of various global uncertainty guided TS algorithms, including BBB, LinFullPost, Neural Linear, and $\pi$-TS-DGF. It is clear that BBB has the worst overall performance and exhibits large variance on its cumulative regrets across different random trials, suggesting that using a diagonal Gaussian variational distribution on the global parameters (neural network weights) leads to poor exploration. LinFullPost performs well in some datasets. For example, it works very well on the Mushroom dataset, which is likely because using Gibbs sampling on global variables makes it simple to move its reward distribution of eating a poisonous mushroom away from the bad local mode of $+5$. However, it clearly suffers from lack of representation power on datasets that violate the linear assumption, such as Covertype, Census, Adult, and Statlog. Neural Linear involves feature extraction using a neural network and keeps the exact linear posterior updates for Thompson sampling, but its representation learning relies heavily on the number of training steps that have been taken, which might be the reason for its relatively poor performance. Since $\pi$-TS-DGF of Zhang et al. (2019) can provide better uncertainty estimation than BBB on the global parameters and more representation power than LinFullPost, it works quite well on some datasets and overall outperforms BBB and LinFullPost. Nevertheless, it does not perform that well on Mushroom and Jester and performs poorly on Wheel, which requires heavy exploration in order to minimize the cumulative regrets.

We then examine the performance of the proposed LU guided TS algorithms, including LU-Gauss and LU-SIVI. It is clear from Figs. 3 and 4 and Table 1 that LU-Gauss in general
performs quite well, except that it provides poor performance on Mushroom. The poor
performance of LU-Gauss on Mushroom, as analyzed in detail in Section (5.1), is likely
because the diagonal Gaussian variational distribution is not flexible enough to encourage
sufficient exploration. To be more specific, as shown in Figs. 1(b) and 2(b), it prevents
the sampled mean rewards of eating some poisonous mushrooms from moving away from
a bad local density mode. By contrast, LU-SIVI performs well across all eight benchmark
datasets. In particular, for the Mushroom dataset that LU-Gauss performs poorly, as shown
in Figs. 1(d) and 2(d), LU-SIVI places most of its sampled mean rewards of eating poisonous
mushrooms clearly below zero. This can be explained by the improved ability of LU-SIVI in
exploration due to the use of a semi-implicit variational distribution that not only is more
flexible, but also remains simple to optimize.

To better compare the overall performance of different algorithms, as shown in Table 1,
for each algorithm, we follow Riquelme et al. (2018) and Sun et al. (2019) to compute
both the Mean Rank and the Mean Value of normalized cumulative regrets over all eight
benchmark datasets. The Mean Rank and Mean Value suggest that LU-SIVI has the best
overall performance, followed by LU-Gauss and π-TS-DGF. Note when the contextual vector
dimension is low, both LU-Gauss and LU-SIVI take more time to run in comparison to both
LinFullPost and Neural Linear. We report the time cost based on an NVidia 1080-TI GPU.
For example, on Mushroom whose contextual vector dimension is 22, both LU-Gauss and
LU-SIVI take about 30 seconds for 2000 training steps, while both LinFullPost and Neural
Linear take about 15 seconds. However, the computational complexity of both LinFullPost
and Neural Linear increases cubically with the dimension of the contextual vector, due to the
need to perform both Cholesky decomposition of the covariance matrix and matrix inversion
when sampling the regression coefficient vector $\beta$. For example, on Census whose contextual
vector dimension is 389, it takes both LU-Gauss and LU-SIVI about 40 seconds to run 2000
training steps, while it takes both LinFullPost and Neural Linear over 700 seconds. For
π-TS-DGF, it takes about 184 seconds on Mushroom and 490 seconds on Census.

6 Conclusion

To address the problem of contextual bandits, we propose Thompson sampling (TS) guided
by local uncertainty (LU). This new TS framework models the reward distribution given
the context using a latent variable model, and uses a pre-posterior contextual variational
distribution to approximately capture the uncertainty of the local latent variable, whose
true posterior depends on both the observed context and the reward that is yet to be
observed. Under this framework, we introduce both LU-Gauss, which uses a diagonal Gaussian
contextual variational distribution, and LU-SIVI, which uses a semi-implicit contextual variational distribution. In comparison to LU-Gauss, LU-SIVI has a more flexible variational distribution that enhances its ability of exploration, leading to improved performance on datasets with complex reward distributions. Experimental results on eight different contextual bandit datasets demonstrate that both LU-Gauss and LU-SIVI well model the uncertainty and provide good performance. In particular, LU-SIVI outperforms the particle-interactive TS algorithm of Zhang et al. (2019), the current state-of-the-art, in having a better overall performance and clearly lower computational complexity. An interesting topic for future research is to integrate both global parameter uncertainty and local latent variable uncertainty under TS to achieve further improved performance.

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## A Model Details

In the implementation, we all use ReLU activation function, except for using the exponential link function for parameterizing the standard deviation of the Gaussian distributions. We set prior distribution \( p(z_t) \) as a normal distribution with mean 0 and standard deviation \( \sigma \mathbf{I} \), where \( \sigma \) is a point estimation with initial value \( \sigma = 1.25 \). Denote the latent dimension as \( H \), number of actions as \( A \), and context dimension as \( C \).

For LU-Gauss: we set the latent dimension of \( z \) as \( H = 50 \). \( \mathcal{T}_\theta \) is a neural network with input \([x, z]\) in dimension \( H + C \), one hidden layer [50], and output in dimension \( A \). We use a point estimation on \( \Sigma_r \). \( \mathcal{T}_{\phi_0} \) is a neural network with input \([x, \epsilon]\) in dimension \( C + C \), one hidden layer [100], and output in dimension 50, where \( \epsilon \) has the same dimension as context dimension. \( \mathcal{T}_{\phi_1} \) is a neural network with input in dimension 50, one hidden layer [50] and
output in dimension $H$. $T_{\varphi_2}$ is a neural network with input in dimension 50, one hidden layer $[50]$, and output in dimension $H$.

For LU-SIVI: we set the latent dimension of $z$ as $H = 50$ and $K = 50$. $T_{\theta}$ is a neural network with input $[x, z]$ in dimension $H + C$, one hidden layer $[50]$, and output in dimension $A$. We use a point estimation on $\Sigma_r$. $T_{\varphi_1}$ is a neural network with input $[x, \epsilon]$ in dimension $C + C$, one hidden layer $[100]$, and output in dimension $H$, where $\epsilon$ has the same dimension as context dimension. $T_{\varphi_2}$ is a neural network with input in dimension $C$, one hidden layer $[50]$, and output in dimension $H$.

## B Comparison with FBNNS

We have tried to make comparison with FBNNS of Sun et al. (2019). The code for FBNNS, however, is too computationally expensive for us to run. For example, the smallest FBNNS model (1x50) used by Sun et al. (2019) is already about 20 times slower than our proposed LU-Gauss and LU-SIVI, let alone larger FBNNS models. For this reason, we directly quote FBNNS’ results reported in Sun et al. (2019), which were obtained based on as few as 10 random trials. Note the following results, which are quoted merely for reference, are not intended for a rigorous comparison as they are not obtained by averaging over the same set of 50 random sequences used by the other algorithms. The Mean Value is 46.0 for FBNNS (1 x 50), 47.0 for (2 x 50), 48.9 for (3 x 50), 45.3 for (1 x 500), 44.2 for (2 x 500), and 44.6 for (3 x 500). Their best Mean Value over the eight datasets is 44.2, from model FBNNS (2 x 500), which is considerably slower to run in comparison to both LU-Gauss and LU-SIVI.

| Dataset     | Context | Action |
|-------------|---------|--------|
| Mushroom    | 22      | 2      |
| Financial   | 21      | 8      |
| Statlog     | 16      | 7      |
| Jester      | 32      | 8      |
| Wheel       | 2       | 5      |
| Covertype   | 54      | 7      |
| Adult       | 94      | 14     |
| Census      | 389     | 9      |

Table 2: Dataset Dimension Details
Algorithm 1: Vanilla Thompson Sampling

**input**: Prior distribution $p_0(\theta)$.

**output**: Fine-tuned posterior distribution $p_T(\theta)$.

**for** $t = 1, \ldots, T$ **do**
  **Observe context** $x_t$.
  **Sample parameters** $\theta_t \sim p_{t-1}(\theta)$.
  **Select action** $a_t = \arg\max_a f(x, a; \theta_t)$.
  **Observe reward** $r_t$.
  **Update posterior distribution** $p_t(\theta)$ with $(x_t, a_t, r_t)$.
**end for**

Algorithm 2: LU-Gauss: Thompson Sampling via Gaussian Local Uncertainty

**Input**: Likelihood $p(r_t | x_t, z_t) = \mathcal{N}(\mu_{r_t}, \Sigma_{r_t})$, prior $p(z) = \mathcal{N}(0, \Sigma_z)$, and variational distribution $q(z_t | x_t) = \mathcal{N}(\mu_{z_t}, \Sigma_{z_t})$; neural networks $T_\theta$, $T_{\phi_0}$, $T_{\phi_1}$, and $T_{\phi_2}$, $t_f = 20$ (training frequency), $t_s = 40$ (the number of mini-batches per training period).

**Output**: Inferred parameters $\Sigma_{r_t}$, $\theta$, $\phi_0$, $\phi_1$, and $\phi_2$.

**Initialize** $\Sigma_r$.

**Initialize dataset** $D_0 = \emptyset$.

**for** $t = 1, \ldots, T$ **do**
  **Observe context** $x_t$
  $h = T_{\phi_0}(x_t)$
  $\mu_{z_t} = T_{\phi_1}(h)$, $\Sigma_{z_t} = T_{\phi_2}(h)$
  **Sample** $z_t \sim \mathcal{N}(\mu_{z_t}, \Sigma_{z_t})$
  $\mu_{r_t} = T_\theta([x_t, z_t])$
  **Select action** $a_t = \arg\max_a \mu_{r_t}$
  **Observe reward** $r_t$
  $D_t = D_{t-1} \cup (x_t, a_t, r_t)$
  **if** $t \mod t_f = 0$ **then**
  **for** iteration $= 1 : t_s$ **do**
    **Draw a minibatch data** $\{(x_i, a_i, r_i)\}_{i=1}^N$
    **Expand** $r_i$ to vector $r_i$ with 0 at unobserved positions
    **Create mask** $\{m_i\}_{i=1}^N$, where $m_i$ are zeros only except $m_i[a_i] = 1$
    **Obtain the action space dimension** $|A|$ for $i = 1 : N$
    $h_i = T_{\phi_0}(x_i)$, $\mu_{z_i} = T_{\phi_1}(h_i)$, $\Sigma_{z_i} = T_{\phi_2}(h_i)$ for $i = 1 : N$
    **Let** $z_i := \mu_{z_i} + \Sigma_{z_i} \odot \epsilon_i$, $\epsilon_i \sim \mathcal{N}(0, I)$ for $i = 1 : N$ where $\odot$ denotes element-wise product
    $\mu_{r_i} = T_\theta([x_i, z_i])$ for $i = 1 : N$
    **Update** $\Sigma_r$, $\theta$, $\phi_0$, $\phi_1$, and $\phi_2$ by using the gradients of:
    $$\frac{1}{N} \sum_{i=1}^N \left[ \log p(r_i | x_i, z_i) \cdot |A| \cdot \log \frac{p(z_i)}{q(z_i | x_i)} \right]$$
  **end for**
  **end if**
**end for**
Algorithm 3: LU-SIVI: Thompson Sampling with Semi-Implicit Local Uncertainty

**Input**: Likelihood \( p(r_t \mid x_t, z_t) = \mathcal{N}(\mu_r, \Sigma_r) \); prior \( p(z) = \mathcal{N}(0, \Sigma_z) \); explicit variational distribution \( q(z_t \mid x_t) = \mathcal{N}(\psi_t, \Sigma_z) \) with reparameterization \( z_t = \mu_z + \Sigma_z \odot \epsilon_t \), \( \epsilon_t \sim \mathcal{N}(0, I) \); selected random noise distribution \( q(\epsilon) \); neural network \( T_\theta, T_{\phi_1}, \) and \( T_{\phi_2}; t_f = 20 \) (training frequency), \( t_s = 40 \) (the number of mini-batches per training period)

**Output**: Fine-tuned parameters \( \Sigma_r, \theta, \phi_1, \phi_2 \).

Initialize parameters \( \Sigma_r, \theta, \phi_1, \phi_2 \).

Initialize dataset \( D_0 = \emptyset \)

for \( t = 1, \ldots, T \) do

Observe new context \( x_t \)

\( \psi_t = T_{\phi_1}([x_t, \epsilon_t]), \) where \( \epsilon_t \sim q(\epsilon) \)

\( \Sigma_{z_t} = T_{\phi_2}(x_t) \)

Sample \( z_t \sim \mathcal{N}(\psi_t, \Sigma_{z_t}) \)

\( \mu_{r_t} = T_\theta([x_t, z_t]) \)

Select \( a_t = \text{argmax} \mu_{r_t} \)

Observe reward \( r_t \)

\( D_t = D_{t-1} \cup (x_t, a_t, r_t) \)

if \( t \mod t_f = 0 \) then

for iteration = 1 : \( t_s \) do

Draw a minibatch data \( \{(x_i, a_i, r_i)\}_{i=1}^N \)

Expand \( r_i \) to vector \( r_i \) with 0 at unobserved positions

Create mask \( \{m_i\}_{i=1}^N \), where \( m_i \) are zeros only except \( m_i[a_i] = 1 \)

Obtain the action space dimension as \(|A|\)

Let \( \psi_{(k)}^{(i)} := T_{\phi_1}([x_i, \epsilon_{(k)}^i]), \epsilon_{(k)}^i \sim q(\epsilon) \) for \( k = 0 : K \)

Compute \( \Sigma_{z_i} = T_{\phi_2}(x_i) \)

Let \( z_i := \psi_{(0)}^i + \Sigma_{z_i} \odot \epsilon_i, \epsilon_i \sim \mathcal{N}(0, I) \)

Compute \( \mu_{r_i} = T_\theta([x_i, z_i]) \)

Update \( \Sigma_r, \theta, \phi_1, \phi_2 \) by using the gradients of:

\[
\frac{1}{N} \sum_{i=1}^N \left[ \log p(r_i \mid \mu_{r_i}, \Sigma_r) \cdot m_i \cdot |A| + \frac{\log p(z_i)}{\log \frac{1}{K+1} \sum_{k=0}^K q(z_i \mid \psi_{(k)}^i, \Sigma_{z_i})} \right]
\]

end for

end if

end for