Neural Contextual Bandits via Reward-Biased Maximum Likelihood Estimation

Yu-Heng Hung  
Department of Computer Science  
National Yang Ming Chiao Tung University, Hsinchu, Taiwan  
hungyh.cs08@nycu.edu.tw

Ping-Chun Hsieh  
Department of Computer Science  
National Yang Ming Chiao Tung University, Hsinchu, Taiwan  
pinghsieh@nctu.edu.tw

Abstract

Reward-biased maximum likelihood estimation (RBMLE) is a classic principle in the adaptive control literature for tackling explore-exploit trade-offs. This paper studies the stochastic contextual bandit problem with general bounded reward functions and proposes NeuralRBMLE, which adapts the RBMLE principle by adding a bias term to the log-likelihood to enforce exploration. NeuralRBMLE leverages the representation power of neural networks and directly encodes exploratory behavior in the parameter space, without constructing confidence intervals of the estimated rewards. We propose two variants of NeuralRBMLE algorithms: The first variant directly obtains the RBMLE estimator by gradient ascent, and the second variant simplifies RBMLE to a simple index policy through an approximation. We show that both algorithms achieve $\tilde{O}(\sqrt{T})$ regret. Through extensive experiments, we demonstrate that the NeuralRBMLE algorithms achieve comparable or better empirical regrets than the state-of-the-art methods on real-world datasets with non-linear reward functions.

1 Introduction

Efficient exploration has been a fundamental challenge in sequential decision-making in unknown environments. As a classic principle originally proposed in the stochastic adaptive control literature for solving unknown Markov decision processes (MDPs), Reward-Biased Maximum Likelihood Estimation (RBMLE) learns an optimal policy by alternating between estimating the unknown model parameters in an “exploratory” manner and applying the optimal control law based on the estimated parameters (Kumar & Becker, 1982; Borkar, 1990; Campi & Kumar, 1998; Prandini & Campi, 2000). Specifically, to resolve the inherent issue of insufficient exploration of maximum likelihood estimation (MLE), RBMLE enforces exploration by incorporating into the likelihood function a bias term in favor of those model parameters that correspond to higher long-term average rewards. This generic exploration scheme has been shown to asymptotically attain the optimal long-term average reward (Kumar & Becker, 1982).

Recently, the RBMLE principle has been adapted to optimize the regrets in stochastic bandit problems, including the classic non-contextual multi-armed bandit problems (Liu et al., 2020) and the contextual bandit problems with generalized linear reward functions (Hung et al., 2021). Moreover, RBMLE has been shown to achieve order-optimal finite-time regret bounds and competitive empirical regret performance in the above settings. Despite the recent progress, the existing RBMLE
bandit algorithms, as well as their regret guarantees, rely heavily on the structural assumptions, such as the absence of contextual information in [Liu et al. (2020)] and linear realizability in [Hung et al. (2021)], and hence are not readily applicable to various real-world bandit applications with more complex reward structures, such as recommender systems and clinical trials.

Motivated by the competitive performance of the RBMLE principle in the bandit problems mentioned above, this paper takes one step further to study RBMLE in contextual bandits with general reward functions. To unleash the full potential of RBMLE in contextual bandits, we leverage the representation power of neural networks to approximate the unknown reward function, as recently adopted by [Zhou et al. (2020); Zhang et al. (2021)]. Built on the neural reward function approximation, this paper extends the RBMLE principle and proposes the first RBMLE bandit algorithm for the contextual bandit problems without the linear realizability assumption. The main contributions of this paper are summarized as follows:

- We propose NeuralRBMLE, which extends the RBMLE principle to the neural contextual bandit problem. By incorporating a surrogate likelihood function and a proper reward-bias term, we first present a prototypic NeuralRBMLE algorithm that enjoys an index form. We then propose two practical approaches to substantiate the prototypic NeuralRBMLE algorithm.
- We formally establish the regret bounds for the two practical NeuralRBMLE algorithms by leveraging the neural tangent kernel technique. Through regret analysis, we validate the flexibility in using any exponential family distribution as the surrogate likelihood function for NeuralRBMLE-GA, thereby opening up a whole new family of neural bandit algorithms. For NeuralRBMLE-PC, we characterize the interplay between the reward-bias term, the regret, and the condition of $\theta$.
- We evaluate NeuralRBMLE and other benchmark algorithms through extensive simulations on various benchmark real-world datasets. The simulation results show that NeuralRBMLE achieves comparable or better empirical regret performance than the benchmark methods.

Notations. Throughout this paper, for any positive integer $K$, we use $[K]$ as a shorthand for the set $\{1, \ldots, K\}$. We use $\| \cdot \|_2$ to denote the $L_2$-norm of a vector. We use boldface fonts for vectors and matrices throughout the paper. Moreover, we use $0$ and $I$ to denote the zero matrices and the identity matrices, respectively.

2 Problem Formulation

In this section, we formally describe the neural contextual bandit problem considered in this paper.

2.1 Contextual Bandits with General Rewards

We consider the stochastic $K$-armed contextual bandit problem, where the total number of rounds $T$ is known. At each decision time $t \in [T]$, the $K$ context vectors $\{x_{t,a} \in \mathbb{R}^d | a \in [K]\}$, which capture the feature information about the arms, are revealed to the learner. Without loss of generality, we assume that $\|x_{t,a}\|_2 \leq 1$, for all $t \in [T]$ and for all $a \in [K]$. Note that we do not impose any statistical assumptions on the contexts, which could possibly be generated by an adversary. Given the contexts, the learner selects an arm $a_t \in [K]$ and obtains the corresponding random reward $r_{t,a_t}$. For ease of notation, we define (i) $x_t := (x_{t,a_1}, \ldots, x_{t,a_T})$, (ii) $r_t := r_{t,a_t}$, (iii) $F_t := (x_1, a_1, r_1, \ldots, x_t)$ as the observation history up to the beginning of time $t$, (iv) $a^*_t := \arg\max_{a \in [K]} E[r_{t,a} | F_t]$, and (v) $r^*_t := r_{t,a^*_t}$. The goal of the learner is to minimize the pseudo regret as

$$R(T) := \mathbb{E} \left[ \sum_{t=1}^{T} (r^*_t - r_t) \right]$$

In the neural contextual bandit problem, the random reward at each time $t$ takes the form of $r_t = h(x_t) + \epsilon_t$, where $h : \mathbb{R}^d \rightarrow [0, 1]$ is an unknown reward function and $\epsilon_t$ is a $\nu$-sub-Gaussian noise conditionally independent of all the other rewards in the past given the context $x_t$ and satisfying $\mathbb{E}[\epsilon_t | x_t] = 0$, and the reward function $h(\cdot)$ is approximated by a neural network through training. Compared to the generalized linear bandit model, here we assume no special structure (e.g., linearity or convexity) on the reward function, except that the reward signal is bounded in $[0, 1]$.

$^1$The assumption of a known horizon is mild as one could apply the standard doubling trick to convert a horizon-dependent algorithm to an anytime one ([Lattimore & Szepesvári, 2020]).
2.2 Neural Function Approximation for Rewards

In this paper, we leverage a neural network to approximate the reward function \( h(\cdot) \). Let \( L \geq 2 \) be the depth of this neural network, \( \sigma(\cdot) = \max\{\cdot, 0\} \) be the Rectified Linear Unit (ReLU) activation function, and \( m_l \) be the width of the \( l \)-th hidden layer, for \( l \in [L - 1] \). We also let \( m_0 = d \) and \( m_L = 1 \). Let \( W_l \in \mathbb{R}^{m_l \times m_{l-1}} \) denote the weight matrix of the \( l \)-th layer of the neural network, for \( l \in [L] \). For ease of exposition, we focus on the case where \( m_l = m \), for all \( l \in [L - 1] \). For ease of notation, we define \( \theta := [\text{vec}(W_1)^\top, \ldots, \text{vec}(W_L)^\top] \in \mathbb{R}^p \), where \( p = m + md + m^2(L - 1) \) denotes the total number of parameters of the neural network. Let \( f(x; \theta) \) denote the output of the neural network with parameters \( \theta \) and input \( x \), i.e.,

\[
f(x; \theta) := \sqrt{m} \cdot W_L \sigma(W_{L-1} \sigma(W_{L-2} \ldots \sigma(W_1 x))).
\]

Let \( g(x; \theta) := \nabla_x f(x; \theta) \) be the gradient of \( f(x; \theta) \), and let \( \theta_0 \) be the initial model parameters selected by the following random initialization steps: (i) For \( l \in [L - 1] \), let \( W_l \) take the form of \( W_l = \begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix} \), where each entry of \( W \) is drawn independently from \( \mathcal{N}(0, 2/m) \). (ii) For the output layer, let \( W_L \) take the form of \( W_L = (w^\top, -w^\top) \), where each entry of \( w \) is drawn independently from \( \mathcal{N}(0, 1/m) \).

3 An Overview of the RBMLE Principle

In this section, we review the generic RBMLE principle in the context of adaptive control for maximizing the long-term average reward of an unknown dynamic system. Consider a discrete-time MDP with a state space \( S \), an action space \( A \), and unknown transition dynamics as well as a reward function that are both dependent on the unknown true parameter \( \theta \) belonging to some known set \( \Theta \). For ease of notation, for any \( \theta \in \Theta \), we denote the transition probabilities under \( \theta \) by \( p(s_t, s_{t+1}, a_t; \theta) := \text{Prob}(s_{t+1}|s_t, a_t) \), where \( p \) is a probability function parameterized by \( \theta \), \( s_t \in S \) and \( a_t \in A \) are the state and the action taken at time \( t \). Let \( J(\pi; \theta) \) be the long-term average reward under policy \( \pi: S \to A \). We let \( J^*(\theta) := \max_\pi J(\pi; \theta) \) denote the optimal long-term average reward for any \( \theta \in \Theta \) and use \( \pi^* := \arg\max_\pi J(\pi; \theta^*) \) to denote an optimal policy for \( \theta^* \).

- **Closed-loop identification issue:** Originally proposed by Mandl (1974), the certainty equivalent (CE) method addresses the optimal control of an unknown dynamic system by first finding the MLE of the true parameter and then following an optimal policy with respect to the MLE. Specifically, the MLE of the true parameter \( \theta^* \) at each time \( t \) can be derived as

\[
\theta_t^\text{MLE} := \arg\max\limits_{\theta \in \Theta} \prod_{i=1}^{t-1} p(s_i, s_{i+1}, a_i; \theta).
\]

Let \( \pi_t^\text{MLE} := \arg\max_\theta J(\pi, \theta_t^\text{MLE}) \) denote an optimal policy for the system with parameter \( \theta_t^\text{MLE} \). Then, it was shown in Kumar & Becker (1982) that under the sequence of policies \( \{\pi_t^\text{MLE}\} \), the sequence of maximum likelihood estimates \( \{\theta_t^\text{MLE}\} \) converges to some estimate \( \theta^\text{MLE} \) in the limit such that for all pairs of \( s, s' \in S \),

\[
p(s, s', \pi^\text{MLE}_t(s); \theta^\text{MLE}_t) = p(s, s', \pi^\text{MLE}_\infty(s); \theta^*_s),
\]

where \( \pi^\text{MLE}_\infty := \arg\max_\pi J(\pi, \theta^\text{MLE}_\infty) \) is an optimal policy for \( \theta^\text{MLE}_\infty \). Notably, \( \pi^\text{MLE}_\infty \) is typically known as the “closed-loop identification” property, which indicates that under the policy \( \pi^\text{MLE}_\infty \), the transition probabilities can be correctly identified only in a “closed-loop” manner. As a result, under the CE approach, it is not guaranteed that all the transition probabilities of the MDP are correctly estimated, and therefore the policy \( \pi^\text{MLE}_\infty \) is not necessarily optimal for the true parameter \( \theta^* \).

- **The inherent bias resulting from MLE:** The above key insight about the CE approach can be made more explicit by Kumar & Becker (1982) by

\[
J(\pi^\text{MLE}_\infty; \theta^\text{MLE}_\infty) = J(\pi^\text{MLE}_\infty; \theta^*_s) \leq J(\pi^*; \theta^*_s),
\]

To make the connection between RBMLE and neural bandits explicit, in Section 3 we slightly abuse the notation \( \theta \) to denote the parameters of the dynamical system.
where the first equality in (5) follows from (4). As $J(\pi^*_\infty; \theta^*_\infty) \equiv J^*(\theta^*_\infty)$ and $J(\pi^*; \theta_*) \equiv J^*(\theta_*)$, (5) indicates that the estimates under CE suffer from an inherent bias that favors the parameters with smaller optimal long-term average rewards than $\theta_*$. 

• **Adding a reward-bias term for correcting the inherent bias of MLE.** To counteract this bias, Kumar & Becker (1982) proposed the RBMLE approach, which directly multiplies the likelihood by an additional reward-bias term $J^*(\theta)^{\alpha(t)}$ with $\alpha(t) > 0$, $\alpha(t) \to \infty$, $\alpha(t) = o(t)$, with the aim of encouraging exploration over those parameters $\theta$ with a potentially larger optimal long-term average reward. That is, the parameter estimate under RBMLE is

$$\theta_t^{\text{RBMLE}} := \arg\max_{\theta \in \Theta} \left\{ J^*(\theta)^{\alpha(t)} \prod_{i=1}^{t-1} p(s_i, s_{i+1}, a_i; \theta) \right\}. \quad (6)$$

Accordingly, the policy induced by RBMLE at each $t$ is $\pi_t^{\text{RBMLE}} := \arg\max_{\pi} J(\pi; \theta_t^{\text{RBMLE}})$. It has been shown in Kumar & Becker (1982) that RBMLE successfully corrects the inherent bias and converges to the optimal policy $\pi^*$ through the following steps: (i) Since $\alpha(t) = o(t)$, the effect of the reward-bias term becomes negligible compared to the likelihood term for large $t$. Hence, the sublinearity of $\alpha(t)$ leads to diminishing exploration and thereby preserves the convergence property similar to that of MLE. As a result, both the limits $\theta_t^{\text{RBMLE}} := \lim_{t \to \infty} \theta_t^{\text{RBMLE}}$ and $\pi_t^{\text{RBMLE}} := \lim_{t \to \infty} \pi_t^{\text{RBMLE}}$ exist, and the result similar to (5) still holds under RBMLE, i.e.,

$$J(\theta_t^{\text{RBMLE}}, \theta_t^{\text{RBMLE}}) \leq J(\pi^*, \theta_*). \quad (7)$$

(ii) Given that $\alpha(t) \to \infty$, the reward-bias term $J^*(\theta)^{\alpha(t)}$, which favors those parameters with higher rewards, remains large enough to undo the inherent bias of MLE. As a result, RBMLE achieves

$$J(\pi_t^{\text{RBMLE}}, \theta_t^{\text{RBMLE}}) \geq J(\pi^*, \theta^*), \quad (8)$$

as proved in Kumar & Becker (1982) Lemma 4. By (7)-(8), we know that the delicate choice of $\alpha(t)$ ensures $\pi_t^{\text{RBMLE}}$ is an optimal policy for the true parameter $\theta_*$. 

Note that the above optimality result implies that RBMLE achieves a sublinear regret, but without any further characterization of the regret bound and the effect of the bias term $\alpha(t)$. In this paper, we adapt the RBMLE principle to neural contextual bandits and design bandit algorithms with regret guarantees.

### 4 RBMLE for Neural Contextual Bandits

In this section, we present how to adapt the generic RBMLE principle described in Section 3 to the neural bandit problem and propose the NeuralRBMLE algorithms.

#### 4.1 A Prototypic NeuralRBMLE Algorithm

By leveraging the RBMLE principle in (6), we propose to adapt the parameter estimation procedure for MDPs in (6) to neural bandits through the following modifications:

• **Likelihood functions via surrogate distributions:** For each time $t \in [T]$, let $\ell^i(F_t; \theta)$ denote the log-likelihood of the observation history $F_t$ under a neural network parameter $\theta$. Notably, different from the likelihood of state transitions in the original RBMLE in (6), here $\ell^i(F_t; \theta)$ is meant to capture the statistical behavior of the received rewards given the contexts. However, one main challenge is that the underlying true reward distributions may not have a simple parametric form and are unknown to the learner. To address this challenge, we use the log-likelihood of *canonical exponential family distributions* as a surrogate for the true log-likelihood. Specifically, the surrogate log-likelihood is chosen as $\log p(r_s | x_s; \theta) = r_s f(x_s; \theta) - b(f(x_s; \theta))$, where $b(\cdot) : \mathbb{R} \to \mathbb{R}$ is a known strongly convex and smooth function with $L_b \leq b''(z) \leq U_b$, for all $z \in \mathbb{R}$. Note that the above log $p(r_s | x_s; \theta)$ is used only for arm selection under NeuralRBMLE.

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4 For brevity, we ignore the normalization function of the canonical exponential families since this term depends only on $r_s$ and is independent of $\theta$. 

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and we do not impose any distributional assumption on the rewards other than sub-Gaussianity. Hence, \( \ell^I(F_t; \theta) \) can be written as

\[
\ell^I(F_t; \theta) := \sum_{s=1}^{t-1} (r_s f(x_s; \theta) - b(f(x_s; \theta))).
\]  

(9)

For example, one candidate choice for (9) is using Gaussian likelihood with \( b(z) = z^2/2 \).

- **Reward-bias term:** We consider one natural choice \( (\max_{a \in [K]} f(x_{t,a}; \theta))^{\alpha(t)} \), which provides a bias in favor of the parameters \( \theta \) with larger estimated rewards.

- **Regularization:** As the RBMLE procedure requires a maximization step, we also incorporate into the reward-biased likelihood a quadratic regularization term \( \frac{m\lambda}{2} \| \theta - \theta_0 \|^2 \) with \( \lambda > 0 \), as typically done in training neural networks. For ease of notation, we define

\[
\ell^I_\lambda(F_t; \theta) := \ell^I(F_t; \theta) - \frac{m\lambda}{2} \| \theta - \theta_0 \|^2.
\]

(10)

Based on the RBMLE principle in (5) and the design in (9)-(10), at each time \( t \), the learner under NeuralRBMLE selects an arm that maximizes \( f(x_{t,a}; \theta^I_t) \), where

\[
\theta^I_t := \arg\max_{\theta} \left\{ \ell^I_\lambda(F_t; \theta) + \alpha(t) \max_{a \in [K]} f(x_{t,a}; \theta) \right\}.
\]

(11)

Inspired by Hung et al. (2021), we can further show that NeuralRBMLE can be simplified to an index strategy by interchanging the two max operations in (11). Now we are ready to present the prototypic NeuralRBMLE algorithm as follows: At each time \( t \),

1. Define the arm-specific RBMLE estimators

\[
\theta^I_{t,a} := \arg\max_{\theta} \left\{ \ell^I_\lambda(F_t; \theta) + \alpha(t) f(x_{t,a}; \theta) \right\}.
\]

(12)

2. Accordingly, for each arm, we construct an index as

\[
I^I_{t,a} := \ell^I_\lambda(F_t; \theta^I_{t,a}) + \alpha(t) f(x_{t,a}; \theta^I_{t,a}).
\]

(13)

Then, it can be shown that the policy induced by the NeuralRBMLE in (11) is equivalent to an index strategy which selects an arm with the largest \( I^I_{t,a} \) at each time \( t \). The proof is similar to that in Hung et al. (2021) and provided in Appendix E.1 for completeness.

**Remark 1.** Note that in (10)-(13) we use exponential family distributions as the surrogate likelihood functions for RBMLE. When the reward distributions are unknown, one could simply resort to some commonly-used distributions, such as the Gaussian likelihood function. On the other hand, when additional structures of the reward distributions are known, this design also enables the flexibility of better matching the true likelihood and the surrogate likelihood. For example, in the context of logistic bandits, the rewards are known to be binary, and hence one can apply the Bernoulli likelihood to obtain the corresponding NeuralRBMLE estimator.

**Remark 2.** The surrogate likelihood function in (9) follows the similar philosophy as that for the generalized linear bandits in Hung et al. (2021). Despite the similarity, one fundamental difference is that the objective function of NeuralRBMLE is no longer concave in \( \theta \). In spite of this, in Section 5 we show that the practical algorithms derived from NeuralRBMLE still enjoy favorable regret bounds with the help of the neural tangent kernel.

### 4.2 Practical NeuralRBMLE Algorithms

One major challenge in implementing the prototypic NeuralRBMLE algorithm in (12)-(13) is that the exact maximizer \( \theta^I_{t,a} \) in (12) can be difficult to obtain since the maximization problem of (12), which involves the neural function approximator \( f(x; \theta) \), is non-convex in \( \theta \). In this section, we proceed to present two practical implementations of NeuralRBMLE algorithm.

- **NeuralRBMLE by gradient ascent (NeuralRBMLE-GA):** To solve the optimization problem in (12), one natural approach is to apply gradient ascent to obtain an approximator \( \tilde{\theta}^I_{t,a} \) for \( \theta^I_{t,a} \), for
Algorithm 1 NeuralRBMLE via Gradient Ascent

1: \textbf{Input:} $\alpha(t), \zeta(t), \lambda, f, \theta_0, \eta, J$
2: \textbf{Initialization:} $\{\hat{\theta}^\dagger(0,i)\}_{i=1}^{K} \leftarrow \theta_0$
3: for $t = 1, 2, \ldots$ do
4: Observe all the contexts $\{x_{t,a}\}_{1 \leq a \leq K}$.
5: for $a = 1, \ldots, K$ do
6: compute $\hat{\theta}_{t,a}$ as the output of $J$-step gradient ascent with step size $\eta$ for solving $12$.
7: end for
8: select an arm $a_t = \text{argmax}_a \{f(x_t, \hat{\theta}_{t,a})\}$ and obtain reward $r_t$.
9: end for

Algorithm 2 NeuralRBMLE via Reward-Bias-Guided Parameter Correction

1: \textbf{Input:} $\alpha(t), \lambda, f, \theta_0, \eta, J$
2: \textbf{Initialization:} $Z_0 \leftarrow \lambda \mathbf{I}, \hat{\theta}_0 \leftarrow \theta_0$
3: for $t = 1, 2, \ldots$ do
4: Observe all the contexts $\{x_{t,a}\}_{1 \leq a \leq K}$.
5: for $a = 1, \ldots, K$ do
6: compute $\hat{\theta}_{t,a} = \hat{\theta} + \frac{\alpha(t)}{m} \cdot Z_{t-1}^{-1} g(x_t, \tilde{\theta}_t)$.
7: end for
8: select an action $a_t = \text{argmax}_a \{f(x_t, \tilde{\theta}_t)\}$ and obtain reward $r_t$.
9: set $\hat{\theta}_t$ as the output of $J$-step gradient ascent with step size $\eta$ for maximizing $\ell^\dagger(\mathcal{F}_t; \theta)$.
10: update $Z_t \leftarrow Z_{t-1} + g(x_t, \hat{\theta}_t) g(x_t, \hat{\theta}_t)^\top / m$.
11: end for

each arm. The pseudo code of NeuralRBMLE-GA is provided in Algorithm 1. Given the recent progress on the neural tangent kernel of neural networks (Jacot et al., 2018; Cao & Gu, 2019), the estimator $\hat{\theta}^\dagger_{t,a}$ serves as a good approximation for $\theta^\dagger_{t,a}$ despite the non-concave objective function in (12). This will be described in more detail in the regret analysis.

• NeuralRBMLE via reward-bias-guided parameter correction (NeuralRBMLE-PC): Note that by (12), finding each $\theta^\dagger_{t,a}$ originally involves solving an optimization problem for each arm. To arrive at a more computationally efficient algorithm, we propose a surrogate index for the original index policy in (13) with Gaussian likelihood. We observe that the main difference among the estimators $\hat{\theta}^\dagger_{t,a}$ of different arms lies in the reward-bias term $\alpha(t) f(x_{t,a}; \theta^\dagger_{t,a})$, as shown in (13).

Based on this observation, we propose to first (i) find a base estimator $\hat{\theta}_t$ without any reward bias and then (ii) approximately obtain the arm-specific RBMLE estimators by involving the neural tangent kernel of neural networks. Define

$$\hat{\theta}^\dagger_t : = \text{argmax}_\theta \{\ell^\dagger(\mathcal{F}_t; \theta)\},$$

Notably, $\hat{\theta}^\dagger_t$ can be viewed as the least squares estimate given $\mathcal{F}_t$ for the neural network $f(\cdot; \theta)$. We apply $J$-step gradient ascent with step size $\eta$ to solve (14), and denote $\hat{\theta}_t$ as the output of gradient ascent. Next, we define

$$Z_t := \lambda \mathbf{I} + \frac{1}{m} \sum_{\tau=1}^{t} g(x_{\tau}, \hat{\theta}_{\tau}) g(x_{\tau}, \hat{\theta}_{\tau})^\top,$$
and construct an approximate estimator for \( \theta_{t,a}^\dagger \) as
\[
\hat{\theta}_{t,a} := \tilde{\theta}_t + \frac{\alpha(t)}{m} Z_{t-1}^{-1} g(x_{t,a}; \tilde{\theta}_t),
\]
where \( \frac{\alpha(t)}{m} Z_{t-1}^{-1} g(x_{t,a}; \tilde{\theta}_t) \) reflects the effect of the reward-bias term on the neural network parameter. Then, we propose a surrogate index \( \tilde{I}_{t,a} \) for the index \( I_{t,a}^\dagger \) as
\[
\tilde{I}_{t,a} := f(x_{t,a}; \tilde{\theta}_t),
\]
for all \( a \in [K] \) and for all \( t \in [T] \). The detailed derivation for the surrogate index \( \tilde{I}_{t,a} \) are provided in Appendix 4. The main advantage of NeuralRBMLE-PC is that at each time step \( t \), the learner only needs to solve one optimization problem for the base estimator \( \tilde{\theta}_t \) and then follow the guidance of \( Z_{t-1}^{-1} g(x_{t,a}; \tilde{\theta}_t) \) that are readily available, instead of solving multiple optimization problems.

5 Regret Analysis of NeuralRBMLE

In this section, we present the regret analysis of the proposed NeuralRBMLE algorithms. To begin with, we introduce the following useful definition of the neural tangent kernel.

**Definition 1.** [Jacot et al. (2018)] For \( i, j \in [TK] \), define
\[
\Sigma_{i,j} := \langle x_i, x_j \rangle, \quad A_{i,j} := \begin{pmatrix} \Sigma_{i,j} & \Sigma_{i,j}^T \\ \Sigma_{i,j}^T & \Sigma_{i,j} \end{pmatrix},
\]
\[
\Sigma_{i,j}^{l+1} := 2 \cdot \mathbb{E}_{(u,v) \sim N(0,A_{i,j})}[\sigma(u)\sigma(v)],
\]
\[
\tilde{H}_{i,j} := \Sigma_{i,j},
\]
\[
\tilde{H}_{i,j}^{l+1} := 2 \tilde{H}_{i,j} E_{(u,v) \sim N(0,\lambda A_{i,j})} [\tilde{\sigma}(u)\tilde{\sigma}(v)] + \Sigma_{i,j}^{l+1},
\]
where \( \tilde{\sigma}(\cdot) \) denotes the derivative of \( \sigma(\cdot) \). Then, we define the neural tangent kernel matrix of an L-layer ReLU network on the training inputs \( \{x_i\}_{i=1}^{TK} \) as
\[
H := \begin{pmatrix} \tilde{H}_{i,j} + \Sigma_{i,j}^{L} / 2 \end{pmatrix}_{TK \times TK}.
\]

Then, for \( i \in [TK] \), we define the effective dimension \( \tilde{d} \) of the NTK matrix on contexts \( \{x_i\} \) as
\[
\tilde{d} := \frac{\log \det(I + H/\lambda)}{\log(1 + TK/\lambda)}.
\]

The effective dimension \( \tilde{d} \) is a data-dependent measure first introduced by Valko et al. (2013) to measure the actual underlying dimension of the set of observed contexts and later adapted to neural bandits (Zhou et al. 2020; Zhang et al. 2021), and \( \tilde{d} \) can be upper bounded in various settings (Chowdhury & Gopalan 2017; Zhang et al. 2021).

Next, we provide the regret bounds of NeuralRBMLE.

**Theorem 1.** Under NeuralRBMLE-GA in Algorithm 7 there exist positive constants \( \{C_{GA,i}\}_{i=1}^J \) such that for any \( \delta \in (0,1) \), if \( \alpha(t) = \Theta(\sqrt{T}) \), \( \eta \leq C_{GA,1}(m \lambda + TmL)^{-1} \), \( J \geq C_{GA,2} T \), and
\[
m \geq C_{GA,3} \max \left\{ T^{16} \lambda^{-7} L^{24} (\log m)^3, \right.
\]
\[
T^6 K^6 L^6 \lambda^{-\frac{\delta}{2}} \left( \log \left( T K L^2 / \delta \right) \right)^{-\frac{1}{2}} \left\} \right.,
\]
then with probability at least 1 - \( \delta \), the regret satisfies
\[
\mathcal{R}(T) \leq C_{GA,4} \sqrt{T} \cdot \tilde{d} \log(1 + TK/\lambda).
\]
The proof is provided in Appendix C.

We highlight the technical novelty of the analysis for NeuralRBMLE-GA as follows. The challenges in establishing the regret bound in Theorem 1 are mainly three-fold:

- (a) In neural bandits, applying the RMLE principle for low regret involves one inherent dilemma – the reward bias and \( \alpha(t) \) need to be large enough to achieve sufficient exploration, while \( \alpha(t) \) needs to be sufficiently small to enable the NTK-based approximation for low regret (cf. Lemma 2). This is one salient difference from the RMLE algorithm for linear bandits (Hung et al., 2021).

- (b) Moreover, as the additional reward-bias term is tightly coupled with the neural network in the objective (11) and the arm-specific estimators in (12), it is technically challenging to quantify the deviation of the learned policy parameter from \( \theta_0 \). This is one salient difference between NeuralRBMLE-GA and the existing neural bandit algorithms (Zhou et al., 2020; Zhang et al., 2021).

- (c) In NeuralRBMLE-GA, the surrogate likelihood is designed to be flexible and takes the general form of an exponential family distribution, instead of a Gaussian distribution as used in the existing neural bandit methods (Zhou et al., 2020; Zhang et al., 2021). As a result, we cannot directly exploit the special parametric form of the Gaussian likelihood in analyzing the RMLE index.

Given the above, we address these issues as follows: (i) We address the issue (b) by carefully quantifying the distance between the learned policy parameters and the initial parameter (cf. Lemmas 10-11) along with the supporting Lemmas 7-9). (ii) We tackle the issue (c) by providing bounds regarding the log-likelihood of the exponential family distributions in analyzing the arm-specific index (cf. Lemmas 12-13). (iii) Finally, based on the above results, we address the issue (a) by choosing a proper \( \alpha(t) \) that achieves low regret and enables NTK-based analysis simultaneously.

**Theorem 2.** Under NeuralRBMLE-PC in Algorithm 2, there exist positive constant \( C_{PC,1} \), \( C_{PC,2} \) and \( C_{PC,3} \) such that for any \( \delta \in (0, 1) \), if \( \alpha(t) = \Theta(\sqrt{t}) \), \( \eta \leq C_{PC,1}(m\lambda + TmL)^{-1} \), and

\[
m \geq C_{PC,2} \max \left\{ T^{21}\lambda^{-7}L^{24}(\log m)^3, \right. \]

\[
T^6K^6L^6\lambda^{-\frac{3}{4}} \left( \log (TKL^2/\delta) \right)^{\frac{3}{2}}, \left. \right\}, \]

the with probability at least \( 1 - \delta \), the regret satisfies

\[
R(T) \leq C_{PC,3} \sqrt{T} \cdot \tilde{d} \log(1 + TK/\lambda).
\]

The proof is provided in Appendix D.

We highlight the challenge and technical novelty of the analysis for NeuralRBMLE-PC as follows: Notably, the main challenge in establishing the regret bound in Theorem 2 lies in that the bias term affects not only the explore-exploit trade-off but also the approximation capability of the NTK-based analysis. Such a three-way trade-off due to the reward-bias term serves as one salient feature of NeuralRBMLE-PC, compared to RMLE for linear bandits (Hung et al., 2021) and other existing neural bandit algorithms (Zhou et al., 2020; Zhang et al., 2021). Despite the above challenges, we are still able to (i) characterize the interplay between regret and the reward-bias \( \alpha(t) \) (cf. (210)-(219) in Appendix D.2), (ii) specify the distance between \( \theta_0 \) and the learned policy parameter \( \hat{\theta}_{t,a} \) induced by the bias term (cf. Lemma 18), and (iii) carefully handle each regret component that involves \( \| g(x^*_t; \hat{\theta}_{1}) \|_2 \) in the regret bound by the technique of completing the square (cf. (221)-(231) in Appendix D.2).

### 6 Numerical Experiments

We evaluate the performance of NeuralRBMLE against the popular benchmark methods through experiments on various real-world datasets, including Adult, Covertype, Magic Telescope, Mushroom, Shuttle (Asuncion & Newman, 2007), and MNIST (LeCun et al., 2010). To construct bandit problems from these datasets, we follow the same procedure as in Zhou et al. (2020); Zhang et al. (2021) by converting classification problems to \( K \)-armed bandit problems with general reward functions. Specifically, we first convert each input feature \( x \in \mathbb{R}^d \) into \( K \) different context vectors, where
Figure 1: Cumulative regret averaged over 10 trials with $T = 1.5 \times 10^4$.

Table 1: Mean final cumulative regret over 10 trials for Figure 1 and Figure 3. The best of each column is highlighted.

| Mean Final Regret | Adult | Covertype | MagicTelescope | MNIST | Mushroom | Shuttle |
|-------------------|-------|-----------|----------------|-------|----------|---------|
| NeuralRBMLE-GA    | 3125.2| 4328.1    | 3342.9         | 1557.8| 313.1    | 335.2   |
| NeuralRBMLE-PC    | 3200.6| 4824.9    | 3630.2         | 2197.7| 580.4    | 817.7   |
| NeuralUCB         | 3154.9| 4697.7    | 3555.2         | 2079.5| 583.8    | 555.0   |
| NeuralTS          | 3179.0| 4813.3    | 3567.1         | 2585.7| 594.5    | 577.7   |
| DeepFPL           | 3174.9| 5207.3    | 3559.2         | 4473.0| 600.1    | 1622.9  |
| BoostedNN         | 3351.4| 5265.3    | 3929.7         | 6437.1| 805.1    | 1323.9  |
| LinRBMLE          | 3121.9| 4929.8    | 3885.0         | 11851.9| 656.0    | 3193.7  |

$x_{t,i} = (0^{d'}, x, 0^d)^{i-1} \in \mathbb{R}^{d'K} \equiv \mathbb{R}^d$ for $i \in [K]$. The learner receives a unit reward if the context is classified correctly, and receives zero reward otherwise. The benchmark methods considered in our experiments include the two state-of-the-art neural contextual bandit algorithms, namely NeuralTS [Zhang et al. (2021)] and NeuralUCB [Zhou et al. (2020)]. Furthermore, we also provide the results of multiple benchmark methods that enforce exploration directly in the parameter space, including BoostedNN [Osband et al. (2016)], the neural variant of random exploration through perturbation (DeepFPL) in [Kveton et al. (2020)], and RBMLE for linear bandits (LinRBMLE) in [Hung et al. (2021)]. For all the neural-network-based algorithms, we set $J = 100$ as the maximum number of steps for gradient decent, choose learning rate $\eta = 0.001$, and update the parameters at each time step. Each trial continues for $T = 15000$ steps except that we set $T = 8000$ in the experiments of Mushroom as the number of data samples in Mushroom is 8124. For $Z_t$ in NeuralRBMLE-PC, NeuralTS, NeuralUCB, we use the inverse of the diagonal elements of $Z_t$ to be the surrogate of $Z_t^{-1}$ to speed up the experiments. Notice that this procedure is also adopted by [Zhou et al. (2020), Zhang et al. (2021)]. To ensure a fair comparison among the algorithms, the hyperparameters of each algorithm are tuned, and the configuration is provided in Appendix F. All the results reported in this section are the average over 10 random seeds.

Effectiveness of NeuralRBMLE. Figure 1 Table 1 and Figure 3 (cf. Appendix H) show the empirical regret performance of each algorithm. We observe that NeuralRBMLE-GA outperforms most of the other benchmark methods under the six real-world datasets, and NeuralRBMLE-PC achieves empirical regrets competitive to the other state-of-the-art neural bandit algorithms. Table 2 in Appendix H shows the standard deviation of the regrets over random seeds. Notably, we observe that the performance of NeuralRBMLE and LinRBMLE appears more consistent across different random seeds than other benchmarks. This suggests that the reward-biased methods empirically enjoy better robustness across different sample paths.

NeuralRBMLE-GA with different likelihood functions. As described in Sections 4.2 and 5 NeuralRBMLE-GA opens up a whole new family of algorithms with provable regret bounds.
Figure 2: Cumulative regret of the three variants of NeuralRBMLE-GA averaged over 10 trials with $T = 1.5 \times 10^4$.

We provide the experiment of NeuralRBMLE-GA with the three different likelihood functions (i) $-\frac{1}{2}(f(x_s; \theta) - r_s)^2$, (ii) $r_s f(x_s; \theta) - \log (1 + e^{f(x_s; \theta)})$ and (iii) $-\frac{1}{2}(f(x_s; \theta) - r_s)^2 + r_s f(x_s; \theta) - \log (1 + e^{f(x_s; \theta)})$ are Gaussian, Bernoulli, and the mixture of Gaussian and Bernoulli likelihood, respectively, and all of them belong to some canonical exponential family. Figure 2 shows the empirical regrets of NeuralRBMLE-GA under different likelihood functions. We can observe that these three variants of NeuralRBMLE-GA have empirical regret competitive to other neural bandit algorithms like NeuralUCB, NeuralTS and DeepFPL. NeuralRBMLE-GA with Gaussian likelihood and the mixture of Gaussian and Bernoulli likelihood are the best in empirical regret. This corroborates the flexibility of NeuralRBMLE-GA in selecting the surrogate likelihood.

7 Related Work

RBMLE algorithms. RBMLE was first proposed by Kumar & Becker (1982) to maximize the long-term average reward for unknown MDPs in the context of adaptive control. Despite being a classic approach of optimal adaptive control, RBMLE has remained largely unknown vis-à-vis the finite-time performance until recently. In Liu et al. (2020), RBMLE has been extended to solve the standard non-contextual multi-armed bandit problems, and its regret bounds have been established under both sub-Gaussian and sub-exponential reward distributions. Subsequently, Hung et al. (2021) proposed to adapt the RBMLE principle and obtain simple index policies for both the standard linear bandits and the generalized linear bandits and accordingly established the order-optimal regret bounds. Moreover, Mete et al. (2021) applied RBMLE to model-based reinforcement learning and established a regret bound for finite MDPs. Despite the above promising results, it remains unexplored how to extend and analyze RBMLE for the more general contextual bandit problems. This paper presents the first RBMLE algorithm that achieves favorable regrets in contextual bandit problems with general reward functions.

Contextual bandits beyond linear realizability. To relax the linear realizability assumption, contextual bandits have been studied from the perspectives of using known general kernels Valko et al. (2013) and the surrogate model provided by Gaussian processes Chowdhury & Gopalan (2017). Moreover, one recent attempt is to leverage the representation power of deep neural networks to learn the unknown bounded reward functions Gu et al. (2021); Kveton et al. (2020); Riquelme et al. (2018); Zahavy & Mannor (2019); Zhou et al. (2020); Zhang et al. (2021); Zhu et al. (2022). Among the above, the prior works most related to this paper are NeuralUCB Zhou et al. (2020) and NeuralTS Zhang et al. (2021), which incorporate the construction of confidence sets of UCB and the posterior sampling technique of TS into the training of neural networks, respectively. Another two recent preprints propose Neural-LinUCB Xu et al. (2020) and NPR Anonymous (2022), which incorporate shallow exploration in the sense of LinUCB and the technique of reward perturbation into neural bandits, respectively. Different from the above neural bandit algorithms, NeuralRBMLE achieves efficient exploration in a fundamentally different manner by following the guidance of the reward-bias term in the parameter space, instead.

*Due to space limitation, a summary of related work on linear bandits is in Appendix [9]*
of using posterior sampling, reward perturbation, or confidence bounds derived from concentration inequalities.

8 Conclusion

This paper presents NeuralRBMLE, the first bandit algorithm that extends the classic RBMLE principle in adaptive control to contextual bandits with general reward functions. Through regret analysis and extensive simulations on real-world datasets, we show that NeuralRBMLE indeed achieves competitive regret performance compared to the state-of-the-art neural bandit algorithms. As a result, we expect that NeuralRBMLE would be a promising solution to real-world bandit problems with complex reward functions.

References

Abbasi-Yadkori, Y., Pál, D., and Szepesvári, C. Improved algorithms for linear stochastic bandits. *Advances in neural information processing systems*, 24:2312–2320, 2011.

Abeille, M., Lazaric, A., et al. Linear Thompson sampling revisited. *Electronic Journal of Statistics*, 11(2):5165–5197, 2017.

Agrawal, S. and Goyal, N. Thompson sampling for contextual bandits with linear payoffs. In *International Conference on Machine Learning*, pp. 127–135, 2013.

Allen-Zhu, Z., Li, Y., and Song, Z. A convergence theory for deep learning via over-parameterization. In *International Conference on Machine Learning*, pp. 242–252. PMLR, 2019.

Anonymous. Learning neural contextual bandits through perturbed rewards. In Submitted to *The Tenth International Conference on Learning Representations*, 2022. URL https://openreview.net/forum?id=7inCJ3MhXt3 under review.

Asuncion, A. and Newman, D. Uci machine learning repository, 2007.

Auer, P. Using confidence bounds for exploitation-exploration trade-offs. *Journal of Machine Learning Research*, 3(Nov):397–422, 2002.

Borkar, V. The Kumar-Becker-Lin scheme revisited. *Journal of Optimization Theory and Applications*, 66(2):289–309, 1990.

Campi, M. C. and Kumar, P. Adaptive linear quadratic Gaussian control: the cost-biased approach revisited. *SIAM Journal on Control and Optimization*, 36(6):1890–1907, 1998.

Cao, Y. and Gu, Q. Generalization bounds of stochastic gradient descent for wide and deep neural networks. In *Advances in Neural Information Processing Systems*, pp. 10836–10846, 2019.

Chowdhury, S. R. and Gopalan, A. On kernelized multi-armed bandits. In *International Conference on Machine Learning*, pp. 844–853, 2017.

Chu, W., Li, L., Reyzin, L., and Schapire, R. Contextual bandits with linear payoff functions. In *International Conference on Artificial Intelligence and Statistics*, pp. 208–214, 2011.

Dani, V., Hayes, T. P., and Kakade, S. M. Stochastic linear optimization under bandit feedback. In *Conference on Learning Theory*, 2008.

Dumitrascu, B., Feng, K., and Engelhardt, B. Pg-ts: Improved Thompson sampling for logistic contextual bandits. In *Advances in neural information processing systems*, pp. 4624–4633, 2018.

Filippi, S., Cappe, O., Garivier, A., and Szepesvári, C. Parametric bandits: The generalized linear case. In *Advances in Neural Information Processing Systems*, pp. 586–594, 2010.

Gu, Q., Karbasi, A., Khosravi, K., Mirrokni, V., and Zhou, D. Batched neural bandits. *arXiv preprint arXiv:2102.13028*, 2021.
Hung, Y.-H., Hsieh, P.-C., Liu, X., and Kumar, P. Reward-biased maximum likelihood estimation for linear stochastic bandits. In *AAAI Conference on Artificial Intelligence*, volume 35, pp. 7874–7882, 2021.

Jacot, A., Gabriel, F., and Hongler, C. Neural tangent kernel: Convergence and generalization in neural networks. *Advances in Neural Information Processing Systems*, 2018.

Jun, K.-S., Bhargava, A., Nowak, R., and Willett, R. Scalable generalized linear bandits: online computation and hashing. In *Advances in Neural Information Processing Systems*, pp. 98–108, 2017.

Kirschner, J. and Krause, A. Information directed sampling and bandits with heteroscedastic noise. In *Conference On Learning Theory*, pp. 358–384, 2018.

Kumar, P. and Becker, A. A new family of optimal adaptive controllers for markov chains. *IEEE Transactions on Automatic Control*, 27(1):137–146, 1982.

Kveton, B., Zaheer, M., Szepesvari, C., Li, L., Ghavamzadeh, M., and Boutilier, C. Randomized exploration in generalized linear bandits. In *International Conference on Artificial Intelligence and Statistics*, pp. 2066–2076, 2020.

Lattimore, T. and Szepesvári, C. *Bandit algorithms*. Cambridge University Press, 2020.

LeCun, Y., Cortes, C., and Burges, C. Mnist handwritten digit database. at&t labs, 2010.

Li, L., Lu, Y., and Zhou, D. Provably optimal algorithms for generalized linear contextual bandits. In *International Conference on Machine Learning*, pp. 2071–2080, 2017.

Liu, X., Hsieh, P.-C., Hung, Y. H., Bhattacharya, A., and Kumar, P. Exploration through reward biasing: Reward-biased maximum likelihood estimation for stochastic multi-armed bandits. In *International Conference on Machine Learning*, pp. 6248–6258. PMLR, 2020.

Mandl, P. Estimation and control in markov chains. *Advances in Applied Probability*, pp. 40–60, 1974.

Mete, A., Singh, R., Liu, X., and Kumar, P. Reward biased maximum likelihood estimation for reinforcement learning. In *Learning for Dynamics and Control*, pp. 815–827, 2021.

Nesterov, Y. Gradient methods for minimizing composite functions. *Mathematical Programming*, 140(1):125–161, 2013.

Osband, I., Blundell, C., Pritzel, A., and Van Roy, B. Deep exploration via bootstrapped dqn. *arXiv preprint arXiv:1602.04621*, 2016.

Prandini, M. and Campi, M. C. Adaptive LQG Control of Input-Output Systems—A Cost-biased Approach. *SIAM Journal on Control and Optimization*, 39(5):1499–1519, 2000.

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*, 2018.

Rusmevichientong, P. and Tsitsiklis, J. N. Linearly parameterized bandits. *Mathematics of Operations Research*, 35(2):395–411, 2010.

Russo, D. and Van Roy, B. An information-theoretic analysis of Thompson sampling. *Journal of Machine Learning Research*, 17(1):2442–2471, 2016.

Russo, D. and Van Roy, B. Learning to optimize via information-directed sampling. *Operations Research*, 66(1):230–252, 2018.

Valko, M., Korda, N., Munos, R., Flaounas, I., and Cristianini, N. Finite-time analysis of kernelised contextual bandits. In *Uncertainty in Artificial Intelligence*, 2013.

Vershynin, R. *High-dimensional probability: An introduction with applications in data science*, volume 47. Cambridge university press, 2018.
Appendix

A Supporting Lemmas for the Regret Analysis

Lemma 1. (Zhou et al., 2020, Lemma 5.1) There exists a positive constant $F_1$ and $\theta^* \in \mathbb{R}^p$ such that for any $\delta \in (0, 1)$ and all observed context vectors $x$, with probability at least $1 - \delta$, under $m \geq F_1^1 K^4 L^6 \log(T^2 K^2 L/\delta^4)$, we have

$$h(x) = \langle g(x; \theta_0), \theta^* - \theta_0 \rangle$$

(28)

$$\sqrt{m} \| \theta^* - \theta_0 \|_2 \leq \sqrt{2} \mathbf{h}^\top \mathbf{H}^{-1} \mathbf{h} \leq S,$$

(29)

where $\mathbf{H}$ is defined in (22), and $\mathbf{h} := [h(x_t, a)]_{t \in [K], a \in [T]}$. According to Zhou et al., 2020, $S$ is a constant when the reward function $h(\cdot)$ belongs to $\mathcal{H}$, the RKHS function space induced by NTK, and $\|h\|_{\mathcal{H}} \leq \infty$.

Lemma 2. (Cao & Gu, 2019, Lemma 4.1) There exist positive constants $F_2$, $F_2^1$, and $F_2^2$, such that for any $\delta \in (0, 1)$ and all observed context vectors $x$, with probability at least $1 - \delta$, if $\tau$ satisfies that

$$F_2^1 m^{-\frac{3}{2}} L^{-\frac{3}{2}} \left[ \log \left(TK L^2/\delta \right) \right]^{\frac{3}{2}} \leq \tau \leq F_2^2 L^{-6} (\log m)^{-\frac{3}{2}},$$

(30)

then for all $\theta$ that satisfies $\| \theta - \theta_0 \|_2 \leq \tau$, we have

$$\| f(x; \theta) - \langle g(x; \theta), \theta - \theta_0 \rangle \| \leq F_2 \tau^1 L^3 \sqrt{m \log m}.$$ (31)

Notice that under the initialization steps in Section 2.2, we have $f(x; \theta_0) = 0$ for all observed context vectors $x$.

Lemma 3. (Allen-Zhu et al., 2019, Theorem 5) There exist positive constants $F_3^1$, $F_3^2$, and $F_3^3$, such that for any $\delta \in (0, 1)$ and all observed context vectors $x$, with probability at least $1 - \delta$, if $\tau$ satisfies that

$$F_3^1 m^{-\frac{3}{2}} L^{-\frac{3}{2}} \max \left\{ (\log m)^{-\frac{3}{2}}, \log (TK/\delta)^{\frac{3}{2}} \right\} \leq \tau \leq F_3^2 L^{-\frac{3}{2}} (\log m)^{-3},$$

(32)

then for all $\theta$ that satisfies $\| \theta - \theta_0 \|_2 \leq \tau$, we have

$$\| g(x; \theta) - g(x; \theta_0) \|_2 \leq F_3 \sqrt{\log m \tau^2} L^3 \| g(x; \theta_0) \|_2.$$ (33)

Lemma 4. (Cao & Gu, 2019, Lemma B.3) There exist positive constants $F_4^1$, $F_4^2$, and $F_4^3$ for any $\delta \in (0, 1)$ and all observed context vectors $x$, with probability at least $1 - \delta$, if $\tau$ satisfies that

$$F_4^1 m^{-\frac{3}{2}} L^{-\frac{3}{2}} \left[ \log TKL^2/\delta \right]^{\frac{3}{2}} \leq \tau \leq F_4^2 L^{-6} (\log m)^{-\frac{3}{2}},$$

(34)

then for all $\theta$ that satisfies $\| \theta - \theta_0 \|_2 \leq \tau$, we have $\| g(x; \theta) \|_2 \leq F_4 \sqrt{m \tau L}$.  

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Lemma 5. (Hoeffding’s inequality) For a sequence of independent, zero-mean, sub-Gaussian random variables $X_1, \ldots, X_t$, we have
\[
P \left\{ \frac{1}{t} \sum_{s=1}^{t} X_s \geq \delta_1 \right\} \leq 2 \exp(-F_{E_{1}}^2),
\]
where $F_{E_{1}}$ is a constant that is independent of $\delta_1$ but dependent on the sub-Gaussianity parameters.

Proof. This is the direct result of Theorem 2.6.2 in Vershynin (2018).

Lemma 6. (Bernstein’s inequality) For a sequence of independent, zero-mean, sub-exponential random variables $X_1, \ldots, X_t$, we have
\[
P \left\{ \frac{1}{t} \sum_{s=1}^{t} X_s \geq \delta_2 \right\} \leq 2 \exp(-\min\{F_{E_{1}}^2, F_{E_{2}}^2\}).
\]
where $F_{E_{1}}, F_{E_{2}}$ are constants that are independent of $\delta_2$ but dependent on the sub-exponentiality parameters.

Proof. This is the direct result of Theorem 2.8.1 in Vershynin (2018).

Lemma 7. For all $t \in [T_0, T]$, with probability at least $1 - \frac{1}{t^2}$, we have
\[
\left| \sum_{s=1}^{t} r_s \right| \leq F_{E_{1}} t \sqrt{\log t},
\]
\[
\sum_{s=1}^{t} r_s^2 \leq F_{E_{2}} t \log t,
\]
where $T_0 = \inf_s \left\{ s \in \mathbb{N} : E_{E_{1}} \left( \frac{2 \log(2s)}{s^2} \right) \leq E_{E_{2}} \left( \frac{2 \log(2s)}{s^2} \right), s \geq 2 \right\}$ and $E_{E_{1}}, E_{E_{2}}$ are absolute constants.

Proof. By Lemma 5 and letting $\delta_1 = \sqrt{\frac{2 \log(2t)}{t^2}}$, for the sub-Gaussian noise $\{\epsilon_s\}_{s=1}^{t}$ which are assumed to be conditionally independent given the contexts $\{x_1, \cdots, x_t\}$, we have
\[
P \left\{ \frac{1}{t} \sum_{s=1}^{t} \epsilon_s \leq \sqrt{\frac{2 \log(2t)}{t^2}} \right\} \geq 1 - 2 \exp(-E_{E_{1}} \frac{2 \log(2t)}{t^2})
\]
\[
= 1 - \frac{1}{2t^2}.
\]
Then, choosing $F_{E_{1}} = \sqrt{\frac{2 \log(2t)}{t^2}}$ and $T_0 \geq 2$, we have proved (37). Similarly, letting $\delta_2 = \sqrt{\frac{2 \log(2t)}{t^2}}$, for all $t$ that satisfies
\[
E_{E_{1}} \left( \frac{2 \log(2t)}{t^2} \right) \leq E_{E_{2}} \left( \frac{2 \log(2t)}{t^2} \right),
\]
we have
\[
P \left\{ \frac{1}{t} \sum_{s=1}^{t} \epsilon_s^2 \leq \delta_2 \right\} \geq 1 - 2 \exp(-\min\{F_{E_{1}}^2, F_{E_{2}}^2\})
\]
\[
= 1 - \frac{1}{2t^2},
\]
where (42) holds by Lemma 5 with $\{\epsilon_s^2\}_{s=1}^{t}$ are sub-exponential random variables. (43) holds by (41). Then, choosing $F_{E_{2}} = \sqrt{\frac{2 \log(2t)}{t^2}}$ and $T_0 \geq 2$, we have proved (38). By combining (40) and (44), we complete the proof by the boundedness of $h(\cdot)$.
B Supporting Lemmas for the Proof of Theorem 1

Define

\[ \mathcal{L}_{t,a}^\dagger(\theta) := \sum_{s=1}^{t-1} \left( b(f(x_s; \theta)) - r_s f(x_s; \theta) \right) + \frac{m\lambda}{2} \| \theta - \theta_0 \|^2 - \alpha(t) f(x_{t,a}; \theta) \quad (45) \]

as the loss function we used in Algorithm 1. Then, according to the update rule of gradient descent with step size \( \eta \) and total number of steps \( J \) used in Algorithm 1, we formally define the parameter \( \tilde{\theta}_{t,a}^\dagger \) here. Define

\[ \tilde{\theta}_{t,a}^\dagger = \theta_{t,a}^\dagger(0) \]

\[ \tilde{\theta}_{t,a}^\dagger = \theta_{t,a}^\dagger(j-1) - \eta \nabla \theta \mathcal{L}_{t,a}^\dagger(\theta_{t,a}^\dagger(j-1)) \]

\[ \tilde{\theta}_{t,a}^\dagger(0) = \theta_0. \]

Then, the following lemma shows the upper bound of the log-likelihood under \( \tilde{\theta}_{t,a}^\dagger \).

**Lemma 8.** There exist a positive constant \( F_{S_1,2} \) and \( F_{S_2} \), which are independent to \( m \) and \( t \), such that for all \( j \in [J] \), \( a \in [K] \), \( t \in [T] \) and under

\[ m \geq \frac{F_{S_1,2} F_{S_2}}{2 \lambda^8 T^7 \lambda^{-8} L^{18}(\log T)^{-4}(\log m)^3}, \quad (49) \]

if \( \alpha(t) = \sqrt{t} \) and \( \tilde{\theta}_{t,a}^\dagger(j) \) that satisfies

\[ \| \tilde{\theta}_{t,a}^\dagger(j) - \theta_0 \|_2 \leq F_{S_1,2} \sqrt{\frac{t \log t}{m \lambda^2}}, \quad (50) \]

then we have

\[ \sum_{s=1}^{t} \left( b(f(x_s; \tilde{\theta}_{t,a}^\dagger(j))) - r_s f(x_s; \tilde{\theta}_{t,a}^\dagger(j)) \right) \leq F_{S_2} \sqrt{\log t} \quad (51) \]

**Proof.** According to the gradient update rule, for all \( j \in [J] \), we have

\[ \mathcal{L}_{t,a}^\dagger(\tilde{\theta}_{t,a}^\dagger) - \frac{m\lambda}{2} \left( \tilde{\theta}_{t,a}^\dagger(j) - \theta_0 \right)^2 \leq \mathcal{L}_{t,a}^\dagger(\theta_{t,a}^\dagger) \leq \mathcal{L}_{t,a}^\dagger(\theta_0) = \sum_{s=1}^{t-1} b(0), \quad (52) \]

where the equality holds due to \( f(x_{t,a}; \theta_0) = 0 \) for all \( a \in [K], t \in [T] \). Rearranging (52), we have

\[ \sum_{s=1}^{t-1} \left( b(f(x_s; \tilde{\theta}_{t,a}^\dagger(j))) - r_s f(x_s; \tilde{\theta}_{t,a}^\dagger(j)) \right) \]

\[ \leq \sum_{s=1}^{t-1} b(0) + \alpha(t) \left( |g(x_{t,a}; \tilde{\theta}_{t,a}^\dagger(j))| + F_{S_1} \left( F_{S_2} \sqrt{\frac{t \log t}{m \lambda^2}} \right)^{\frac{4}{3}} L^3 \sqrt{m \log m} \right) \]

\[ \leq \sum_{s=1}^{t-1} b(0) + \alpha(t) E_{S_1} F_{S_2} \sqrt{L \frac{t \log t}{m \lambda^2}} + \alpha(t) E_{S_1} F_{S_2} \sqrt{\frac{t \log t}{m \lambda^2}}^{\frac{4}{3}} L^3 \sqrt{m \log m} \]

\[ = (t-1)b(0) + \alpha(t) E_{S_1} F_{S_2} \sqrt{L \frac{t \log t}{m \lambda^2}} + \alpha(t) E_{S_1} F_{S_2} \sqrt{t \log t \lambda^2} \]

where (53) holds by substituting the reward-biased term by Lemma 2 and (54) holds due to Lemma 4 and Cauchy–Schwarz inequality. Notice that (49) satisfies the conditions of \( m \) in both Lemma 2 and Lemma 4. Then, by letting \( \alpha(t) = \sqrt{t}, \ m \geq \frac{F_{S_1,2} F_{S_2}}{2 \lambda^8 T^7 \lambda^{-8} L^{18}(\log T)^{-4}(\log m)^3} \) and \( F_{S_2} = 3 \max\{b(0), 2E_{S_1} F_{S_2} \sqrt{\frac{L}{\lambda^2}}, 1\} \), we complete the proof. \( \square \)
Lemma 9. For all \( j \in [J], \ a \in [K], \ t \in [T] \) and \( m \) satisfies that \( m \geq \tilde{C}_1 T^7 \lambda^{-7} L^{21} (\log m)^3 \), we have
\[
\sum_{s=1}^{t} |b'(f(x_s; \tilde{\theta}_{t,a}^{(j)}))| \leq E_{[t]} \sqrt{\log t} \tag{56}
\]
where \( E_{[t]} \) is an absolute constant.

Proof. First, we start by obtaining an upper bound of \( \sum_{s=1}^{t} |f(x_s; \tilde{\theta}_{t,a}^{(j)})| \). By Lemma 8 we have
\[
E_{[t]} \sqrt{\log t} \geq \sum_{s=1}^{t} \left( b(f(x_s; \tilde{\theta}_{t,a}^{(j)})) - r_s f(x_s; \tilde{\theta}_{t,a}^{(j)}) \right) \tag{57}
\]
\[
= \sum_{s=1}^{t} \left( b(f(x_s; \theta_0)) + b'(f(x_s; \theta_0))(f(x_s; \tilde{\theta}_{t,a}^{(j)}) - f(x_s; \theta_0)) + \frac{L_b}{2} (f(x_s; \tilde{\theta}_{t,a}^{(j)}) - f(x_s; \theta_0))^2 - r_s f(x_s; \tilde{\theta}_{t,a}^{(j)}) \right) \tag{58}
\]
\[
= \sum_{s=1}^{t} \left( b(0) + b'(0) f(x_s; \tilde{\theta}_{t,a}^{(j)}) + \frac{L_b}{2} f(x_s; \tilde{\theta}_{t,a}^{(j)})^2 - r_s f(x_s; \tilde{\theta}_{t,a}^{(j)}) \right) \tag{59}
\]
\[
= \sum_{s=1}^{t} \left( L_b (f(x_s; \tilde{\theta}_{t,a}^{(j)}) + \frac{b'(0) - r_s}{L_b})^2 + b(0) - \frac{(b'(0) - r_s)^2}{2L_b} \right) \tag{60}
\]
where (58) holds because \( b'(\cdot) \) is \( L_b \)-strongly convex, (59) holds by \( f(x; \theta_0) = 0 \) for all vector \( x \). Then, reorganizing the terms in (60) and applying Lemma 7 to find bounds for the terms that involve \( r_s \), with probability at least \( 1 - \frac{1}{T} \), we have
\[
F_{[t]} \sqrt{\log t} \geq \sum_{s=1}^{t} \left( f(x_s; \tilde{\theta}_{t,a}^{(j)}) + \frac{b'(0) - r_s}{L_b} \right)^2, \tag{61}
\]
where \( F_{[t]} = E_{[t]} + b(0) + \frac{b'(0)^2}{L_b} + \frac{L_b}{2L_b} + \frac{L_b}{2L_b} \). Applying Cauchy–Schwarz inequality to (61), we have
\[
F_{[t]} \sqrt{\log t} \cdot \sum_{s=1}^{t} 1^2 \geq \sum_{s=1}^{t} \left( f(x_s; \tilde{\theta}_{t,a}^{(j)}) + \frac{b'(0) - r_s}{L_b} \right)^2 \cdot \sum_{s=1}^{t} 1^2 \tag{62}
\]
\[
\geq \left( \sum_{s=1}^{t} \left( f(x_s; \tilde{\theta}_{t,a}^{(j)}) + \frac{b'(0) - r_s}{L_b} \right)^2 \right) \tag{63}
\]
Reorganizing (63) and applying Lemma 7 we have
\[
\sum_{s=1}^{t} |f(x_s; \tilde{\theta}_{t,a}^{(j)})| \leq F_{[t]} t \sqrt{\log t}, \tag{64}
\]
where \( F_{[t]} = F_{[t]} + \frac{b'(0)}{L_b} + \frac{L_b}{2L_b} \) is a positive constant. Then, by Taylor’s Theorem and the fact that \( b''(z) \leq U_b \), for all \( z \), we have
\[
\sum_{s=1}^{t} |b'(f(x_s; \tilde{\theta}_{t,a}^{(j)}))| \leq \sum_{s=1}^{t} |b'(f(x_s; \theta_0))| + \sum_{s=1}^{t} U_b |f(x_s; \tilde{\theta}_{t,a}^{(j)}) - f(x_s; \theta_0)| \tag{65}
\]
\[
= \sum_{s=1}^{t} |b'(0)| + \sum_{s=1}^{t} U_b |f(x_s; \tilde{\theta}_{t,a}^{(j)})| \tag{66}
\]
\[
\leq F_{[t]} \sqrt{\log t}, \tag{67}
\]
where (66) hold by \( f(x; \theta_0) = 0 \) for all vector \( x \). (67) holds by (64) and choosing \( F_{[t]} = b'(0) + U_b F_{[t]} \). Then, we complete the proof. \( \square \)
Then, for all $x$, derive an upper bound for the regularization term of $L$ as the loss function under the approximation in the NTK regime. Then, given the update rule of $\theta_t$, we start by considering a collection of scalar variables as follows:

$\tilde{\theta}^{(t)}_{t,a} = \tilde{\theta}^{(0)}_{t,a}$ \hfill (70)

$\tilde{\theta}^{(j)}_{t,a} = \tilde{\theta}^{(j-1)}_{t,a} - \eta \nabla_{\theta_t} \mathcal{L}_{t,a}(\tilde{\theta}^{(j-1)}_{t,a})$ \hfill (71)

$\tilde{\theta}^{(0)}_{t,a} = \theta_0$ \hfill (72)

The next lemma given an upper bound of the term $\|\tilde{\theta}^{(j)}_{t,a} - \theta_0\|_2$ for all $j \in [J]$.

**Lemma 10.** For all $j \in [J]$, $t \in [T]$ and $a \in [K]$, we have

$$
\left\|\tilde{\theta}^{(j)}_{t,a} - \theta_0\right\|_2 \leq E_{10} \sqrt{\frac{t \log t}{m\lambda^2}}
$$

**Proof.** We start by considering a collection of scalar variables $\{x_s\}_{s=1}^t$ and studying the function $\sum_{s=1}^{t-1} (b(x_s) - r_s x_s)$. For each $x_s$, define $x^*_s := \arg\min_x \{b(x) - r_s x\}$. Due to the strong convexity of the log-likelihood of an exponential family, it is easy to show that $x^*_s = \arg\min_x \{b(x) - r_s x\} = b^{-1}(r_s)$. \hfill (74)

Then, for all $x_s \in \{x_s\}_{s=1}^{t-1}$, we have

$$
\sum_{s=1}^{t-1} (b(x_s) - r_s x_s) \geq \sum_{s=1}^{t-1} (b(x^*_s) - r_s x^*_s) \geq (t - 1)b\left(\frac{1}{t-1} \sum_{s=1}^{t-1} b^{-1}(r_s)\right) - \sum_{s=1}^{t-1} r_s b^{-1}(r_s) \geq E_{10} t - \frac{1}{L_b} E_{10} t \log t \geq -E_{10} t \log t,
$$

where (75), (76) hold by (74), (77) holds by Jensen’s inequality, (78) holds by the fact that $b(\cdot)$ is a strongly convex function, Lemma 3 and that $E_{10}$ is a positive constant. Based on this, we can derive an upper bound for the regularization term of $\mathcal{L}_{t,a}(\tilde{\theta}^{(j)}_{t,a})$.

$$
\frac{m\lambda}{2} \left\|\tilde{\theta}^{(j)}_{t,a} - \theta_0\right\|_2^2 \leq \sum_{s=1}^{t-1} \left(b(\langle g(x_s; \theta_0), \tilde{\theta}^{(j)}_{t,a} - \theta_0\rangle) - r_s \langle \tilde{\theta}^{(j)}_{t,a} - \theta_0\rangle \right) + \frac{m\lambda}{2} \left\|\tilde{\theta}^{(j)}_{t,a} - \theta_0\right\|_2^2 - \alpha(t) \left\|g(x_t; \theta_0), \tilde{\theta}^{(j)}_{t,a} - \theta_0\right\|_2
$$

$$
+ E_{10} t \log t + \alpha(t) \left\|g(x_t; \theta_0)\right\|_2 \cdot \left\|\tilde{\theta}^{(j)}_{t,a} - \theta_0\right\|_2 \leq \mathcal{L}_{t,a}(\tilde{\theta}^{(j)}_{t,a}) + E_{10} t \log t + E_{10} \sqrt{tmL} \left\|\tilde{\theta}^{(j)}_{t,a} - \theta_0\right\|_2
$$

$$
\leq \mathcal{L}_{t,a}(\theta_0) + E_{10} t \log t + E_{10} \sqrt{tmL} \left\|\tilde{\theta}^{(j)}_{t,a} - \theta_0\right\|_2,
$$

where $\mathcal{L}_{t,a}(\tilde{\theta}^{(j)}_{t,a})$, $\mathcal{L}_{t,a}(\tilde{\theta}^{(j)}_{t,a})$, and $\mathcal{L}_{t,a}(\theta_0)$ are the loss functions defined in the NTK regime.
where \( (80) \) holds by \( (79) \) and Cauchy–Schwarz inequality, \( (81) \) holds by Lemma 4 and \( (82) \) holds by the rule of gradient descent. Then, by solving the quadratic equation induced by \( (82) \), we have

\[
\left\| \hat{\theta}_{t,a}^{(j)} - \theta_0 \right\|_2 \leq \frac{4E_\text{tr}L}{m\lambda} + \sqrt{\frac{2L_{t,a}(\theta_0)}{m\lambda}} + \sqrt{\frac{2E_{\text{tr}}t \log t}{m\lambda}} + \frac{E_{\text{tr}}^2 L}{m\lambda^2} \tag{83}
\]

\[
\leq E_\text{tr} \sqrt{\frac{t \log t}{m\lambda^2}}, \tag{84}
\]

where \( E_\text{tr} = 4 \max\{E_{\text{tr}} \sqrt{t}, 2b(0), 2E_{\text{tr}}^2, E_{\text{tr}}^2 L\} \) is a positive constant.

The next lemma gives an upper bound of the term \( \left\| \hat{\theta}_{t,a}^{(j)} - \theta_0 \right\|_2 \), for each \( j \in [J] \).

**Lemma 11.** For all \( j \in [J], t \in [T] \) and \( a \in [K] \), we have

\[
\left\| \hat{\theta}_{t,a}^{(j)} - \theta_0 \right\|_2 \leq E_{\text{tr}} \sqrt{\frac{t \log t}{m\lambda^2}} \tag{85}
\]

where \( E_{\text{tr}} = 2E_\text{tr} \) is a positive constant.

**Proof.** Let’s prove this lemma by induction. It is straightforward to verify that \( (85) \) holds if \( j = 0 \).

Next, we assume that \( \left\| \hat{\theta}_{t,a}^{(j)} - \theta_0 \right\|_2 \leq E_{\text{tr}} \sqrt{\frac{t \log t}{m\lambda^2}} \) holds. By plugging \( (47) \) and \( (71) \), we have

\[
\left\| \hat{\theta}_{t,a}^{(j+1)} - \hat{\theta}_{t,a}^{(j)} \right\|_2 = \left\| \hat{\theta}_{t,a}^{(j)} - \hat{\theta}_{t,a}^{(j)} - \eta \sum_{s=1}^{t} g(x_s; \hat{\theta}_{t,a}^{(j)}) \left( b'(f(x_s; \hat{\theta}_{t,a}^{(j)})) - r_s \right) 
\]

\[+ \eta \sum_{s=1}^{t} g(x_s; \theta_0) \left( b'(g(x_s; \theta_0, \hat{\theta}_{t,a}^{(j)}) - \hat{\theta}_{t,a}^{(j)}) - r_s \right) 
\]

\[= \left\| (1 - \eta m\lambda)(\hat{\theta}_{t,a}^{(j)} - \hat{\theta}_{t,a}^{(j)}) - \eta \sum_{s=1}^{t} \left( g(x_s; \hat{\theta}_{t,a}^{(j)}) - g(x_s; \theta_0) \right) \left( b'(f(x_s; \hat{\theta}_{t,a}^{(j)})) - r_s \right) 
\]

\[- \eta \sum_{s=1}^{t} g(x_s; \theta_0) \left( b'(g(x_s; \theta_0, \hat{\theta}_{t,a}^{(j)}) - b'(g(x_s; \theta_0, \hat{\theta}_{t,a}^{(j)}) - b'(g(x_s; \theta_0, \hat{\theta}_{t,a}^{(j)}) - \theta_0)) \right) 
\]

\[+ \eta \alpha(t)(g(x_t; \hat{\theta}_{t,a}^{(j)}) - g(x_t; \theta_0)) \right\|_2 \tag{86}
\]

For the term \( b'(f(x_s; \hat{\theta}_{t,a}^{(j)})) - b'(g(x_s; \theta_0, \hat{\theta}_{t,a}^{(j)} - \theta_0)) \), by mean-value theorem, there exists a set of positive constants \( \{ E_{10,1,s} \}_{s=1}^{t-1} \) with \( E_{10,1,s} \in [L_b, U_b] \) for every \( s \in \{1, \ldots, t-1\} \), such that

\[
b'(f(x_s; \hat{\theta}_{t,a}^{(j)})) - b'(g(x_s; \theta_0, \hat{\theta}_{t,a}^{(j)} - \theta_0)) = E_{10,1,s} \left( f(x_s; \hat{\theta}_{t,a}^{(j)}) - g(x_s; \theta_0, \theta_0) \right), \tag{88}
\]
where (88) hold by $L_b \leq b''(\cdot) \leq U_b$. Then, plugging (88) into (87), we have
\[
\left\| \tilde{\theta}_{t,a}^{(j+1)} - \tilde{\theta}_{t,a}^{(j+1)} \right\|_2 \\
= (1 - \eta m \lambda) \left( \tilde{\theta}_{t,a}^{(j)} - \tilde{\theta}_{t,a}^{(j)} \right) - \eta \sum_{s=1}^{t-1} \left( g(x_s; \tilde{\theta}_{t,a}^{(j)}) - g(x_s; \theta_0) \right) \left( b'(f(x_s; \tilde{\theta}_{t,a}^{(j)})) - r_s \right) \\
- \eta \sum_{s=1}^{t-1} E_{t,a}^s g(x_s; \theta_0) \left( f(x_s; \tilde{\theta}_{t,a}^{(j)}) - (g(x_s; \theta_0), \tilde{\theta}_{t,a}^{(j)} - \theta_0) + (g(x_s; \theta_0), \tilde{\theta}_{t,a}^{(j)} - \tilde{\theta}_{t,a}^{(j)}) \right) \\
+ \eta \alpha(t) \left( g(x_{t,a}; \tilde{\theta}_{t,a}^{(j)}) - g(x_{t,a}; \theta_0) \right) \right\|_2 \\
\leq \left\| I - \eta (m \lambda I + \sum_{s=1}^{t-1} E_{t,a}^s g(x_s; \theta_0) g(x_s; \theta_0)^T) \left( \tilde{\theta}_{t,a}^{(j)} - \tilde{\theta}_{t,a}^{(j)} \right) \right\|_2 \\
:\equiv I_1 \\
+ \eta \left\| \sum_{s=1}^{t-1} \left( g(x_s; \tilde{\theta}_{t,a}^{(j)}) - g(x_s; \theta_0) \right) \left( b'(f(x_s; \tilde{\theta}_{t,a}^{(j)})) - r_s \right) \right\|_2 \\
=: I_2 \\
+ \eta \left\| \sum_{s=1}^{t-1} g(x_s; \theta_0) \left( E_{t,a}^s f(x_s; \tilde{\theta}_{t,a}^{(j)}) - (g(x_s; \theta_0), \tilde{\theta}_{t,a}^{(j)} - \theta_0) \right) \right\|_2 \\
=: I_3 \\
+ \eta \alpha(t) \left\| g(x_{t,a}; \tilde{\theta}_{t,a}^{(j)}) - g(x_{t,a}; \theta_0) \right\|_2 , \\
=: I_4,
\]
where (90) holds by triangle inequality. For $I_1$, we have
\[
I_1 = \left\| I - \eta (m \lambda I + \sum_{s=1}^{t-1} E_{t,a}^s g(x_s; \theta_0) g(x_s; \theta_0)^T) \left( \tilde{\theta}_{t,a}^{(j)} - \tilde{\theta}_{t,a}^{(j)} \right) \right\|_2 \\
\leq \left\| I - \eta (m \lambda I + \sum_{s=1}^{t-1} E_{t,a}^s g(x_s; \theta_0) g(x_s; \theta_0)^T) \right\|_2 \cdot \left\| \tilde{\theta}_{t,a}^{(j)} - \tilde{\theta}_{t,a}^{(j)} \right\|_2 \\
\leq \left\| I - \eta (m \lambda I + U_b t E_{t,a}^s) \right\|_2 \cdot \left\| \tilde{\theta}_{t,a}^{(j)} - \tilde{\theta}_{t,a}^{(j)} \right\|_2 \\
\leq (1 - \eta m \lambda) \left\| \tilde{\theta}_{t,a}^{(j)} - \tilde{\theta}_{t,a}^{(j)} \right\|_2 ,
\]
where (91) holds by the definition of spectral norm, (92) holds by Lemma 4 $E_{t,a}^s \leq U_b$ for all $s \in [l]$, and eigenvalue property of the spectral norm. (93) holds by the choice of $\eta$ with $\eta \leq (m \lambda + \hat{C}_3 t m L)^{-1}$ and $\hat{C}_3 = E_{t,a}^s U_b$. For $I_2$, we have
\[
I_2 = \eta \left\| \sum_{s=1}^{t-1} \left( g(x_s; \tilde{\theta}_{t,a}^{(j)}) - g(x_s; \theta_0) \right) \left( b'(f(x_s; \tilde{\theta}_{t,a}^{(j)})) - r_s \right) \right\|_2 \\
\leq \eta \left\| \sum_{s=1}^{t-1} \left( b'(f(x_s; \tilde{\theta}_{t,a}^{(j)})) - r_s \right) \cdot \left\| g(x_s; \tilde{\theta}_{t,a}^{(j)}) - g(x_s; \theta_0) \right\|_2 \\
\leq \eta \left\| \sum_{s=1}^{t-1} \left| b'(f(x_s; \tilde{\theta}_{t,a}^{(j)})) - r_s \right| \cdot \left\| g(x_s; \tilde{\theta}_{t,a}^{(j)}) - g(x_s; \theta_0) \right\|_2 \\
\leq \eta E_{t,a}^s \left( \frac{\lambda^2}{m \log m} \left( \frac{l \log l}{m \lambda^2} \right)^{\frac{1}{2}} \right)^{\frac{3}{2}} L^2 ,
\]
where (94) holds by the choice of $\eta$, (95) holds by Lemma 4, (96) holds by the choice of $\eta$ with $\eta \leq (m \lambda + \hat{C}_3 t m L)^{-1}$ and $\hat{C}_3 = E_{t,a}^s U_b$. For $I_3$, we have
\[
I_3 = \eta \left\| \sum_{s=1}^{t-1} g(x_s; \theta_0) \left( E_{t,a}^s f(x_s; \tilde{\theta}_{t,a}^{(j)}) - (g(x_s; \theta_0), \tilde{\theta}_{t,a}^{(j)} - \theta_0) \right) \right\|_2 \\
\leq \eta E_{t,a}^s \left( \frac{\lambda^2}{m \log m} \left( \frac{l \log l}{m \lambda^2} \right)^{\frac{1}{2}} \right)^{\frac{3}{2}} L^2 ,
\]
where (97) holds by the choice of $\eta$ with $\eta \leq (m \lambda + \hat{C}_3 t m L)^{-1}$ and $\hat{C}_3 = E_{t,a}^s U_b$.
where \((96)\) holds by Lemma \(3\), \((97)\) holds by Lemma \(2\), and \(\mathcal{F}_{11, \omega} := E_{11}^3 + E_{10}\).

For \(I_3\), we have

\[I_3 = \eta \left\| \sum_{s=1}^{t-1} g(x_s; \theta_0) \left( F_{11, \omega} (f(x_s; \tilde{\theta}_{t,a}^{(j)}) - g(x_s; \theta_0), \tilde{\theta}_{t,a}^{(j)} - \theta_0) \right) \right\|_2 \tag{98}\]

\[\leq \eta U_0 \left\| \sum_{s=1}^{t-1} f(x_s; \tilde{\theta}_{t,a}^{(j)}) - g(x_s; \theta_0), \tilde{\theta}_{t,a}^{(j)} - \theta_0 \right\|_2 \tag{99}\]

\[\leq \eta U_0 F_{2} \left( F_{11} \left( \frac{t \log t}{m \lambda^2} \right)^{\frac{1}{2}} L^3 \sqrt{m \log m} \cdot \sum_{s=1}^{t-1} \left\| g(x_s; \theta_0) \right\|_2 \right) \tag{100}\]

\[\leq \eta U_0 F_{2} \left( F_{11} \left( \frac{t \log t}{m \lambda^2} \right)^{\frac{1}{2}} L^3 \sqrt{m \log m} \cdot E_{11} \sqrt{mL} \right) \tag{101}\]

\[\leq \eta E_{11} \beta m^{\frac{1}{4}} (\log t)^{\frac{1}{4}} (\log m)^{\frac{1}{4}} \lambda^{-\frac{1}{4}} L^2, \tag{102}\]

where \((92)\) holds by \(E_{11, \omega} \leq U_0\) for all \(s \in [t]\), \((100)\) holds by Lemma \(2\) and triangle inequality, \((101)\) holds by Lemma \(3\) and \((102)\) holds by \(E_{11} := E_{11}^1 + U_0 E_{2} \). For \(I_4\), we have

\[I_4 = \eta \alpha(t) \left\| g(x; \tilde{\theta}_{t,a}^{(j)}) - g(x; \theta_0) \right\|_2 \tag{103}\]

\[\leq \eta \alpha(t) \beta \sqrt{m \log m} \left( F_{11} \left( \frac{t \log t}{m \lambda^2} \right)^{\frac{1}{2}} L^2 \right) \tag{104}\]

\[= \eta \beta \sqrt{t} m^{\frac{1}{2}} (\log t)^{\frac{1}{2}} (\log m)^{\frac{1}{2}} \lambda^{-\frac{1}{2}} L^2, \tag{105}\]

where \((104)\) holds by Lemma \(3\), \((105)\) holds by \(\alpha(t) = \sqrt{t}\), and \(E_{11} := E_{11}^1 + E_{10}\). Therefore, combining \((93)\), \((97)\), \((102)\), and \((105)\), we have

\[\left\| \tilde{\theta}_{t,a}^{(j+1)} - \tilde{\theta}_{t,a}^{(j)} \right\|_2 \leq (1 - \eta \lambda m) \left\| \tilde{\theta}_{t,a}^{(j)} - \tilde{\theta}_{t,a}^{(j)} \right\|_2 + \sum_{s=2}^{t} I_s \tag{106}\]

\[\leq F_{11} \beta m^{\frac{1}{2}} (\log t)^{\frac{1}{2}} (\log m)^{\frac{1}{2}} \lambda^{-\frac{1}{2}} L^2, \tag{107}\]

where \(F_{11} := 3 \max\{E_{11}, \beta, F_{11}, F_{11} \}\). Notice that \((107)\) holds by the formula of geometric series and the fact that \(\lambda \leq 1\). Then, by triangle inequality, we have

\[\left\| \tilde{\theta}_{t,a}^{(j+1)} - \theta_0 \right\|_2 \leq \left\| \tilde{\theta}_{t,a}^{(j+1)} - \tilde{\theta}_{t,a}^{(j)} \right\|_2 + \left\| \tilde{\theta}_{t,a}^{(j)} - \theta_0 \right\|_2 \tag{108}\]

\[\leq F_{11} \beta m^{\frac{1}{2}} (\log t)^{\frac{1}{2}} (\log m)^{\frac{1}{2}} \lambda^{-\frac{1}{2}} L^2 + E_{10} \left( \frac{t \log t}{m \lambda^2} \right)^{\frac{1}{2}} \tag{109}\]

\[\leq 2F_{10} \left( \frac{t \log t}{m \lambda^2} \right)^{\frac{1}{2}} \tag{110}\]

\[= F_{11} \left( \frac{t \log t}{m \lambda^2} \right)^{\frac{1}{2}}, \tag{111}\]

where \((109)\) holds by \((107)\) and Lemma \(10\), \((110)\) holds by choosing an \(m\) that satisfies

\[m \geq F_{10}^{1/6} F_{11} \frac{F_{11}}{F_{10}} T^7 (\log T)(\log m)^3 \lambda^{-8} L^{21}, \tag{112}\]

and \((111)\) holds by letting \(E_{11} := 2F_{10}\). By mathematical induction, we complete the proof. \(\square\)
C Regret Bound of NeuralRBMLE-GA

Recall that
\[
\ell_n(F_t; \theta) = \sum_{s=1}^{t-1} \left( r_s \langle g(x_s; \theta_0), \theta - \theta_0 \rangle - b(\langle g(x_s; \theta_0), \theta - \theta_0 \rangle) \right) - \frac{m\lambda}{2} \| \theta - \theta_0 \|^2_2 \quad (113)
\]
\[
\bar{Z}_t = \lambda \cdot I + \frac{1}{m} \sum_{s=1}^{t-1} g(x_s; \theta_0) g(x_s; \theta_0)^\top
\]
\[
\theta_{t,a} := \arg \max_{\theta} \{ \ell_n(F_t; \theta) + \alpha(t) \langle g(x_{t,a}; \theta_0), \theta - \theta_0 \rangle \}
\]
\[
I_{t,a} := \ell_n(F_t; \theta_{t,a}) + \alpha(t) \zeta(t) (g(x_{t,a}; \theta_0), \theta_{t,a} - \theta_0)
\]

To begin with, we introduce the following several useful lemmas specific to the regret bound of NeuralRBMLE-GA. The following lemma shows the difference between the model parameter \( \tilde{\theta}_{t,a} \), which we actually used in index comparison, and \( \theta_{t,a} \), which is the optimal solution to \( \min \{L_{t,a}(\theta)\} \).

**Lemma 12.** For all \( a \in [K], t \in [T] \), we have
\[
\left\| \tilde{\theta}_{t,a} - \theta_{t,a} \right\|_2 \leq F_{12} I_2 \frac{m}{2} \frac{(\log t)^{\frac{3}{2}}}{(mL + m\lambda)} + F_{12} I_2 \frac{m}{2} \frac{\log t}{(mL + m\lambda)} + \sqrt{\frac{t \log t}{m\lambda^2}}
\]

**Proof.** Note that \( L_{t,a}(\theta) \) is \( m\lambda \)-strongly convex and \( E_{12} \), \((tmL + m\lambda)\)-smooth for an absolute constant \( E_{12} \). By the convergence theorem of gradient descent for a strongly convex and smooth function (Theorem 5, Nesterov [2013]), if \( \eta \leq \frac{m\lambda + \frac{1}{2}m}{(tmL + m\lambda)} \), we have
\[
\left\| \tilde{\theta}_{t,a} - \theta_{t,a} \right\|_2 \leq \left( \frac{m\lambda}{(tmL + m\lambda) + 1} \right)^{\frac{1}{2}} \left\| \theta_{t,a} - \theta_0 \right\|_2
\]
\[
= F_{12} I_2 \left\| \theta_{t,a} - \theta_0 \right\|_2 ,
\]
where \( F_{12} I_2 := \left( \frac{m\lambda}{(tmL + m\lambda) + 1} \right)^{\frac{1}{2}} \leq 1 \). For the term \( \left\| \theta_{t,a} - \theta_0 \right\|_2 \), we have
\[
\frac{m\lambda}{2} \left\| \theta_{t,a} - \theta_0 \right\|_2^2 \leq L_{t,a}(\theta_{t,a}) + F_{10} t \log t + \alpha(t) \left\| g(x_{t,a}; \theta_0) \right\|_2 \cdot \left\| \theta_{t,a} - \theta_0 \right\|_2
\]
\[
\leq L_{t,a}(\theta_0) + F_{10} t \log t + F_{23} \sqrt{mL} \left\| \theta_{t,a} - \theta_0 \right\|_2
\]
\[
\leq F_{10} t \log t + F_{23} \sqrt{mL} \left\| \theta_{t,a} - \theta_0 \right\|_2 ,
\]
where (120) holds by (107) and Cauchy–Schwarz inequality, (122) holds by the rule of gradient descent, Lemma 4 \( \alpha(t) = \sqrt{t} \), and (122) holds by the definition \( F_{10} := 2 \max \{ b(0), F_{10} I_2 \} \). By solving (122), we have
\[
\left\| \theta_{t,a} - \theta_0 \right\|_2 \leq F_{12} I_2 \frac{t \log t}{m\lambda^2}
\]
Combining (119) and (122), we have
\[
\left\| \tilde{\theta}_{t,a} - \theta_{t,a} \right\|_2 \leq F_{12} I_2 F_{12} I_2 \frac{t \log t}{m\lambda^2}
\]
Then, by triangle inequality, we have
\[
\left\| \tilde{\theta}_{t,a} - \theta_{t,a} \right\|_2 \leq \left\| \tilde{\theta}_{t,a} - \theta_{t,a} \right\|_2
\]
\[
\leq F_{12} I_2 F_{12} I_2 \frac{t \log t}{m\lambda^2} ,
\]
where (126) holds by (107) and (124). The proof is complete. \( \square \)
Lemma 13. For all \( a \in [K], t \in [T] \), we have

\[
\left| I_{t,a} - \ell^\dagger_F(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) - \alpha(t)\zeta(t)f(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) \right|
\leq \left( F_{13} \right) \left( t \log t + \alpha(t)\zeta(t) \right) \left( F_{12} \right) \left( t \log t \right) \left( F_{12} \frac{L^3}{m\lambda^2} \right) \left( F_{12} \frac{L^3}{m\lambda^2} \right) + E_{13} \left( \frac{m\lambda^2}{2} \right) \frac{t \log t}{m\lambda^2} \left( F_{12} \frac{L^3}{m\lambda^2} \right) \left( F_{12} \frac{L^3}{m\lambda^2} \right)
\]

Proof. By the definition of \( I_{t,a} \), we have

\[
\left| I_{t,a} - \ell^\dagger_F(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) - \alpha(t)\zeta(t)f(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) \right|
\leq \ell_F(x_{t,a}; \theta_{t,a}) - \ell^\dagger_F(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) + \alpha(t)\zeta(t) \left| f(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) - \langle g(x_{t,a}; \theta_0), \theta_{t,a} - \theta_0 \rangle \right|
\]

where \( (128) \) holds by triangle inequality. For \( K_1 \), we have

\[
K_1 = \left| \ell_F(x_{t,a}; \theta_{t,a}) - \ell^\dagger_F(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) \right|
\leq \ell_F(x_{t,a}; \theta_{t,a}) - \ell^\dagger_F(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) + \frac{m\lambda^2}{2} \left| \theta_{t,a} - \theta_0 \right|_2 \left| \tilde{\theta}_{t,a}^\dagger - \theta_0 \right|_2 \quad (129)
\]

where \( (130) \) holds by triangle inequality. Then, for \( \ell_F(x_{t,a}; \theta_{t,a}) - \ell^\dagger_F(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) \), we have

\[
\left| \ell_F(x_{t,a}; \theta_{t,a}) - \ell^\dagger_F(x_{t,a}; \tilde{\theta}_{t,a}^\dagger) \right|
\leq \sum_{s=1}^{t-1} \left| b(g(x_s; \theta_0)^\top (\theta_{t,a} - \theta_0)) - b(f(x_s; \tilde{\theta}_{t,a}^\dagger)) - r_s(g(x_s; \theta_0)^\top (\theta_{t,a} - \theta_0) - f(x_s; \tilde{\theta}_{t,a}^\dagger)) \right|
\]

\[
\leq \sum_{s=1}^{t-1} \left| b'(g(x_s; \theta_0)^\top (\theta_{t,a} - \theta_0)) - f(x_s; \tilde{\theta}_{t,a}^\dagger) - r_s(g(x_s; \theta_0)^\top (\theta_{t,a} - \theta_0) - f(x_s; \tilde{\theta}_{t,a}^\dagger)) \right|
\]

\[
+ U_b \sum_{s=1}^{t-1} \left( g(x_s; \theta_0)^\top (\theta_{t,a} - \theta_0) - f(x_s; \tilde{\theta}_{t,a}^\dagger) \right)^2 \quad (131)
\]

where \( (128) \) holds by triangle inequality.
where (132) holds by Taylor’s theorem and \( b(\cdot) \) is a \( U_b \)-smooth function and (133) holds by introducing \( E_{131} := 2 \max \{ U_b, E_{121} \} \). Notice that for all vector \( \mathbf{x} \) and \( a \in [K], t \in [T] \), we have
\[
\| \mathbf{g}(\mathbf{x}; \theta_0) \|^2 \leq E_{131} t \log t \frac{t \log t}{m \lambda^2} \frac{2}{\sqrt{m \log m}} L^3 \sqrt{m \log m}
\]
\[
+ E_{111} t \log t \frac{t \log t}{m \lambda^2} \frac{2}{\sqrt{m \log m}} L^3 \sqrt{m \log m}
\]
For all arm \( K \) by Lemma 11, Lemma 12 and (135) holds by Lemma 14.
\]
\[
\| \mathbf{g}(\mathbf{x}; \theta_0) \|^2 \leq E_{131} t \log t \frac{t \log t}{m \lambda^2} \frac{2}{\sqrt{m \log m}} L^3 \sqrt{m \log m}
\]
where (134) holds by Lemma 4 and Lemma 12. For \( m_\lambda \) we have
\[
\| \mathbf{g}(\mathbf{x}; \theta_t) - \mathbf{g}(\mathbf{x}; \theta_0) \|_2^2 - \| \mathbf{g}(\mathbf{x}; \theta_t) - \mathbf{g}(\mathbf{x}; \theta_0) \|_2^2
\]
where (135) holds by triangle inequality, and (137) holds by \( \alpha^2 - b^2 = (a + b)(a - b) \), (136) holds by triangle inequality, and (137) holds by Lemma 11, Lemma 12 and \( E_{132} = 2 \max \{ E_{111}, E_{121} \} \). Combining (133), (134) and (137), we have
\[
K_1 \leq E_{131} t \log t \frac{t \log t}{m \lambda^2} \frac{2}{\sqrt{m \log m}} L^3 \sqrt{m \log m}
\]
\[
+ E_{111} t \log t \frac{t \log t}{m \lambda^2} \frac{2}{\sqrt{m \log m}} L^3 \sqrt{m \log m}
\]
For \( K_2 \), by (134) we have
\[
K_2 = \alpha(t) \zeta(t) \left| \mathbf{g}(\mathbf{x}_{t,a}; \theta_t) - \mathbf{g}(\mathbf{x}_{t,a}; \theta_0) \right|
\]
\[
\leq \alpha(t) \zeta(t) \left( E_{131} t \log t \frac{t \log t}{m \lambda^2} \frac{2}{\sqrt{m \log m}} L^3 \sqrt{m \log m}
\]
\[
+ E_{111} t \log t \frac{t \log t}{m \lambda^2} \frac{2}{\sqrt{m \log m}} L^3 \sqrt{m \log m}
\]
Then, combining (138) and (140), we complete the proof. 

**Lemma 14.** For all arm \( i, j \in [K] \) and \( t \in [T] \), there exists \( \theta' = \kappa \theta_{t,i} + (1 - \kappa) \theta_{t,j} \) for some \( \kappa \in (0, 1) \), we have
\[
0 \leq (\mathbf{g}(\mathbf{x}_{t,i}; \theta_0) + \mathbf{g}(\mathbf{x}_{t,j}; \theta_0))^\top (\theta_{t,j} - \theta_{t,i}) + \frac{\alpha(t)}{m} \left( \| \mathbf{g}(\mathbf{x}_{t,i}; \theta_0) \|^2_{U_i^{-1}} - \| \mathbf{g}(\mathbf{x}_{t,j}; \theta_0) \|^2_{U_j^{-1}} \right)
\]
where
\[ U_0 := \lambda \cdot I + \frac{1}{m} \sum_{s=1}^{t-1} b''(\langle g(x_s; \theta_0), \theta' - \theta_0 \rangle) g(x_s; \theta_0) g(x_s; \theta_0) \top, \]
(142)

Proof. By the first-order necessary condition of \( \theta_{t,i} \) and \( \theta_{t,j} \) for any two arms \( i, j \in [K] \), we have
\[ \sum_{s=1}^{t-1} \left( r_s g(x_s; \theta_0) - b'\left( \langle g(x_s; \theta_0), \theta_{t,i} - \theta_0 \rangle \right) g(x_s; \theta_0) \right) - m\lambda(\theta_{t,i} - \theta_0) + \alpha(t) g(x_{t,i}; \theta_0) = 0, \]
(143)
\[ \sum_{s=1}^{t-1} \left( r_s g(x_s; \theta_0) - b'\left( \langle g(x_s; \theta_0), \theta_{t,j} - \theta_0 \rangle \right) g(x_s; \theta_0) \right) - m\lambda(\theta_{t,j} - \theta_0) + \alpha(t) g(x_{t,j}; \theta_0) = 0. \]
(144)

After multiplying both sides of (143)-(144) by \( g(x_{t,j}; \theta_0) + g(x_{t,i}; \theta_0) \top U_t^{-1} \) and taking the difference between (143)-(144), we have
\[ 0 = \left( g(x_{t,i}; \theta_0) + g(x_{t,j}; \theta_0) \right) \top U_t^{-1} \left( \alpha(t) g(x_{t,i}; \theta_0) - \alpha(t) g(x_{t,j}; \theta_{t,i}) \right) + m\lambda(\theta_{t,j} - \theta_{t,i}) + \sum_{s=1}^{t-1} \left( b'\left( \langle g(x_s; \theta_0), \theta_{t,j} - \theta_0 \rangle \right) - b'\left( \langle g(x_s; \theta_0), \theta_{t,i} - \theta_0 \rangle \right) \right) g(x_s; \theta_0) \]
\[ = \frac{\alpha(t)}{m} \left( \|g(x_{t,i}; \theta_0)\|^2_{U_t^{-1}} - \|g(x_{t,j}; \theta_0)\|^2_{U_t^{-1}} \right) + \left( g(x_{t,i}; \theta_0) + g(x_{t,j}; \theta_0) \right) \top U_t^{-1} \]
\[ \cdot \left( m\lambda \cdot I + \sum_{s=1}^{t-1} b''\left( \langle g(x_s; \theta_0), \theta' - \theta_0 \rangle \right) g(x_s; \theta_0) g(x_s; \theta_0) \top \right) \left( \theta_{t,j} - \theta_{t,i} \right) \]
\[ = \frac{\alpha(t)}{m} \left( \|g(x_{t,i}; \theta_0)\|^2_{U_t^{-1}} - \|g(x_{t,j}; \theta_0)\|^2_{U_t^{-1}} \right) + \left( g(x_{t,i}; \theta_0) + g(x_{t,j}; \theta_0) \right) \top (\theta_{t,j} - \theta_{t,i}), \]
(145)
where (146) holds by mean-value theorem with \( \theta' = \kappa \theta_{t,i} + (1 - \kappa) \theta_{t,j} \) for some \( \kappa \in (0, 1) \), and (147) holds by the definition of \( U_t \) in (142).

\[ \text{Lemma 15. For all arm } a \in [K], \text{ we have} \]
\[ \|\hat{\theta}_t - \theta_{t,a}\|_{Z_t} \leq \frac{\alpha(t)}{mL_b} \|g(x_{t,a}; \theta_0)\|_{Z_t^{-1}}. \]
(148)

Moreover, for any pair of arms \( i, j \in [K] \), we have
\[ \ell_x(F_t; \theta_{t,i}) - \ell_x(F_t; \theta_{t,j}) \leq \frac{U_0 \alpha(t)^2}{mL_b^2} \|g(x_{t,j}; \theta_0)\|^2_{Z_t^{-1}}. \]
(149)

Proof. Recall that for all \( a \in [K] \), we have
\[ \hat{\theta}_t = \arg\max_{\theta} \{ \ell_x(F_t; \theta) \} \]
(150)
\[ \theta_{t,a} = \arg\max_{\theta} \{ \ell_x(F_t; \theta) + \alpha(t) f(x_{t,a}; \theta) \}. \]
(151)

By considering the first-order necessary condition of \( \hat{\theta}_t \) and \( \theta_{t,a} \), we obtain
\[ \alpha(t) g(x_{t,a}; \theta_0) = \ell_x'(F_t; \hat{\theta}_t) - \ell_x'(F_t; \theta_{t,a}) \]
\[ = -\frac{1}{m} \sum_{s=1}^{t-1} \frac{1}{m} b''\left( \langle g(x_s; \theta_0), \theta'' - \theta_0 \rangle \right) g(x_s; \theta_0) g(x_s; \theta_0) \top \left( \hat{\theta}_t - \theta_{t,a} \right), \]
(152)
\[ := U_t. \]
where (153) holds by mean-value theorem with \( \theta'' = \kappa' \hat{\theta}_t + (1 - \kappa') \theta_{t,a} \) for some \( \kappa' \in (0, 1) \). Multiplying both sides of (152) by \( (\hat{\theta}_t - \theta_{t,a})^\top \), we have

\[
\alpha(t)(\hat{\theta}_t - \theta_{t,a})^\top g(x_t; \theta_0) = -m(\hat{\theta}_t - \theta_{t,a})^\top \tilde{U}_t(\hat{\theta}_t - \theta_{t,a}).
\]  

(154)

By applying Cauchy–Schwarz inequality to the left hand side of (154), we have

\[
\frac{\alpha(t)}{m}(\hat{\theta}_t - \theta_{t,a})^\top g(x_t; \theta_0) \leq \frac{\alpha(t)}{m} \| \hat{\theta}_t - \theta_{t,a} \|_{Z_t} \cdot \| g(x_t; \theta_0) \|_{Z_t^{-1}}.
\]  

(155)

For the right hand side of (154), by the fact that \( \tilde{U}_t \hat{\theta}_t \leq U_b \hat{\theta}_t \) for all \( \theta \) and Cauchy–Schwarz inequality, we have

\[
\frac{\alpha(t)}{m} \| \hat{\theta}_t - \theta_{t,a} \|_{Z_t} \geq L_b \| \hat{\theta}_t - \theta_{t,a} \|_{Z_t}^2.
\]  

(156)

Then, by combining (155) and (156), we have

\[
\| \hat{\theta}_t - \theta_{t,a} \|_{Z_t} \leq \frac{\alpha(t)}{mL_b} \| g(x_t; \theta_0) \|_{Z_t^{-1}}.
\]  

(157)

Moreover, we have

\[
\ell_{\lambda}(F_{t,i}; \theta_{t,i}) - \ell_{\lambda}(F_{t,j}; \bar{\theta}_t) = m \| \hat{\theta}_t - \theta_{t,j} \|_{Z_t}^2
\]  

(158)

\[
= mU_b \| \hat{\theta}_t - \theta_{t,j} \|_{Z_t}^2 \quad \text{(159)}
\]

\[
\leq \frac{U_b \alpha(t)^2}{mL_b^2} \| g(x_t; \theta_0) \|_{Z_t^{-1}}^2,
\]  

(160)

where (158) holds due to \( \hat{\theta}_t = \arg \max \ell_{\lambda}(F_{t,i}; \theta) \), (159) holds by mean value theorem with \( \theta'' = \kappa \bar{\theta}_t + (1 - \kappa) \theta_{t,j} \) for some \( \kappa \in (0, 1) \), (160) holds by the fact that \( \tilde{U}_t \leq U_b \bar{\theta}_t \), and (161) holds due to (157). Hence, the proof is complete.

**C.1 Proof of Theorem 1**

Define

\[
G_1 = \left\{ \sum_{s=1}^{t} r_s \leq E_{\mathcal{T}}^1 \sqrt{t \log t} \right\}
\]  

(162)

\[
G_2 = \left\{ \sum_{s=1}^{t} r_s^2 \leq E_{\mathcal{T}}^2 t \log t \right\}
\]  

(163)

as the good events. By Lemma 7, we have \( \mathbb{P}(G_1, G_2) = 1 - \frac{1}{\sqrt{t}} \). To begin with, we start by obtaining an upper bound for the immediate regret of NeuralRBMLE-GA described in Algorithm 1. Under events \( G_1 \) and \( G_2 \), the expected immediate regret can be derived as

\[
\mathbb{E}[r^*_t - r_t] = h(x^*_t) - h(x_t)
\]  

(164)

\[
= g(x^*_t; \theta_0), \theta^* - \theta_0 - g(x_t; \theta_0), \theta^* - \theta_0
\]  

(165)

\[
= g(x^*_t; \theta_0), \theta^* - \theta_t + g(x^*_t; \theta_0), \theta_t - \theta_0 - g(x_t; \theta_0), \theta^* - \theta_0
\]  

(166)

\[
= g(x^*_t; \theta_0), \theta^* - \theta_t - g(x_t; \theta_0), \theta^* - \theta_0 + g(x_t; \theta_0), \theta_{t,a} - \theta_t
\]

\[
+ g(x^*_t; \theta_0), \theta_{t,a} - \theta_0 + \frac{\alpha(t)}{m} \left( \| g(x_t; \theta_0) \|_{\tilde{U}_t^{-1}}^2 - \| g(x^*_t; \theta_0) \|_{\tilde{U}_t^{-1}}^2 \right),
\]  

(167)

where (165) holds by Lemma 1, (166) is obtained by adding and subtracting \( \theta_t \), and (167) holds due to Lemma 14. Then, applying Lemma 13 to the index policy of Algorithm 1, we have
\[
\mathbb{E}[r_t^* - r_t] \leq \langle g(x_t^*; \theta_0), \theta^* - \theta_t \rangle - \langle g(x_t; \theta_0), \theta^* - \theta_t \rangle + \langle g(x_t; \theta_t), \theta_t - \theta_0 \rangle + \frac{\ell(x; \theta) - \ell(x; \theta_t)}{\alpha(t)} + 2F_{1}(m, t) \\
+ \frac{\alpha(t)}{m} \left( \|g(x_t; \theta_0)\|_{U_t^{-1}}^2 - \|g(x_t^*; \theta_0)\|_{U_t^{-1}}^2 \right) + \frac{\alpha(t)}{m} \left( \|g(x_t; \theta_0)\|_{U_t^{-1}}^2 - \|g(x_t^*; \theta_0)\|_{U_t^{-1}}^2 \right) + 2F_{1}(m, t).
\]

(168)

\[
\leq \langle g(x_t^*; \theta_0), \theta^* - \theta_t \rangle + \langle g(x_t; \theta_0), \theta_t - \theta^* \rangle + 2F_{1}(m, t) \\
+ \frac{U_b \alpha(t)}{m L_b^2 \zeta(t)} \|g(x_t^*; \theta_0)\|_{U_t^{-1}}^2 + \frac{\alpha(t)}{m} \left( \frac{1}{U_b} \frac{g(x_t; \theta_0)}{\sqrt{m}} Z_t^{-1} - \frac{1}{L_b} \frac{g(x_t; \theta_0)}{\sqrt{m}} Z_t^{-1} \right),
\]

(170)

where (169) holds by Lemma 15 and (170) holds by the fact that \(L_b Z_t \leq U_t \leq L_b Z_t\) and

\[
\|g(x_t; \theta_0)\|_{U_t^{-1}}^2 - \|g(x_t^*; \theta_0)\|_{U_t^{-1}}^2 \leq \frac{1}{U_b} \|g(x_t; \theta_0)\|_{Z_t^{-1}}^2 - \frac{1}{L_b} \|g(x_t^*; \theta_0)\|_{Z_t^{-1}}^2.
\]

(171)

Regarding the term \(\langle g(x_t^*; \theta_0), \theta^* - \theta_t \rangle\), we have

\[
\langle g(x_t^*; \theta_0), \theta^* - \theta_t \rangle \leq \sqrt{m} \|\theta^* - \theta_t\|_{Z_t} \cdot \frac{g(x_t^*; \theta_0)}{\sqrt{m}} \|Z_t^{-1}\|
\]

(172)

\[
\leq \left( \sqrt{m} \|\theta^* - \theta_t\|_{Z_t} + \frac{\alpha(t)}{\sqrt{m} L_b} \|g(x_t; \theta_0)\|_{Z_t^{-1}} \right) \cdot \frac{g(x_t^*; \theta_0)}{\sqrt{m}} \|Z_t^{-1}\|
\]

(173)

\[
\leq \left( \sqrt{m} \|\theta^* - \theta_t\|_{Z_t} + \frac{\alpha(t)}{\sqrt{m} L_b} \|g(x_t; \theta_0)\|_{Z_t^{-1}} \right) \cdot \frac{g(x_t^*; \theta_0)}{\sqrt{m}} \|Z_t^{-1}\|
\]

(174)

where (172) holds by the Cauchy–Schwarz inequality, (173) holds by the triangle inequality, and (174) holds by (157). Similarly, for the term \(\langle g(x_t; \theta_0), \theta_t^* - \theta^* \rangle\), we have

\[
\langle g(x_t; \theta_0), \theta_t^* - \theta^* \rangle \leq \left( \sqrt{m} \|\theta^* - \theta_t\|_{Z_t} + \frac{\alpha(t)}{\sqrt{m} L_b} \|g(x_t^*; \theta_0)\|_{Z_t^{-1}} \right) \cdot \frac{g(x_t; \theta_0)}{\sqrt{m}} \|Z_t^{-1}\|
\]

(175)

Plugging (170), (174) and (175) into (170), we obtain

\[
\mathbb{E}[r_t^* - r_t] \leq \left( \sqrt{m} \|\theta^* - \theta_t\|_{Z_t} + \frac{\alpha(t)}{\sqrt{m} L_b} \|g(x_t; \theta_0)\|_{Z_t^{-1}} \right) \cdot \frac{g(x_t^*; \theta_0)}{\sqrt{m}} \|Z_t^{-1}\|
\]

(176)

+ \left( \sqrt{m} \|\theta^* - \theta_t\|_{Z_t} + \frac{\alpha(t)}{\sqrt{m} L_b} \|g(x_t^*; \theta_0)\|_{Z_t^{-1}} \right) \cdot \|g(x_t; \theta_0)\|_{Z_t^{-1}}
\]

\[
+ \frac{U_b \alpha(t)}{L_b^2 \zeta(t)} \|g(x_t^*; \theta_0)\|_{U_t^{-1}}^2 + \frac{\alpha(t)}{m} \left( \frac{1}{U_b} \frac{g(x_t; \theta_0)}{\sqrt{m}} Z_t^{-1} - \frac{1}{L_b} \frac{g(x_t^*; \theta_0)}{\sqrt{m}} Z_t^{-1} \right).
\]

\[
\mathbb{E}[r_t^* - r_t] \leq \Psi \left( \frac{g(x_t^*; \theta_0)}{\sqrt{m}} \|Z_t^{-1}\| \right), \quad \text{where } \Psi(x) = \left( \sqrt{m} \|\theta^* - \theta_t\|_{Z_t} + \frac{2\alpha(t)}{\sqrt{m} L_b} \|g(x_t; \theta_0)\|_{Z_t^{-1}} \right) x + \left( \frac{U_b \alpha(t)}{L_b^2 \zeta(t)} \right) x^2.
\]

(177)
By completing the square, for any \( t \in \{t' \in \mathbb{N} : \frac{L_b}{L_\xi(t')^2} \leq 1 \} \), we have that for any \( x \in \mathbb{R} \),

\[
\Psi(x) \leq \frac{\left( \sqrt{m} \left\| \theta^* - \hat{\theta} \right\|_{Z_t} + \frac{2\alpha(t)}{\sqrt{m} U_b} \left\| g(x_t; \theta_0) \right\|_{Z_t^{-1}} \right)^2}{4 \left( \frac{\alpha(t)}{L_b} - \frac{U_b \alpha(t)}{L_\xi(t)} \right)} \leq \frac{\left( \sqrt{m} \left\| \theta^* - \hat{\theta} \right\|_{Z_t} + \frac{2\alpha(t)}{\sqrt{m} U_b} \left\| g(x_t; \theta_0) \right\|_{Z_t^{-1}} \right)^2}{4 \alpha(t)}
\]

(178)

Therefore, combining (176) and (180), we obtain

\[
\mathbb{E}[r_t^* - r_t] \leq \sqrt{m} \left\| \theta^* - \hat{\theta} \right\|_{Z_t} \cdot \left\| \frac{g(x_t; \theta_0)}{\sqrt{m}} \right\|_{Z_t^{-1}} + \frac{\alpha(t)}{mL_b} \left\| \frac{g(x_t; \theta_0)}{\sqrt{m}} \right\|_{Z_t^{-1}}^2 + \Psi \left( \left\| \frac{g(x_t^*; \theta_0^*)}{\sqrt{m}} \right\|_{Z_t^{-1}} \right)
\]

(181)

\[
\leq 2\sqrt{m} \left\| \theta^* - \hat{\theta} \right\|_{Z_t} \cdot \left\| \frac{g(x_t; \theta_0)}{\sqrt{m}} \right\|_{Z_t^{-1}} + \frac{2\alpha(t) t}{mU_b} \left\| \frac{g(x_t; \theta_0)}{\sqrt{m}} \right\|_{Z_t^{-1}}^2 + \frac{mL_b}{4\alpha(t)} \left\| \theta^* - \hat{\theta} \right\|_{Z_t}^2 + 2\mathcal{E}(m, t).
\]

(182)

Regarding the total regret \( \mathcal{R}(T) \) defined in (1), we have

\[
\mathcal{R}(T) = \mathbb{E} \left[ \sum_{t=1}^T (r_t^* - r_t) \right] G_1, G_2] + \mathbb{E} \left[ 1 | G_1^2 \cup G_2^2 \right] + T \mathcal{R}\mathcal{E}(m, t)
\]

(183)

\[
\leq 2\sqrt{m} \sum_{t=1}^T \left\| \theta^* - \hat{\theta} \right\|_{Z_t} \cdot \left\| \frac{g(x_t; \theta_0)}{\sqrt{m}} \right\|_{Z_t^{-1}} + \sum_{t=1}^T \frac{2\alpha(t) t}{mU_b} \left\| \frac{g(x_t; \theta_0)}{\sqrt{m}} \right\|_{Z_t^{-1}}^2
\]

\[
+ \sum_{t=1}^T \frac{4\alpha(t) t}{mL_b} \left\| \theta^* - \hat{\theta} \right\|_{Z_t}^2 + T \sum_{t=1}^T \frac{1}{t^2} + 2\mathcal{E}\mathcal{R}(m, t).
\]

(184)

Then, by [Abassi-Yadkori et al. 2011, Theorem 2], for any \( \delta \in (0, 1) \), with probability at least \( 1 - \delta \), we have

\[
\sqrt{m} \left\| \theta^* - \hat{\theta} \right\|_{Z_t} \leq \sqrt{\log \frac{\det Z_t}{\det \lambda} - 2 \log \delta + \frac{\lambda^2 S}{\lambda}} \leq \sqrt{\tilde{d} \log \left( 1 + \frac{TK}{\lambda} \right)} + 1 - 2 \log \delta + \frac{\lambda^2 S}{\lambda} := \bar{\gamma}_t,
\]

(185)

where (186) holds by (Zhou et al. 2020, B.19). For \( \sum_{t=1}^T \frac{2\alpha(t)}{mU_b} \left\| g(x_t; \theta_0) \right\|_{Z_t^{-1}}^2 \), we have

\[
\sum_{t=1}^T \frac{2\alpha(t)}{mU_b} \left\| g(x_t; \theta_0) \right\|_{Z_t^{-1}}^2 \leq \sum_{t=1}^T \min \left\{ \frac{2\alpha(t)}{mU_b} \left\| g(x_t; \theta_0) \right\|_{Z_t^{-1}}, 1 \right\}
\]

(187)

\[
\leq \sum_{t=1}^T \frac{2\alpha(t)}{U_b} \min \left\{ \left\| \frac{g(x_t; \theta_0)}{\sqrt{m}} \right\|_{Z_t^{-1}}^2, 1 \right\}
\]

(188)

\[
\leq \frac{4\alpha(T)}{U_b} \log \frac{\det Z_t}{\det \lambda} \leq \frac{4\alpha(T) T \log \left( 1 + \frac{TK}{\lambda} \right) + 1}{U_b}
\]

(189)
where (187) holds by $\mathbb{E}[\nu_i^* - r_i] \leq 1$, and (188) holds for any $\{t' \in \mathbb{N} : \frac{\alpha(t')}{T} \geq 1\}$, (189) holds by (Abbasi-Yadkori et al., 2011, Lemma 11), and (190) holds by (Zhou et al., 2020, B.19). Then, we have

$$R(T) \leq 2\gamma T \sqrt{\frac{d \log \left(1 + \frac{TK}{\lambda}\right)}{1 + \frac{2\alpha(T)}{U_b} \left(d \log \left(1 + \frac{TK}{\lambda}\right) + 1\right) + \frac{4\alpha(T)}{mL_b} \gamma^2_T + \log T + 2T \mathcal{K}(m, t)}},$$

$$\mathcal{O}\left(\sqrt{T \log T}\right),$$

where (192) holds by the choice of $m$.

### D Regret Bound of NeuralRBMLE-PC

#### D.1 Supporting Lemmas for the Proof of Theorem 2

**Lemma 16.** (Zhou et al., 2020, Lemma 5.2) There exist positive constants $\{F_{i, 17}\}_{i=1}^5$, such that for all $\delta \in (0, 1)$, if $\eta \leq F_{i, 17}(TmL + \lambda)^{-1}$ and

$$m \geq F_{i, 17} \max \left\{ \left. T^7 \lambda^{-7} L^{21} (\log m)^3, \lambda^{-\frac{7}{2}} L^{-\frac{1}{2}} \left(\log \frac{TKL^2}{\delta}\right)^{\frac{1}{2}} \right\} \right.,$$

with probability at least $1 - \delta$, for all $t \in [T]$, we have $\left\| \hat{\theta}_t - \theta_0 \right\|_2 \leq 2\sqrt{\frac{\gamma(t)}{m}}$ and $\left\| \theta^* - \hat{\theta}_t \right\|_{z_t, i} \leq \frac{\gamma(t)}{\sqrt{m}}$, where

$$\gamma(t) = \sqrt{\left(1 + F_{i, 17} \right) m^{-\frac{1}{2}} \sqrt{\log mlT^4 t^4 \lambda^{-\frac{1}{2}}} \left(\log \frac{TKL^2}{\delta}\right)^{\frac{1}{2}}} \cdot \left(\nu \sqrt{\frac{\log \text{det} Z_t}{\text{det} \lambda_T}} + F_{i, 17} \right) m^{-\frac{1}{2}} \sqrt{\log mlT^4 t^4 \lambda^{-\frac{1}{2}}} \left(\log \frac{TKL^2}{\delta}\right)^{\frac{1}{2}} + \left(\lambda + F_{i, 17} T L\right) \left(1 - \eta m \lambda\right) \frac{1}{2} m^{-\frac{1}{2}} \sqrt{\log mlT^4 t^4 \lambda^{-\frac{1}{2}}} \left(1 + \frac{t}{\lambda}\right) \right).$$

Notice that according to the proof of Lemma 5.4 in (Zhou et al., 2020), we have

$$\log \frac{\text{det} Z_t}{\text{det} \lambda_T} \leq -d \log(1 + T K / \lambda) + F_{i, 17} m^{-\frac{1}{2}} \sqrt{\log mlT^4 t^4 \lambda^{-\frac{1}{2}}}.$$

**Lemma 17.** (Zhou et al., 2020, Lemma 5.4) There exist positive constants $\{F_{i, 17}\}_{i=1}^3$, such that for all $t \in [T]$ and $\delta \in (0, 1)$, if $\eta \leq F_{i, 17}(TmL + \lambda)^{-1}$ and $m$ satisfies that

$$m \geq F_{i, 17} \max \left\{ T^7 \lambda^{-7} L^{21} (\log m)^3, T^6 K^6 L^6 \left(\log \left(\frac{TKL^2}{\delta}\right)\right)^{\frac{1}{2}} \right\},$$

with probability at least $1 - \delta$, we have

$$\sum_{t=1}^T \min \left\{ \left. \left\| g(x_t, \hat{\theta}_t) \right\|_m \right\|_{z_{t-1}}^2, 1 \right\} \leq 2d \log(1 + T K / \lambda) + 2 + F_{i, 17} m^{-\frac{1}{2}} \sqrt{\log mlT^4 T^4 \lambda^{-\frac{1}{2}}},$$

where $d$ is the effective dimension defined in (23).

**Lemma 18.** For all $a \in [K]$, $t \in [T]$, we have

$$\left\| \hat{\theta}_{t,a} - \theta_0 \right\|_2 \leq 2 \sqrt{\frac{t}{m} + F_{i, 17} \frac{\alpha(t)}{m} \sqrt{m}},$$

where $F_{i, 17}$ is a positive constant. Moreover, by choosing $\alpha(t) = \sqrt{t}$ and defining $F_{i, 17} = 2 \max\{2, F_{i, 17}\}$, we have $\left\| \hat{\theta}_{t,a} - \theta_0 \right\|_2 \leq F_{i, 17} \sqrt{\frac{t}{m}}$. 

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Proof. Recall that \( \hat{\theta}_{t,a} = \hat{\theta}_t + \frac{\alpha(t)}{m} \cdot Z_{t-1}^{-1} g(x_{t,a}; \hat{\theta}_t) \). By triangle inequality, we have

\[
\| \hat{\theta}_{t,a} - \theta_0 \|_2 \leq \| \hat{\theta}_t - \theta_0 \|_2 + \frac{\alpha(t)}{m} \cdot \| Z_{t-1}^{-1} g(x_{t,a}; \hat{\theta}_t) \|_2.
\] (199)

Then, by Lemma 16, we can verify that \( \| \hat{\theta}_t - \theta_0 \|_2 \) satisfies the condition of Lemma 4. Therefore, we have

\[
\| \hat{\theta}_{t,a} - \theta_0 \|_2 \leq 2\sqrt{\frac{t}{m \lambda}} + \frac{\alpha(t)}{m} \cdot \| Z_{t-1}^{-1} g(x_{t,a}; \hat{\theta}_t) \|_2
\] (200)

\[
\leq 2\sqrt{\frac{t}{m \lambda}} + \frac{\alpha(t)}{m} \sqrt{L} \cdot \| Z_{t-1}^{-1} \|_2
\] (201)

\[
\leq 2\sqrt{\frac{t}{m \lambda}} + \frac{\alpha(t)}{m} \sqrt{L \lambda},
\] (202)

where (200) holds by Lemma 16, (201) holds by Lemma 4 and Cauchy–Schwarz inequality, and (202) holds by the fact that \( \| Z_{t-1}^{-1} \|_2 \leq \frac{1}{\lambda} \), for all \( t \in [T] \). By letting \( E_{18} := E_{16} \sqrt{L \lambda} \), we complete the proof.

D.2 Proof of Theorem 2

By Lemmas 16, 18 the choice of \( m \), and choosing \( \alpha(t) = \sqrt{t} \), we can verify that Lemmas 2 hold when \( \theta = \theta_{t,a} \) and \( \theta = \hat{\theta}_t \), for all \( t \in [T], a \in [K] \). Then, we start by the index comparison of NeuralRBMLE-PC in Algorithm 2 as follows:

\[
f(x_t; \hat{\theta}_{t,a}) \geq f(x_t^*; \hat{\theta}_{t,a}^*)
\] (203)

\[
\implies 2E_{18} \left( \frac{t}{m \lambda} \right)^{\frac{3}{4}} L^3 \sqrt{m \log m} + \langle g(x_t; \theta_0), \hat{\theta}_{t,a} - \theta_0 \rangle \geq \langle g(x_t^*; \theta_0), \hat{\theta}_{t,a}^* - \theta_0 \rangle \]

(204)

\[
\implies 2E_{18} \left( \frac{t}{m \lambda} \right)^{\frac{3}{4}} L^3 \sqrt{m \log m} + \| \hat{\theta}_{t,a} - \theta_0 \|_2 \cdot \| g(x_t; \theta_0) - g(x_t; \hat{\theta}_t) \|_2
\]

\[
+ \| \hat{\theta}_{t,a} - \theta_0 \|_2 \cdot \| g(x_t^*; \theta_0) - g(x_t^*; \hat{\theta}_t) \|_2 + \langle g(x_t; \hat{\theta}_t), \hat{\theta}_{t,a} - \theta_0 \rangle \geq \langle g(x_t^*; \theta_0), \hat{\theta}_{t,a}^* - \theta_0 \rangle
\]

(205)

\[
\implies 2E_{18} \left( \frac{t}{m \lambda} \right)^{\frac{3}{4}} L^3 \sqrt{m \log m} + 2E_{18} \left( \frac{t}{m \lambda} \right)^{\frac{3}{4}} L^3 \sqrt{m \log m} \left( 2 \sqrt{\frac{t}{m \lambda}} \right)^{\frac{3}{4}} L^2
\]

\[
+ \langle g(x_t; \hat{\theta}_t), \hat{\theta}_{t,a} - \theta_0 \rangle \geq \langle g(x_t^*; \theta_0), \hat{\theta}_{t,a}^* - \theta_0 \rangle,
\] (206)

where (204) follows from Lemma 2, (205) is obtained by adding and subtracting \( g(x_t; \hat{\theta}_t) \) as well as \( g(x_t^*; \hat{\theta}_t) \) at the same time and then applying the Cauchy–Schwarz inequality, and (206) follows from Lemma 5, Lemma 4 and Lemma 18. For ease of notation, we use \( E_{PC,1} \) to denote the pre-constant of \( D_1 \). By (206), we further have

\[
\langle g(x_t; \hat{\theta}_t), \hat{\theta}_{t,a} - \theta_0 \rangle + E_{PC,1} t^2 \log m \lambda^{-\frac{3}{2}} \sqrt{L^2 \lambda} \geq \langle g(x_t^*; \hat{\theta}_t), \hat{\theta}_{t,a}^* - \theta_0 \rangle
\] (207)

\[
\implies \langle g(x_t; \hat{\theta}_t), \hat{\theta}_t + \frac{\alpha(t)}{m} Z_{t-1}^{-1} g(x_t; \hat{\theta}_t) - \theta_0 \rangle - \langle g(x_t^*; \hat{\theta}_t), \hat{\theta}_t + \frac{\alpha(t)}{m} Z_{t-1}^{-1} g(x_t^*; \hat{\theta}_t) - \theta_0 \rangle + D_1 \geq 0
\] (208)

\[
\implies \langle g(x_t; \hat{\theta}_t), \hat{\theta}_t - \theta_0 \rangle + \frac{\alpha(t)}{m} \| g(x_t; \hat{\theta}_t) \|_{Z_{t-1}^{-1}}^2 - \left( \langle g(x_t^*; \hat{\theta}_t), \hat{\theta}_t - \theta_0 \rangle + \frac{\alpha(t)}{m} \| g(x_t^*; \hat{\theta}_t) \|_{Z_{t-1}^{-1}}^2 \right) + D_1 \geq 0.
\] (209)
Now we are ready to derive the regret bound of NeuralRBMLE-PC. To begin with, we quantify the immediate regret at each step $t$ as

$$h(x_t^*) - h(x_t) = \langle g(x_t^*; \theta_t), \theta^* - \theta_0 \rangle - \langle g(x_t; \theta_t), \theta^* - \theta_0 \rangle \leq \langle g(x_t^*; \tilde{\theta}_t), \theta^* - \theta_0 \rangle - \langle g(x_t; \tilde{\theta}_t), \theta^* - \theta_0 \rangle + \|\theta^* - \theta_0\|_2 \left( \left\| g(x_t^*; \theta_0) - g(x_t^*; \tilde{\theta}_t) \right\|_2 + \left\| g(x_t; \theta_0) - g(x_t; \tilde{\theta}_t) \right\|_2 \right),$$

where \((210)\) follows directly from Lemma 1, \((211)\) holds by adding and subtracting $g(x_t^*; \tilde{\theta}_t)$ as well as $g(x_t; \tilde{\theta}_t)$ at the same time and then applying the Cauchy-Schwarz inequality, \((212)\) follows from Lemma 1, Lemma 3, Lemma 4 and \(\sqrt{2h \log m} \leq S\). For \(\langle g(x_t^*; \tilde{\theta}_t), \theta^* - \theta_0 \rangle\), due to Lemma 16, Theorem 2 in [Abbasi-Yadkori et al. 2011], and the fact that

$$\max_{a:||a||_2 \leq c} \langle a, x \rangle = \langle a, b \rangle + c \sqrt{a^T A^{-1} a},$$

we have

$$\langle g(x_t^*; \tilde{\theta}_t), \theta^* - \theta_0 \rangle \leq \langle g(x_t^*; \tilde{\theta}_t), \tilde{\theta}_t - \theta_0 \rangle + \frac{\gamma(t)}{\sqrt{m}} \left\| g(x_t^*; \tilde{\theta}_t) \right\|_{Z_t^{-1}}$$

$$= \langle g(x_t^*; \tilde{\theta}_t), \tilde{\theta}_t - \theta_0 \rangle + \frac{\gamma(t)}{\sqrt{m}} \left\| g(x_t^*; \tilde{\theta}_t) \right\|_{Z_t^{-1}} + \frac{\alpha(t)}{m} \left\| g(x_t^*; \tilde{\theta}_t) \right\|_{Z_t^{-1}}^2 - \frac{\alpha(t)}{m} \left\| g(x_t^*; \tilde{\theta}_t) \right\|_{Z_t^{-1}}^2 + D_1$$

where \((213)\) holds by completing the square with respect to \(\left\| g(x_t^*; \tilde{\theta}_t) \right\|_{Z_t^{-1}}\). Then, combining \((212)\) and \((213)\), we obtain

$$h(x_t^*) - h(x_t) \leq \langle g(x_t^*; \tilde{\theta}_t), \tilde{\theta}_t - \theta_0 \rangle + \frac{\alpha(t)}{m} \left\| g(x_t^*; \tilde{\theta}_t) \right\|_{Z_t^{-1}}^2 + \frac{\gamma(t)^2}{4\alpha(t)} + (g(x_t^*; \tilde{\theta}_t), \theta^* - \theta_0) + D_1 + D_2.$$
Moreover, we have
\[
\langle g(x_t; \hat{\theta}_t), \hat{\theta}_t - \theta_0 \rangle - \langle g(x_t; \hat{\theta}_t), \theta^* - \theta_0 \rangle 
\leq \max_{\theta: \|\theta - \hat{\theta}_t\|_{\mathcal{Z}_t} \leq \gamma(t)} \left\{ \langle g(x_t; \hat{\theta}_t), \theta - \theta_0 \rangle - \langle g(x_t; \hat{\theta}_t), \theta^* - \theta_0 \rangle \right\} 
\leq \max_{\theta: \|\theta - \hat{\theta}_t\|_{\mathcal{Z}_t} \leq \gamma(t)} \left\{ \|g(x_t; \hat{\theta}_t)\|_{\mathcal{Z}_t} \cdot \|\theta - \hat{\theta}_t\|_{\mathcal{Z}_t} + \|g(x_t; \hat{\theta}_t)\|_{\mathcal{Z}_t} \cdot \|\theta^* - \hat{\theta}_t\|_{\mathcal{Z}_t} \right\} 
\leq \frac{2\gamma(t)}{\sqrt{m}} \|g(x_t; \hat{\theta}_t)\|_{\mathcal{Z}_t}, 
\tag{225}
\]
where (224) holds by the Cauchy-Schwarz inequality, and (225) follows directly from the fact that \(\|\theta - \hat{\theta}_t\|_{\mathcal{Z}_t} \leq \frac{\gamma(t)}{\sqrt{m}}\) and Lemma 16. Therefore, plugging (225) into (220), with probability at least \(1 - \delta\), we have
\[
h(x^*_t) - h(x_t) \leq \frac{2\gamma(t)}{\sqrt{m}} \|g(x_t; \hat{\theta}_t)\|_{\mathcal{Z}_t} + \frac{\alpha(t)}{m} \|g(x_t; \hat{\theta}_t)\|^2_{\mathcal{Z}_t} + \frac{\gamma(t)^2}{4\alpha(t)} + D_1 + D_2. 
\tag{226}
\]
Notice that we cannot directly minimize (226) by the inequality of arithmetic and geometric means to obtain the reward-bias term because \(\{\theta_t, a_t\}_{t \in [T], a \in [K]}\) need to satisfy the constrains of Lemma 24. According to Lemma 13 and the choice of \(\alpha(t) = \sqrt{T}\), we can further bound the summation of the immediate regret over time step \(t\) as follows:
\[
\sum_{t=1}^{T} h(x^*_t) - h(x_t) 
\leq 2\gamma(T) \sum_{t=1}^{T} \frac{\|g(x_t; \hat{\theta}_t)\|_{\mathcal{Z}_t}}{\sqrt{m}} + \frac{T}{\sqrt{T}} \sum_{t=1}^{T} \frac{\|g(x_t; \hat{\theta}_t)\|^2_{\mathcal{Z}_t}}{\sqrt{m}} + \frac{\sum_{t=1}^{T} \gamma(t)^2}{4\sqrt{T}} + T(D_1 + D_2). 
\tag{227}
\]
\[
\leq 2\gamma(T) \sum_{t=1}^{T} \min \left\{ \frac{\|g(x_t; \hat{\theta}_t)\|_{\mathcal{Z}_t}}{\sqrt{m}}, 1 \right\} + \frac{T}{\sqrt{T}} \sum_{t=1}^{T} \min \left\{ \frac{\|g(x_t; \hat{\theta}_t)\|^2_{\mathcal{Z}_t}}{\sqrt{m}}, 1 \right\} + \frac{\sum_{t=1}^{T} \gamma(t)^2}{4\sqrt{T}} + T(D_1 + D_2), 
\tag{228}
\]
where (228) holds by the fact that \(h(x^*_t) - h(x_t)\) is upper bounded by 1. For \(2\gamma(T) \sum_{t=1}^{T} \min \left\{ \frac{\|g(x_t; \hat{\theta}_t)\|_{\mathcal{Z}_t}}{\sqrt{m}}, 1 \right\}\), we have
\[
2\gamma(T) \sum_{t=1}^{T} \min \left\{ \frac{\|g(x_t; \hat{\theta}_t)\|_{\mathcal{Z}_t}}{\sqrt{m}}, 1 \right\} \leq 2\gamma(T) \sqrt{T} \sum_{t=1}^{T} \min \left\{ \frac{\|g(x_t; \hat{\theta}_t)\|^2_{\mathcal{Z}_t}}{\sqrt{m}}, 1 \right\} 
\leq 2\sqrt{T} \gamma(T) \sqrt{2d\log(1 + TK/\lambda) + 2 + E_{17} m^{-\frac{7}{6}} \sqrt{\log mL^4 T^\frac{7}{6}}}, 
\tag{229}
\]
where (229) holds by Cauchy–Schwarz inequality, and (230) holds by Lemma 17. For \(\sqrt{T} \sum_{t=1}^{T} \min \left\{ \frac{\|g(x_t; \hat{\theta}_t)\|^2_{\mathcal{Z}_t}}{\sqrt{m}}, 1 \right\}\), we have
\[
\sqrt{T} \sum_{t=1}^{T} \min \left\{ \frac{\|g(x_t; \hat{\theta}_t)\|^2_{\mathcal{Z}_t}}{\sqrt{m}}, 1 \right\} \leq \sqrt{T} \left( 2d\log(1 + TK/\lambda) + 2 + E_{17} m^{-\frac{7}{6}} \sqrt{\log mL^4 T^\frac{7}{6}} \right), 
\tag{231}
\]
where (231) holds by Lemma 17. For \(\sum_{t=1}^{T} \frac{\gamma(t)^2}{4\sqrt{T}}\), we have
\[
\sum_{t=1}^{T} \frac{\gamma(t)^2}{4\sqrt{T}} \leq \sqrt{T} \gamma(T)^2. 
\tag{232}
\]
Notice that when $m \geq T^{10} \lambda^{-7} L^{24} (\log m)^3$, we have $\gamma(T) = \mathcal{O}\left(\sqrt{d \log(1 + TK/\lambda)}\right)$. For $T(D_1 + D_2)$, we have

$$T(D_1 + D_2) = T \left( E_{PC,D_1,D_2} \sum_{t=1}^{T} m^{-\frac{3}{2}} \lambda^{-\frac{3}{4}} L^2 \sqrt{\log m} + 2 Sm^{-\frac{3}{2}} \sqrt{\log m} \sum_{t=1}^{T} m L^2 \lambda^{-\frac{3}{4}} L^2 \right)$$

(233)

Similarly, $T(D_1 + D_2)$ will not affect the regret bound under the choice of $m$. Then, substituting (230), (231) and (232) into (228), we have $\sum_{t=1}^{T} h(x_t^*) - h(x_t) = \mathcal{O}(\sqrt{T \log T})$.

### E Index Derivations of the NeuralRBMLE Algorithms

#### E.1 Equivalence Between NeuralRBMLE in (11) and the Index Strategy in (12)-(13)

Recall (11) that $\theta_t^*$ denotes a maximizer of the following problem:

$$\max_{\theta} \left\{ f^t(F_t; \theta) + \alpha(t) \cdot \max_{1 \leq a \leq K} f(x_{t,a}; \theta) - \frac{m \lambda}{2} \| \theta - \theta_0 \|^2 \right\}. \tag{235}$$

Define

$$\hat{\theta}_t := \arg\max_{\theta} f(x_{t,a}; \theta_t^*), \tag{236}$$

$$\theta_t^* := \arg\max_{\theta} \left\{ f^t(F_t; \theta) + \alpha(t) \cdot f(x_{t,a}; \theta) - \frac{\lambda}{2} \| \theta - \theta_0 \|^2 \right\}. \tag{237}$$

For each arm $a$, consider an estimator $\hat{\theta}_{t,a}^\dagger \in \theta_{t,a}^\dagger$. Subsequently, define an index set

$$\hat{A}_t := \arg\max_{1 \leq a \leq K} \left\{ f^t(F_t; \hat{\theta}_{t,a}^\dagger) + \alpha(t) \cdot f(x_{t,a}; \theta_{t,a}^\dagger) - \frac{\lambda}{2} \| \theta_{t,a}^\dagger - \theta_0 \|^2 \right\}. \tag{238}$$

**Lemma 19.** For all $t \in [T]$, we have

$$\hat{A}_t = \hat{A}_t^\dagger. \tag{239}$$

**Proof.** Substituting $f(x_{t,a}; \theta_t^*)$ for $\hat{\theta}_{t,a}^\dagger$ and $f(x_{t,a}; \theta_{t,a}^\dagger)$ for $\hat{\theta}_{t,a}^\dagger$, we can obtain (239) by reusing the same analysis as that of Theorem 3 in [Hung et al. (2021)].

#### E.2 Derivation of the Surrogate Index of NeuralRBMLE-PC

Recall that $\hat{\theta}_t$ is the least-squares estimate.

**Lemma 20.** For all $a \in [K]$, all $t \in [T]$, any $\theta$ that satisfies $\| \theta - \theta_0 \|_2 \leq \tau$, and $m$ that satisfies

$$m \geq 2(\max \{ E_{22}, E_{23} \})^{\delta T_{16} L^2 14 (\log m)^3}, \tag{240}$$

we have

$$f(x_{t,a}; \theta) - \langle g(x_{t,a}; \hat{\theta}_t), \theta - \theta_0 \rangle \leq \frac{1}{T^2}. \tag{241}$$

**Proof.** By Lemma 2, we have

$$f(x_{t,a}; \theta) - \langle g(x_{t,a}; \hat{\theta}_t), \theta - \theta_0 \rangle \leq \langle g(x_{t,a}; \theta_0), \theta - \theta_0 \rangle - \langle g(x_{t,a}; \hat{\theta}_t), \theta - \theta_0 \rangle + E_{23} \sqrt{m \log(m)} \tag{242} \leq E_{23} L^2 \sqrt{m \log(m)} + E_{23} L^2 \sqrt{m \log(m)} \tag{243} \leq \frac{1}{T^2}, \tag{244}$$

where (243) holds by Lemma 3 and Lemma 4, and (244) holds by (240). Then, we complete the proof.
Lemma [20] shows that we can approximate the forward value of the neural network: \( f(x; \theta) \) by the inner product of \( \theta - \theta_0 \) and \( g(x; \hat{\theta}_t) \), which is the gradient in the \( \hat{\theta}_t \)-induced NTK regime. Then, we take the following steps to approximate \( I_{t,a}^\dagger \), the true NeuralRBMLE index, by the surrogate index of NeuralRBMLE-PC. Define

\[
\hat{\theta}_t := \theta_0 + \left( \frac{1}{m} \sum_{s=1}^{t-1} g(x_s; \hat{\theta}_t) g(x_s; \hat{\theta}_t)^T + \lambda I \right)^{-1} \cdot \left( \frac{1}{m} \sum_{s=1}^{t-1} r_s g(x_s; \hat{\theta}_t) \right) \tag{245}
\]

as the approximation of \( \hat{\theta}_t \) in the \( \hat{\theta}_t \)-induced NTK regime. Recall that the true index of NeuralRBMLE is

\[
I_{t,a}^\dagger = \ell^\dagger_{\lambda}(F_t; \theta_{t,a}) + \alpha(t)f(x_{t,a}; \theta_{t,a}). \tag{246}
\]

By Lemma [20] we can use \( \langle g(x; \hat{\theta}_t), \theta - \theta_0 \rangle \) to replace \( f(x; \theta) \) in \( I_{t,a}^\dagger \). Then, we can obtain a surrogate of \( \hat{\theta}_t \) defined in (16) as

\[
\hat{\theta}_{t,a} = \arg\max_\theta \left\{ -\frac{1}{2} \sum_{s=1}^{t-1} \langle g(x_s; \hat{\theta}_t), \theta - \theta_0 \rangle - r_s \right\}^2 - \frac{m\lambda}{2} \| \theta - \theta_0 \|_2^2 + \alpha(t) \langle g(x_{t,a}; \hat{\theta}_t), \theta - \theta_0 \rangle \right\}. \tag{247}
\]

By the first-order necessary optimality condition of \( \hat{\theta}_{t,a} \), we have

\[
\hat{\theta}_{t,a} = \theta_0 + \left( \frac{1}{m} \sum_{s=1}^{t-1} g(x_s; \hat{\theta}_t) g(x_s; \hat{\theta}_t)^T + \lambda I \right)^{-1} \cdot \left( \frac{1}{m} \sum_{s=1}^{t-1} r_s g(x_s; \hat{\theta}_t) \right) = \hat{\theta}_t + \frac{\alpha(t)}{m} Z_{t-1} g(x_{t,a}; \hat{\theta}_t) \tag{248}
\]

\[
\approx \hat{\theta}_t + \frac{\alpha(t)}{m} Z_{t-1} g(x_{t,a}; \hat{\theta}_t) \tag{249}
\]

\[
= \hat{\theta}_{t,a}. \tag{250}
\]

where (249) holds by the definition of \( \hat{\theta}_t \) in (245), (250) holds by \( \hat{\theta}_t \approx \hat{\theta}_t \) in \( \hat{\theta}_t \)-induced NTK regime, and (251) holds due to (16). Then, we have obtained the surrogate arm-specific RBMLE estimators \( \hat{\theta}_{t,a} \) for Algorithm [2].

### F Detailed Configuration of Experiments

To ensure a fair comparison among the algorithms, the hyper-parameters of each algorithm are tuned as follows: For \( \nu \) relative to exploration ratio, NeuralTS, NeuralUCB, NeuralRBMLE, DeepFPL, and LinRBMLE, we do grid search on \( \{1, 10^{-1}, 10^{-3}, 10^{-5}\} \). For BootstrappedNN, we refer to Zhou et al. [2020] and then set the transition probability as 0.8, and we use 10 neural networks to estimate the unknown reward function. For \( \lambda \) used in ridge regression, we set \( \lambda = 1 \) for LinRBMLE as suggested by Hung et al. [2021], and set \( \lambda = 0.001 \) for NeuralTS, NeuralUCB, and NeuralRBMLE. We choose \( \alpha(t) = \nu \sqrt{t} \) in both NeuralRBMLE-GA, NeuralRBMLE-PC and LinRBMLE, where \( \nu \) is tuned in the same way as other benchmarks. For the benchmark methods, we leverage the open-source implementation provided by NeuralTS [Zhang et al. 2021] available at https://openreview.net/forum?id=tkAtoZkcUnm.

### G Related Work on Linear Contextual Bandits

Linear stochastic contextual bandit problems have been extensively studied in the literature. For example, the celebrated Upper Confidence Bound (UCB) method and its variants enforce exploration through constructing confidence sets and have been applied to both linear bandits [Auer 2002; Dani et al. 2008; Rusmevichientong & Tsitsiklis 2010; Abbasi-Yadkori et al. 2011; Chu et al. 2011].
and generalized linear bandits Filippi et al. (2010); Li et al. (2017); Jun et al. (2017) with provably optimal regret bounds. Another popular line of exploration techniques is using randomized exploration. For example, from a Bayesian perspective, Thompson sampling (TS) achieves exploration in linear bandits Agrawal & Goyal (2013); Russo & Van Roy (2016); Abeille et al. (2017) and generalized linear bandits Dumitrascu et al. (2018); Kveton et al. (2020) by sampling the parameter from the posterior distribution. Kveton et al. (2020) proposed a follow-the-perturbed-leader algorithm for generalized linear bandits to achieve efficient exploration through perturbed rewards. Another popular randomized approach is information-directed sampling Russo & Van Roy (2018); Kirschner & Krause (2018), which determine the action sampling distribution by maximizing the ratio between the squared expected regret and the information gain. The above list of works is by no means exhaustive and is only meant to provide an overview of the research progress in this domain.

While the above prior studies offer useful insights into efficient exploration, they share the common limitation that the reward functions are required to satisfy the linear realizability assumption.

### Additional Experimental Results

| Std. of Final Regret | Adult | Covertype | MagicTelescope | MNIST | Mushroom | Shuttle |
|----------------------|-------|-----------|----------------|-------|----------|---------|
| NeuralRBMLE-GA       | 28.05 | 50.97     | 32.91          | 29.80 | 19.60    | 11.50   |
| NeuralRBMLE-PC       | 115.96| 88.91     | 137.96         | 82.28 | 57.91    | 48.37   |
| NeuralUCB            | 42.21 | 62.67     | 97.44          | 86.48 | 40.74    | 79.00   |
| NeuralTS             | 36.67 | 87.34     | 125.69         | 179.94| 44.46    | 75.92   |
| DeepFPL              | 53.88 | 536.48    | 93.77          | 1255.68| 43.25   | 824.98  |
| BoostrappedNN        | 133.52| 126.23    | 55.25          | 630.02| 64.31    | 311.51  |
| LinRBMLE             | **24.97**| 99.99     | **27.20**      | 279.36| 20.23    | 71.27   |

Figure 3: Cumulative regret averaged over 10 trials with $T = 1.5 \times 10^4$. 

(a) Covertype (b) MagicTelescope (c) Adult