A. Proof of Additional Results in Section 4

A.1. Verification of Remark 4.4

Suppose there exists a mapping \( \psi : \mathbb{R}^d \to \mathbb{R}^{\hat{d}} \) satisfying \( \| \psi(x) \|_2 \leq 1 \) which maps any context \( x \in \mathbb{R}^d \) to the Hilbert space \( \mathcal{H} \) associated with the Gram matrix \( H \in \mathbb{R}^{TK \times TK} \) over contexts \( \{ x^i \}_{i=1}^{TK} \). Then \( H = \Psi^T \Psi \), where \( \Psi = [\psi(x^1), ..., \psi(x^{TK})] \in \mathbb{R}^{\hat{d} \times TK} \). Thus, we can bound the effective dimension \( \hat{d} \) as follows

\[
\hat{d} = \frac{\log \det(I + H/\lambda)}{\log(1 + TK/\lambda)} = \frac{\log \det(I + \Psi \Psi^T/\lambda)}{\log(1 + TK/\lambda)} \leq \hat{d} \cdot \frac{\log \|I + \Psi \Psi^T/\lambda\|_2}{\log(1 + TK/\lambda)}.
\]

where the second equality holds due to the fact that \( \det(I + A^T A/\lambda) = \det(I + AA^T/\lambda) \) holds for any matrix \( A \), and the inequality holds since \( \det A \leq \|A\|^2 \) for any \( A \in \mathbb{R}^{\hat{d} \times \hat{d}} \). Clearly, \( \hat{d} \leq \hat{d} \) as long as \( \|I + \Psi \Psi^T/\lambda\|_2 \leq 1 + TK/\lambda \). Indeed,

\[
\|I + \Psi \Psi^T/\lambda\|_2 \leq 1 + \|\Psi \Psi^T\|_2/\lambda \leq 1 + \sum_{i=1}^{TK} \|\psi(x^i)\psi(x^i)^T\|_2/\lambda \leq 1 + TK/\lambda,
\]

where the first inequality is due to triangle inequality and the fact \( \lambda \geq 1 \), the second inequality holds due to the definition of \( \Psi \) and triangle inequality, and the last inequality is by \( \|\psi(x^i)\|_2 \leq 1 \) for any \( 1 \leq i \leq TK \).

A.2. Verification of Remark 4.8

Let \( K(\cdot, \cdot) \) be the NTK kernel, then for \( i, j \in [TK] \), we have \( H_{i,j} = K(x^i, x^j) \). Suppose that \( h \in \mathcal{H} \), then \( h \) can be decomposed as \( h = h_H + h_\perp \), where \( h_H(x) = \sum_{i=1}^{TK} \alpha_i K(x, x^i) \) is the projection of \( h \) to the function space spanned by \( \{ K(x, x^i) \}_{i=1}^{TK} \) and \( h_\perp \) is the orthogonal part. By definition we have \( h(x^i) = h_H(x^i) \) for \( i \in [TK] \), thus

\[
\alpha = H \alpha, \quad h = [h(x^1), ..., h(x^{TK})]^T = [h_H(x^1), ..., h_H(x^{TK})]^T = \left[ \sum_{i=1}^{TK} \alpha_i K(x^1, x^i), ..., \sum_{i=1}^{TK} \alpha_i K(x^{TK}, x^i) \right]^T = H \alpha,
\]

which implies that \( \alpha = H^{-1} h \). Thus, we have

\[
\|h\|_\mathcal{H} \geq \|h_H\|_\mathcal{H} = \sqrt{\alpha^T H \alpha} = \sqrt{h^T H^{-1} H H^{-1} h} = \sqrt{h^T H^{-1} h}.
\]

A.3. Proof of Corollary 4.9

Proof of Corollary 4.9. Notice that \( R_T \leq T \) since \( 0 \leq h(x) \leq 1 \). Thus, with the fact that with probability at least \( 1 - \delta \), (4.3) holds, we can bound \( \mathbb{E}[R_T] \) as

\[
\mathbb{E}[R_T] \leq (1 - \delta) \left( 3\sqrt{T} \sqrt{d \log(1 + TK/\lambda)} + 2 \left[ \sqrt{d \log(1 + TK/\lambda)} + 2 - 2 \log \delta \right] + 2 \sqrt{\lambda S} + (\lambda + C_2 TL)(1 - \eta m \lambda)^{1/2} \sqrt{\lambda/\lambda} + 1 \right) + \delta T. \tag{A.1}
\]

Taking \( \delta = 1/T \) completes the proof.

\( \square \)

B. Proof of Lemmas in Section 5

B.1. Proof of Lemma 5.1

We start with the following lemma:
Lemma B.1. Let \( G = [g(x^1; \theta_0), \ldots, g(x^{TK}; \theta_0)]/\sqrt{m} \in \mathbb{R}^{p \times (TK)} \). Let \( H \) be the NTK matrix as defined in Definition 4.1. For any \( \delta \in (0, 1) \), if

\[
m = \Omega \left( \frac{L^6 \log(TKL/\delta)}{\epsilon^4} \right),
\]

then with probability at least \( 1 - \delta \), we have

\[
\|G^T G - H\|_F \leq TK\epsilon.
\]

We begin to prove Lemma 5.1.

Proof of Lemma 5.1. By Assumption 4.2, we know that \( \lambda_0 > 0 \). By the choice of \( m \), we have \( m \geq \Omega(L^6 \log(TKL/\delta)/\epsilon^4) \), where \( \epsilon = \lambda_0/(2TK) \). Thus, due to Lemma B.1, with probability at least \( 1 - \delta \), we have \( \|G^T G - H\|_F \leq TK\epsilon = \lambda_0/2 \). That leads to

\[
G^T G \geq H - \|G^T G - H\|_F I \geq H - \lambda_0/2 \geq H/2 > 0,
\]

where the first inequality holds due to the triangle inequality, the third and fourth inequality holds due to \( H \geq \lambda_0 I > 0 \). Thus, suppose the singular value decomposition of \( G \) is \( G = PAQ^\top \), \( P \in \mathbb{R}^{n \times TK} \), \( A \in \mathbb{R}^{TK \times TK} \), \( Q \in \mathbb{R}^{TK \times TK} \), we have \( A > 0 \). Now we are going to show that \( \theta^* = \theta_0 + PA^{-1}Q^\top h/\sqrt{m} \) satisfies (5.1). First, we have

\[
G^T \sqrt{m}(\theta^* - \theta_0) = QA P^\top PA^{-1} Q^\top h = h,
\]

which suggests that for any \( i \), \( \langle g(x^i; \theta_0), \theta^* - \theta_0 \rangle = h(x^i) \). We also have

\[
m\|\theta^* - \theta_0\|_2^2 = h^\top QA^{-2}Q^\top h = h^\top (G^T G)^{-1} h \leq 2h^\top H^{-1} h,
\]

where the last inequality holds due to (B.1). This completes the proof. \( \square \)

B.2. Proof of Lemma 5.2

In this section we prove Lemma 5.2. For simplicity, we define \( \mathbf{Z}_t, \mathbf{b}_t, \bar{\gamma}_t \) as follows:

\[
\mathbf{Z}_t = \lambda I + \sum_{i=1}^t g(x_{i,a}; \theta_0)g(x_{i,a}; \theta_0)^\top / m,
\]

\[
\mathbf{b}_t = \sum_{i=1}^t r_{i,a} g(x_{i,a}; \theta_0) / \sqrt{m},
\]

\[
\bar{\gamma}_t = \nu \sqrt{\log \frac{\det \mathbf{Z}_t}{\det \lambda I}} - 2 \log \delta + \sqrt{\lambda S}.
\]

We need the following lemmas. The first lemma shows that the network parameter \( \theta_t \) at round \( t \) can be well approximated by \( \theta_0 + \mathbf{Z}_t^{-1} \mathbf{b}_t / \sqrt{m} \).

Lemma B.2. There exist constants \( \{ \bar{C}_i \}_{i=1}^5 > 0 \) such that for any \( \delta > 0 \), if for all \( t \in [T] \), \( \eta, m \) satisfy

\[
2 \sqrt{t/(m \lambda)} \geq \bar{C}_1 m^{-3/2} L^{-3/2} [\log(TKL^2/\delta)]^{3/2},
\]

\[
2 \sqrt{t/(m \lambda)} \leq \bar{C}_2 \min \{ L^{-6} [\log m]^{-3/2}, (m(\lambda \eta)^2 L^{-6} t^{-1} (\log m)^{-1} )^{3/8} \},
\]

\[
\eta \leq \bar{C}_3 (m \lambda + tmL)^{-1},
\]

\[
m^{1/6} \geq \bar{C}_4 \sqrt{\log m L^{7/2} t^{7/6} \lambda^{-7/6} (1 + \sqrt{t/\lambda})},
\]

then with probability at least \( 1 - \delta \), we have that \( \|\theta_t - \theta_0\|_2 \leq 2 \sqrt{t/(m \lambda)} \) and

\[
\|\theta_t - \theta_0 - \mathbf{Z}_t^{-1} \mathbf{b}_t / \sqrt{m}\|_2 \leq (1 - \eta m \lambda)^{1/2} \sqrt{t/(m \lambda)} + \bar{C}_5 m^{-2/3} \sqrt{\log m L^{7/2} t^{5/3} \lambda^{-5/3} (1 + \sqrt{t/\lambda})}.
\]
Next lemma shows the error bounds for $\bar{Z}_t$ and $Z_t$.

**Lemma B.3.** There exist constants $\{C_i\}_{i=1}^5 > 0$ such that for any $\delta > 0$, if $m$ satisfies that
\[
C_1m^{-3/2}L^{-3/2}[\log(TKL^2/\delta)]^{3/2} \leq 2\sqrt{t/(m\lambda)} \leq C_2L^{-6}[\log m]^{-3/2}, \quad \forall t \in [T],
\]
then with probability at least $1 - \delta$, for any $t \in [T]$, we have
\[
\|Z_t\|_2 \leq \lambda + C_3 t L, \\
\|Z_t - \bar{Z}_t\|_F \leq C_4 m^{-1/6} \sqrt{\log mL^4 t^{7/6} \lambda^{-1/6}}, \\
\left| \log \frac{\det(Z_t)}{\det(\lambda)} - \log \frac{\det(\bar{Z}_t)}{\det(\lambda)} \right| \leq C_5 m^{-1/6} \sqrt{\log mL^4 t^{5/3} \lambda^{-1/6}}.
\]

With above lemmas, we prove Lemma 5.2 as follows.

**Proof of Lemma 5.2.** By Lemma B.2 we know that $\|\theta_t - \theta_0\|_2 \leq 2\sqrt{t/(m\lambda)}$. By Lemma 5.1, with probability at least $1 - \delta$, there exists $\theta^*$ such that for any $1 \leq t \leq T$,
\[
h(x_{t,a_t}) = \langle g(x_{t,a_t}; \theta_0) / \sqrt{m}, \sqrt{m}(\theta^* - \theta_0) \rangle, \quad (B.2)
\]
\[
\sqrt{m}\|\theta^* - \theta_0\|_2 \leq \sqrt{2h^T \mathbf{H}^{-1} \mathbf{H}} \leq S, \quad (B.3)
\]
where the second inequality holds since $S \geq \sqrt{2h^T \mathbf{H}^{-1} \mathbf{H}}$ in the statement of Lemma 5.2. Thus, conditioned on (B.2) and (B.3), by Theorem 2 in Abbasi-Yadkori et al. (2011), with probability at least $1 - \delta$, for any $1 \leq t \leq T$, $\theta^*$ satisfies that
\[
\|\sqrt{m}(\theta^* - \theta_0) - \bar{Z}_t^{-1}b_t\|_{Z_t} \leq \tilde{\gamma}_t. \quad (B.4)
\]
We now prove that $\|\theta^* - \theta_t\|_{Z_t} \leq \gamma_t / \sqrt{m}$. From the triangle inequality,
\[
\|\theta^* - \theta_t\|_{Z_t} \leq \underbrace{\|\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m}\|_{Z_t}}_{I_1} + \underbrace{\|\theta_t - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m}\|_{Z_t}}_{I_2}. \quad (B.5)
\]
We bound $I_1$ and $I_2$ separately. For $I_1$, we have
\[
I_1^2 = (\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m})^T Z_t (\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m}) \\
= (\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m})^T Z_t (\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m}) \\
+ (\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m})^T (Z_t - \bar{Z}_t)(\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m}) \\
\leq (\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m})^T Z_t (\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m}) \\
+ \frac{\|Z_t - \bar{Z}_t\|^2}{\lambda} (\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m})^T Z_t (\theta^* - \theta_0 - \bar{Z}_t^{-1}b_t / \sqrt{m}) \\
\leq (1 + \|Z_t - \bar{Z}_t\|^2 / \lambda) \tilde{\gamma}_t^2 / m, \quad (B.6)
\]
where the first inequality holds due to the fact that $x^T A x \leq x^T B x \cdot \|A\|_2 / \lambda_{\min}(B)$ for some $B \succ 0$ and the fact that $\lambda_{\min}(\bar{Z}_t) \geq \lambda$, the second inequality holds due to (B.4). We have
\[
\|\bar{Z}_t - Z_t\|_2 \leq \left\| Z_t - \bar{Z}_t \right\|_F \leq C_1 m^{-1/6} \sqrt{\log mL^4 t^{7/6} \lambda^{-1/6}}, \quad (B.7)
\]
where the first inequality holds due to the fact that $\|A\|_2 \leq \|A\|_F$, the second inequality holds due to Lemma B.3. We also have
\[
\tilde{\gamma}_t = \nu \sqrt{\log \frac{\det \bar{Z}_t}{\det(\lambda)} - 2 \log \delta + \sqrt{\lambda} S} \\
= \nu \sqrt{\log \frac{\det \bar{Z}_t}{\det(\lambda)} + \log \frac{\det Z_t}{\det(\lambda)} - \log \frac{\det \bar{Z}_t}{\det(\lambda)}} - 2 \log \delta + \sqrt{\lambda} S \\
\leq \nu \sqrt{\log \frac{\det Z_t}{\det(\lambda)} + C_2 m^{-1/6} \sqrt{\log mL^4 t^{5/3} \lambda^{-1/6}} - 2 \log \delta + \sqrt{\lambda} S}, \quad (B.8)
\]
where $C_1, C_2 > 0$ are two constants, the inequality holds due to Lemma B.3. Substituting (B.7) and (B.8) into (B.6), we have

$$I_1 \leq \sqrt{1 + \|Z_t - \bar{Z}_t\|^2 / \lambda\gamma_t / \sqrt{m}}$$

$$\leq \sqrt{1 + C_1 m^{-1/6} \sqrt{\log m L^4 t^{7/6} \lambda^{-7/6}} / \sqrt{m}}$$

$$\cdot \left( v \sqrt{\log \det \Lambda t} + C_2 m^{-1/6} \sqrt{\log m L^4 t^{5/3} \lambda^{-1/6}} - 2 \log \delta + \sqrt{\lambda S} \right).$$  \hspace{1cm} (B.9)

For $I_2$, we have

$$I_2 = \|\theta_t - \theta_0 - \bar{Z}_t^{-1} b_t / \sqrt{m}\|_{Z_t}$$

$$\leq \|Z_t\|_2 \cdot \|\theta_t - \theta_0 - \bar{Z}_t^{-1} b_t / \sqrt{m}\|_2$$

$$\leq (\lambda + C_3 t L) \|\theta_t - \theta_0 - \bar{Z}_t^{-1} b_t / \sqrt{m}\|_2$$

$$\leq (\lambda + C_3 t L) \left( (1 - \eta m \lambda)^{1/2} \sqrt{t / (m \lambda)} + m^{-2/3} \sqrt{\log m L^7 / t^{5/3} \lambda^{-5/3}(1 + \sqrt{t / \lambda})} \right).$$  \hspace{1cm} (B.10)

where $C_3 > 0$ is a constant, the first inequality holds since for any vector $a$, the second inequality holds due to $\|Z_t\|_2 \leq \lambda + C_3 t L$ by Lemma B.3, the third inequality holds due to Lemma B.2. Substituting (B.9) and (B.10) into (B.5), we obtain $\|\theta^* - \hat{\theta}\|_{Z_t} \leq \gamma_t / \sqrt{m}$. This completes the proof. \hfill \Box

### B.3. Proof of Lemma 5.3

The proof starts with three lemmas that bound the error terms of the function value and gradient of neural networks.

**Lemma B.4** (Lemma 4.1, Cao & Gu (2019)). There exist constants $\{\bar{C}_1\}_{i=1}^3 > 0$ such that for any $\delta > 0$, if $\tau$ satisfies that

$$\bar{C}_1 m^{-3/2} L^{-3/2} \log(TKL^2 / \delta)^{3/2} \leq \tau \leq \bar{C}_2 L^{-6} \log m^{-3/2},$$

then with probability at least $1 - \delta$, for all $\bar{\theta}, \tilde{\theta}$ satisfying $\|\bar{\theta} - \theta_0\|_2 \leq \tau, \|\tilde{\theta} - \theta_0\|_2 \leq \tau$ and $j \in [TK]$ we have

$$\left| f(x^j; \bar{\theta}) - f(x^j; \tilde{\theta}) - \langle g(x^j; \bar{\theta}), \bar{\theta} - \tilde{\theta} \rangle \right| \leq \bar{C}_3 \tau^{4/3} L^3 \sqrt{m \log m}.$$

**Lemma B.5** (Theorem 5, Allen-Zhu et al. (2019)). There exist constants $\{\bar{C}_1\}_{i=1}^3 > 0$ such that for any $\delta \in (0, 1)$, if $\tau$ satisfies that

$$\bar{C}_1 m^{-3/2} L^{-3/2} \max\{\log^{-3/2} m, \log^{3/2}(TK / \delta)\} \leq \tau \leq \bar{C}_2 L^{-9/2} \log^{-3} m,$$

then with probability at least $1 - \delta$, for all $\|\theta - \theta_0\|_2 \leq \tau$ and $j \in [TK]$ we have

$$\|g(x^j; \theta) - g(x^j; \theta_0)\|_2 \leq \bar{C}_3 \sqrt{\log m \tau^{1/3} L^3} \|g(x^j; \theta_0)\|_2.$$

**Lemma B.6** (Lemma B.3, Cao & Gu (2019)). There exist constants $\{\bar{C}_1\}_{i=1}^3 > 0$ such that for any $\delta > 0$, if $\tau$ satisfies that

$$\bar{C}_1 m^{-3/2} L^{-3/2} \log(TKL^2 / \delta)^{3/2} \leq \tau \leq \bar{C}_2 L^{-6} \log m^{-3/2},$$

then with probability at least $1 - \delta$, for any $\|\theta - \theta_0\|_2 \leq \tau$ and $j \in [TK]$ we have $\|g(x^j; \theta)\|_F \leq \bar{C}_3 \sqrt{m L}$.

**Proof of Lemma 5.3.** We follow the regret bound analysis in Abbasi-Yadkori et al. (2011); Valko et al. (2013). Denote $\alpha^*_t = \arg\max_{a \in [K]} h(x^t, a)$ and $C_t = \{\theta : \|\theta - \theta_0\|_{Z_t} \leq \gamma_t / \sqrt{m}\}$. By Lemma 5.2, for all $1 \leq t \leq T$, we have $\|\theta_t - \theta_0\|_2 \leq 2 \sqrt{t / (m \lambda)}$ and $\theta^* \in C_t$. By the choice of $m$, Lemmas B.4, B.5 and B.6 hold. Thus, $h(x^t, a^*_t) - h(x^t, a_t)$ can
be bounded as follows:

$$h(x_{t,a_{t}^{*}}) - h(x_{t,a}) = \langle g(x_{t,a}; \theta_{0}), \theta^{*} - \theta_{0} \rangle - \langle g(x_{t,a_{t}^{*}}; \theta_{0}), \theta^{*} - \theta_{0} \rangle$$

$$\leq \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle - \langle g(x_{t,a}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle + \|\theta^{*} - \theta_{0}\|_{2} \|g(x_{t,a_{t}^{*}}; \theta_{t}) - g(x_{t,a_{t}^{*}}; \theta_{t-1})\|_{2} + \|g(x_{t,a_{t}^{*}}; \theta_{t}) - g(x_{t,a}; \theta_{0})\|_{2}$$

$$\leq \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle - \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle + C_{1} \sqrt{h^{1}\mathbb{H}^{-1} \pi m^{-1/6}} \sqrt{\log m t^{1/6} \lambda^{-1/6} L^{7/2}}$$

$$\leq \max_{\theta \in C_{t-1}} \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta - \theta_{0} \rangle - \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle + C_{1} \sqrt{h^{1}\mathbb{H}^{-1} \pi m^{-1/6}} \sqrt{\log m t^{1/6} \lambda^{-1/6} L^{7/2}}, \quad \quad \text{(B.11)}$$

where the equality holds due to Lemma 5.1, the first inequality holds due to triangle inequality, the second inequality holds due to Lemmas 5.1, B.5, B.6, the third inequality holds due to $\theta^{*} \in C_{t-1}$. Denote

$$\tilde{U}_{t,a} = \langle g(x_{t,a}; \theta_{t-1}), \theta_{t-1} - \theta_{0} \rangle + \gamma_{t-1} \sqrt{\varrho_{t-1}} g(x_{t,a}; \theta_{t-1}) / m,$$

then we have $\tilde{U}_{t,a} = \max_{\theta \in C_{t-1}} \langle g(x_{t,a}; \theta_{t-1}), \theta - \theta_{0} \rangle$ due to the fact that

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

Recall the definition of $U_{t,a}$ from Algorithm 1, we also have

$$|U_{t,a} - \tilde{U}_{t,a}| = \left| f(x_{t,a}; \theta_{t-1}) - \langle g(x_{t,a}; \theta_{t-1}), \theta_{t-1} - \theta_{0} \rangle \right|$$

$$= \left| f(x_{t,a}; \theta_{t-1}) - f(x_{t,a}; \theta_{0}) - \langle g(x_{t,a}; \theta_{t-1}), \theta_{t-1} - \theta_{0} \rangle \right|$$

$$\leq C_{2} m^{-1/6} \sqrt{\log m t^{3/2} \lambda^{-2/3} L^{3}}, \quad \quad \text{(B.12)}$$

where $C_{2} > 0$ is a constant, the second equality holds due to $f(x_{t}; \theta_{0}) = 0$ by the random initialization of $\theta_{0}$, the inequality holds due to Lemma B.4 with the fact $||\theta_{t-1} - \theta_{0}||_{2} \leq 2 \sqrt{t/(m \lambda)}$. Since $\theta^{*} \in C_{t-1}$, then $I_{1}$ in (B.11) can be bounded as

$$\max_{\theta \in C_{t-1}} \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta - \theta_{0} \rangle - \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle$$

$$= \tilde{U}_{t,a_{t}^{*}} - \langle g(x_{t,a_{t}^{*}}; \theta_{t}), \theta^{*} - \theta_{0} \rangle$$

$$\leq U_{t,a_{t}^{*}} - \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle + C_{2} m^{-1/6} \sqrt{\log m t^{3/2} \lambda^{-2/3} L^{3}}$$

$$\leq U_{t,a} - \langle g(x_{t,a}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle + C_{2} m^{-1/6} \sqrt{\log m t^{3/2} \lambda^{-2/3} L^{3}}$$

$$\leq \tilde{U}_{t,a} - \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle + 2C_{2} m^{-1/6} \sqrt{\log m t^{3/2} \lambda^{-2/3} L^{3}}, \quad \quad \text{(B.13)}$$

where the first inequality holds due to (B.12), the second inequality holds since $a_{t} = \arg \max_{a} U_{t,a}$, the third inequality holds due to (B.12). Furthermore,

$$\tilde{U}_{t,a_{t}^{*}} - \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle$$

$$= \max_{\theta \in C_{t-1}} \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta - \theta_{0} \rangle - \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{0} \rangle$$

$$= \max_{\theta \in C_{t-1}} \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta - \theta_{t-1} \rangle - \langle g(x_{t,a_{t}^{*}}; \theta_{t-1}), \theta^{*} - \theta_{t-1} \rangle$$

$$\leq \max_{\theta \in C_{t-1}} \|\theta - \theta_{t-1}\|_{Z_{t-1}} \|g(x_{t,a_{t}^{*}}; \theta_{t-1})\|_{Z_{t-1}^{-1}} + \|\theta^{*} - \theta_{t-1}\|_{Z_{t-1}} \|g(x_{t,a_{t}^{*}}; \theta_{t-1})\|_{Z_{t-1}^{-1}}$$

$$\leq 2 \gamma_{t-1} \|g(x_{t,a_{t}^{*}}; \theta_{t-1})\| / \sqrt{m} ||Z_{t-1}^{-1} ||^{-1}, \quad \quad \text{(B.14)}$$
where the second inequality holds due to Hölder inequality, the second inequality holds due to Lemma 5.2. Combining (B.11), (B.13) and (B.14), we have

\[
\begin{align*}
\frac{h(x_{t,a}) - h(x_{t,a'})}{t} & \leq 2\gamma_t -1 \frac{\|g(x_{t,a}; \theta_{t-1})/\sqrt{m}\|_{\mathbb{Z}^{-1}}}{z_{t-1}^1} + C_1 \sqrt{h^\top H^{-1} h m^{-1/6} \sqrt{\log m t^{1/6} \lambda^{-1/6} L^{7/2}}} \\
& \quad + 2C_2 m^{-1/6} \sqrt{\log m t^{2/3} \lambda^{-2/3} L^3} \\
& \leq \min \left\{ 2\gamma_t -1 \frac{\|g(x_{t,a}; \theta_{t-1})/\sqrt{m}\|_{\mathbb{Z}^{-1}}}{z_{t-1}^1} + C_1 \sqrt{h^\top H^{-1} h m^{-1/6} \sqrt{\log m t^{1/6} \lambda^{-1/6} L^{7/2}}} \\
& \quad + 2C_2 m^{-1/6} \sqrt{\log m t^{2/3} \lambda^{-2/3} L^3}, 1 \right\} \leq \min \left\{ 2\gamma_t -1 \frac{\|g(x_{t,a}; \theta_{t-1})/\sqrt{m}\|_{\mathbb{Z}^{-1}}^2}{z_{t-1}^1}, 1 \right\} + C_1 \sqrt{h^\top H^{-1} h m^{-1/6} \sqrt{\log m t^{1/6} \lambda^{-1/6} L^{7/2}}} \\
& \quad + 2C_2 m^{-1/6} \sqrt{\log m t^{2/3} \lambda^{-2/3} L^3} \
\end{align*}
\]

where the second inequality holds due to the fact that \(0 \leq h(x_{t,a}) - h(x_{t,a'}) \leq 1\), the third inequality holds due to the fact that \(\min\{a + b, 1\} \leq \min\{a, 1\} + b\), the fourth inequality holds due to the fact \(\gamma_{t-1} \geq \sqrt{\lambda} S \geq 1\). Finally, by the fact that \(\sqrt{2hH^{-1}h} \leq S\), the proof completes. \(\square\)

B.4. Proof of Lemma 5.4

In this section we prove Lemma 5.4, we need the following lemma from Abbasi-Yadkori et al. (2011).

Lemma B.7 (Lemma 11, Abbasi-Yadkori et al. (2011)). We have the following inequality:

\[
\sum_{t=1}^T \min \left\{ \frac{\|g(x_{t,a}; \theta_{t-1})/\sqrt{m}\|_{\mathbb{Z}^{-1}}^2}{z_{t-1}^1}, 1 \right\} \leq 2 \log \frac{\det Z_T}{\det \lambda^T}.
\]

Proof of Lemma 5.4. First by the definition of \(\gamma_t\), we know that \(\gamma_t\) is a monotonic function w.r.t. \(\det Z_t\). By the definition of \(Z_t\), we know that \(Z_T \geq Z_t\), which implies that \(\det Z_t \leq \det Z_T\). Thus, \(\gamma_t \leq \gamma_T\). Second, by Lemma B.7 we know that

\[
\sum_{t=1}^T \min \left\{ \frac{\|g(x_{t,a}; \theta_{t-1})/\sqrt{m}\|_{\mathbb{Z}^{-1}}^2}{z_{t-1}^1}, 1 \right\} \leq 2 \log \frac{\det Z_T}{\det \lambda^T} \leq 2 \log \frac{\det Z_T}{\det \lambda^T} + C_1 m^{-1/6} \sqrt{\log m L^4 T^{5/3} \lambda^{-1/6}},
\]

where the second inequality holds due to Lemma B.3. Next we are going to bound \(\log \det Z_T\). Denote \(G = [g(x^1; \theta_0)/\sqrt{m}, \ldots, g(x^{TK}; \theta_0)/\sqrt{m}] \in \mathbb{R}^{p \times (TK)}\), then we have

\[
\begin{align*}
\log \frac{\det Z_T}{\det \lambda^T} &= \log \det \left(I + \sum_{t=1}^T g(x_{t,a}; \theta_0)g(x_{t,a}; \theta_0)^\top / (m\lambda)\right) \\
& \leq \log \det \left(I + \sum_{t=1}^{TK} g(x^i; \theta_0)g(x^i; \theta_0)^\top / (m\lambda)\right) \\
& = \log \det \left(I + GG^\top / \lambda\right) \\
& = \log \det \left(I + G^\top G / \lambda\right).
\end{align*}
\]
where the inequality holds naively, the third equality holds since for any matrix $A \in \mathbb{R}^{p \times TK}$, we have $\det(I + AA^T) = \det(I + A^TA)$. We can further bound (B.17) as follows:

$$
\log \det \left( I + G^T G \right) = \log \det \left( I + H / \lambda + (G^T G - H) / \lambda \right) \\
\leq \log \det \left( I + H / \lambda \right) + \langle (I + H / \lambda)^{-1}, (G^T G - H) / \lambda \rangle \\
\leq \log \det \left( I + H / \lambda \right) + \| (I + H / \lambda)^{-1} \|_F \| G^T G - H \|_F / \lambda \\
\leq \log \det \left( I + H / \lambda \right) + \sqrt{TK} \| G^T G - H \|_F \\
\leq \log \det \left( I + H / \lambda \right) + 1 \\
= \tilde{d}\log(1 + TK / \lambda) + 1, \tag{B.18}
$$

where the first inequality holds due to the concavity of $\log \det(\cdot)$, the second inequality holds due to the fact that $\langle A, B \rangle \leq \|A\|_F \|B\|_F$, the third inequality holds due to the facts that $I + H / \lambda \succeq I$, $\lambda \geq 1$ and $\|A\|_F \leq \sqrt{TK} \|A\|_2$ for any $A \in \mathbb{R}^{TK \times TK}$, the fourth inequality holds by Lemma B.1 with the choice of $m$, the fifth inequality holds by the definition of effective dimension in Definition 4.3, and the last inequality holds due to the choice of $\lambda$. Substituting (B.18) into (B.17), we obtain that

$$
\log \frac{\det Z_T}{\det \lambda I} \leq \tilde{d}\log(1 + TK / \lambda) + 1. \tag{B.19}
$$

Substituting (B.19) into (B.16), we have

$$
\sum_{t=1}^{T} \min \left\{ \left\| g(x_{t,\cdot}; \theta_{t-1}) / \sqrt{m} \right\|_{Z_{t-1}}^2, 1 \right\} \leq 2\tilde{d}\log(1 + TK / \lambda) + 2 + C_1 m^{-1/6} \sqrt{\log m} L^4 T^{5/3} \lambda^{-1/6}. \tag{B.20}
$$

We now bound $\gamma_T$, which is

$$
\gamma_T = \sqrt{1 + C_1 m^{-1/6} \sqrt{\log m} L^4 T^{7/6} \lambda^{-7/6}} \\
\cdot \left( \nu \sqrt{\log \frac{\det Z_T}{\det \lambda I}} + C_2 m^{-1/6} \sqrt{\log m} L^4 T^{5/3} \lambda^{-1/6} - 2 \log \delta + \sqrt{\lambda S} \right) \\
+ (\lambda + C_3 TL) \left( (1 - \eta m \lambda)^{1/2} T / (m \lambda) + m^{-2/3} \sqrt{\log m} L^7 / T^{5/3} \lambda^{-5/3} (1 + \sqrt{T / \lambda}) \right) \\
\leq \sqrt{1 + C_1 m^{-1/6} \sqrt{\log m} L^4 T^{7/6} \lambda^{-7/6}} \\
\cdot \left( \nu \sqrt{\log \frac{\det Z_T}{\det \lambda I}} + 2C_2 m^{-1/6} \sqrt{\log m} L^4 T^{5/3} \lambda^{-1/6} - 2 \log \delta + \sqrt{\lambda S} \right) \\
+ (\lambda + C_3 TL) \left( (1 - \eta m \lambda)^{1/2} T / (m \lambda) + m^{-2/3} \sqrt{\log m} L^7 / T^{5/3} \lambda^{-5/3} (1 + \sqrt{T / \lambda}) \right), \tag{B.21}
$$

Neural Contextual Bandits with UCB-based Exploration
where the inequality holds due to Lemma B.3. Finally, we have

\[
\sum_{t=1}^{T} \gamma_{t-1} \min \left\{ \|g(x_{t, i}; \theta_{t-1})/\sqrt{m}\|_{Z_{t-1}}^2, 1 \right\}
\leq \gamma_T \sum_{t=1}^{T} \min \left\{ \|g(x_{t, i}; \theta_{t-1})/\sqrt{m}\|_{Z_{t-1}}^2, 1 \right\}
\leq \sqrt{\log \det Z_T \det Z_T + C_1 m^{-1/6} \sqrt{\log mL^4 T^{5/3} \lambda^{-1/6}} \left[ 1 + C_1 m^{-1/6} \sqrt{\log mL^4 T^{7/6} \lambda^{-7/6}} \right.}
\cdot \left( \nu \sqrt{\log \det Z_T \det Z_T + 2C_2 m^{-1/6} \sqrt{\log mL^4 T^{5/3} \lambda^{-1/6}} - 2 \log \delta + \sqrt{\lambda S} \right)
+ (\lambda + C_3 TL) \left[ (1 - \eta m\lambda)^{-1/2} \sqrt{T/(m\lambda)} + m^{-3/2} \sqrt{\log mL^2 T^{5/3} \lambda^{-5/3}(1 + \sqrt{T/\lambda})} \right]
\leq \sqrt{\bar{d} \log(1 + TK/\lambda)} + 1 + C_1 m^{-1/6} \sqrt{\log mL^4 T^{5/3} \lambda^{-1/6}} \left[ 1 + C_1 m^{-1/6} \sqrt{\log mL^4 T^{7/6} \lambda^{-7/6}} \right.}
\cdot \left( \nu \sqrt{\bar{d} \log(1 + TK/\lambda)} + 2C_2 m^{-1/6} \sqrt{\log mL^4 T^{5/3} \lambda^{-1/6}} - 2 \log \delta + \sqrt{\lambda S} \right)
+ (\lambda + C_3 TL) \left[ (1 - \eta m\lambda)^{-1/2} \sqrt{T/(m\lambda)} + m^{-3/2} \sqrt{\log mL^2 T^{5/3} \lambda^{-5/3}(1 + \sqrt{T/\lambda})} \right],
\]

where the first inequality holds due to the fact that \(\gamma_{t-1} \leq \gamma_T\), the second inequality holds due to (B.20) and (B.21), the third inequality holds due to (B.19). This completes our proof. \(\square\)

### C. Proofs of Technical Lemmas in Appendix B

#### C.1. Proof of Lemma B.1

In this section we prove Lemma B.1, we need the following lemma from Arora et al. (2019):

**Lemma C.1 (Theorem 3.1, Arora et al. (2019)).** Fix \(\epsilon > 0\) and \(\delta \in (0, 1)\). Suppose that

\[
m = \Omega \left( \frac{L^6 \log(L/\delta)}{\epsilon^4} \right),
\]

then for any \(i, j \in [TK]\), with probability at least \(1 - \delta\) over random initialization of \(\theta_0\), we have

\[
|\langle g(x_i^j, \theta_0), g(x_j^j, \theta_0) \rangle/m - H_{i,j}| \leq \epsilon.
\]

**Proof of Lemma B.1.** Taking union bound over \(i, j \in [TK]\), we have that if

\[
m = \Omega \left( \frac{L^6 \log(T^2 K^2 L/\delta)}{\epsilon^4} \right),
\]

then with probability at least \(1 - \delta\), (C.1) holds for all \((i, j) \in [TK] \times [TK]\). Therefore, we have

\[
\|G^T G - H\|_F = \sqrt{\sum_{i=1}^{TK} \sum_{j=1}^{TK} |\langle g(x_i^j, \theta_0), g(x_j^j, \theta_0) \rangle/m - H_{i,j}|^2} \leq TK \epsilon.
\]

\(\square\)
We also define the following auxiliary sequence $\theta = (\theta(0), \ldots, \theta(t))$. Then the update rule of $\theta(j)$ can be written as follows:

$$
\theta(j+1) = \theta(j) - \eta \left[ f(j) - y \right] + m\lambda (\theta(j) - \theta(0)).
$$

(C.2)

Next lemma gives an upper bound of the distance between auxiliary sequence $\| \theta(j+1) - \theta(j) \|_2$.

**Lemma C.4.** There exist constants $\bar{C}_1, \bar{C}_2 > 0$ such that for any $\delta > 0$, if $\tau$ satisfies that

$$
\bar{C}_1 m^{-3/2} L^{-3/2} |\log(TKL^2/\delta)|^{3/2} \leq \tau \leq \bar{C}_2 L^{-6} |\log m|^{-3/2},
$$

then with probability at least $1 - \delta$, for any $j \in [J]$, $\| \theta(j) - \theta(0) \|_2 \leq \tau$, we have the following inequalities for any $j, s \in [J]$,

$$
\| J(j) \|_F \leq \bar{C}_4 \sqrt{tm} L,
$$

(C.3)

$$
\| J(j) - J(0) \|_F \leq \bar{C}_5 \sqrt{tm \log m} \tau^{1/3} L^{7/2},
$$

(C.4)

$$
\| f(s) - f(j) - [ J(j) ]^T ( \theta(s) - \theta(j) ) \|_2 \leq \bar{C}_6 \tau^{4/3} L^3 \sqrt{tm \log m},
$$

(C.5)

$$
\| y \|_2 \leq \sqrt{t}.
$$

(C.6)

Next lemma gives an upper bound for $\| f(j) - y \|_2$.

**Lemma C.3.** There exist constants $\{ \bar{C}_i \}_{i=1}^4 > 0$ such that for any $\delta > 0$, if $\tau, \eta$ satisfy that

$$
\bar{C}_1 m^{-3/2} L^{-3/2} |\log(TKL^2/\delta)|^{3/2} \leq \tau \leq \bar{C}_2 L^{-6} |\log m|^{-3/2},
$$

$$
\eta \leq \bar{C}_3 (m\lambda + tmL)^{-1},
$$

$$
\tau^{8/3} \leq \bar{C}_4 m(\lambda \eta)^2 L^{-6} t^{-1} (\log m)^{-1},
$$

then with probability at least $1 - \delta$, for any $j \in [J]$, $\| \theta(j) - \theta(0) \|_2 \leq \tau$, we have that for any $j \in [J]$, $\| f(j) - y \|_2 \leq 2\sqrt{t}$.

Next lemma gives an upper bound of the distance between auxiliary sequence $\| \tilde{\theta}(j) - \theta(0) \|_2$.

**Lemma C.4.** There exist constants $\{ \bar{C}_i \}_{i=1}^3 > 0$ such that for any $\delta \in (0, 1)$, if $\tau, \eta$ satisfy that

$$
\bar{C}_1 m^{-3/2} L^{-3/2} |\log(TKL^2/\delta)|^{3/2} \leq \tau \leq \bar{C}_2 L^{-6} |\log m|^{-3/2},
$$

$$
\eta \leq \bar{C}_3 (tmL + m\lambda)^{-1},
$$

then with probability at least $1 - \delta$, we have that for any $j \in [J]$,

$$
\| \tilde{\theta}(j) - \theta(0) \|_2 \leq \sqrt{t/(m\lambda)},
$$

$$
\| \tilde{\theta}(j) - \theta(0) - Z^{-1} \tilde{b} / \sqrt{m} \|_2 \leq (1 - \eta m\lambda)^{3/2} \sqrt{t/(m\lambda)}.
$$

\[\text{Neural Contextual Bandits with UCB-based Exploration}\]
With above lemmas, we prove Lemma B.2 as follows.

**Proof of Lemma B.2.** Set $\tau = 2/\sqrt{t/(m\lambda)}$. First we assume that $\|\theta^{(j)} - \theta^{(0)}\|_2 \leq \tau$ for all $0 \leq j \leq J$. Then with this assumption and the choice of $m, \tau$, we have that Lemma C.2, C.3 and C.4 hold. Then we have

$$\|\theta^{(j+1)} - \tilde{\theta}^{(j+1)}\|_2 = \|\theta^{(j)} - \tilde{\theta}^{(j)} - \eta(J^{(j)} - J^{(0)}) (f^{(j)} - y) - \eta m \lambda (\theta^{(j)} - \tilde{\theta}^{(j)}) - \eta J^{(0)} (f^{(j)} - [J^{(0)}]^T (\tilde{\theta}^{(j)} - \theta^{(0)}))\|_2$$

$$= \|(1 - \eta m \lambda) (\theta^{(j)} - \tilde{\theta}^{(j)}) - \eta (J^{(j)} - J^{(0)}) (f^{(j)} - y)$$

$$- \eta J^{(0)} [f^{(j)} - [J^{(0)}]^T (\tilde{\theta}^{(j)} - \theta^{(0)}) + [J^{(0)}]^T (\theta^{(j)} - \tilde{\theta}^{(j)})]\|_2$$

$$\leq \eta \left\| \left( J^{(j)} - J^{(0)} \right) (f^{(j)} - y) \right\|_2 + \eta \left\| J^{(0)} \right\|_2 \left\| f^{(j)} - J^{(0)} (\theta^{(j)} - \theta^{(0)}) \right\|_2$$

$$+ \left\| \left[ I - \eta (m \lambda I + H^{(0)}) \right] (\tilde{\theta}^{(j)} - \theta^{(j)}) \right\|_2,$$  \hspace{1cm} (C.7)

where the inequality holds due to triangle inequality. We now bound $I_1, I_2$ and $I_3$ separately. For $I_1$, we have

$$I_1 \leq \eta \|J^{(j)} - J^{(0)}\|_2 \|f^{(j)} - y\|_2 \leq \eta C_2 t \sqrt{m \log m t^{1/3} L^{7/2}},$$  \hspace{1cm} (C.8)

where $C_2 > 0$ is a constant, the first inequality holds due to the definition of matrix spectral norm and the second inequality holds due to (C.4) in Lemma C.2 and Lemma C.3. For $I_2$, we have

$$I_2 \leq \eta \|J^{(0)}\|_2 \|f^{(j)} - J^{(0)} (\theta^{(j)} - \theta^{(0)})\|_2 \leq \eta C_3 t m L^{7/2} \tau^{4/3} \sqrt{\log m},$$  \hspace{1cm} (C.9)

where $C_3 > 0$, the first inequality holds due to matrix spectral norm, the second inequality holds due to (C.3) and (C.5) in Lemma C.2 and the fact that $f^{(0)} = 0$ by random initialization over $\theta^{(0)}$. For $I_3$, we have

$$I_3 \leq \|I - \eta (m \lambda I + H^{(0)})\|_2 \|\tilde{\theta}^{(j)} - \theta^{(j)}\|_2 \leq (1 - \eta m \lambda) \|\tilde{\theta}^{(j)} - \theta^{(j)}\|_2,$$ \hspace{1cm} (C.10)

where the first inequality holds due to spectral norm inequality, the second inequality holds since

$$\eta (m \lambda I + H^{(0)}) = \eta (m \lambda I + [J^{(0)}]^T J^{(0)}) \leq \eta (m \lambda I + C_1 t m L^2 I) \leq I,$$

for some $C_1 > 0$, the first inequality holds due to (C.3) in Lemma C.2, the second inequality holds due to the choice of $\eta$. Substituting (C.8), (C.9) and (C.10) into (C.7), we obtain

$$\|\theta^{(j+1)} - \tilde{\theta}^{(j+1)}\|_2 \leq (1 - \eta m \lambda) \|\theta^{(j)} - \tilde{\theta}^{(j)}\|_2 + C_4 \left( \eta t \sqrt{m \log m t^{1/3} L^{7/2}} + \eta t m L^{7/2} \tau^{4/3} \sqrt{\log m} \right),$$ \hspace{1cm} (C.11)

where $C_4 > 0$ is a constant. By recursively applying (C.11) from 0 to $j$, we have

$$\|\theta^{(j+1)} - \tilde{\theta}^{(j+1)}\|_2 \leq C_4 \frac{\eta t \sqrt{m \log m t^{1/3} L^{7/2}} + \eta t m L^{7/2} \tau^{4/3} \sqrt{\log m}}{\eta m \lambda} \leq C_5 m^{-2/3} \sqrt{\log m} L^{7/2} t^{5/3} \lambda^{-5/3} (1 + \sqrt{t/\lambda})$$

$$\leq \frac{\tau}{2},$$ \hspace{1cm} (C.12)

where $C_5 > 0$ is a constant, the equality holds by the definition of $\tau$, the last inequality holds due to the choice of $m$, where $m^{1/6} \geq C_6 \sqrt{\log m} L^{7/2} t^{5/6} \lambda^{-7/6} (1 + \sqrt{t/\lambda})$, and $C_6 > 0$ is a constant. Thus, for any $j \in [J]$, we have

$$\|\theta^{(j)} - \theta^{(0)}\|_2 \leq \|\tilde{\theta}^{(j)} - \theta^{(0)}\|_2 + \|\theta^{(j)} - \tilde{\theta}^{(j)}\|_2 \leq \sqrt{t/(m\lambda)} + \tau/2 = \tau,$$ \hspace{1cm} (C.13)
where the first inequality holds due to triangle inequality, the second inequality holds due to Lemma C.4. (C.13) suggests that our assumption \( \|\theta^{(j)} - \theta^{(0)}\|_2 \leq \tau \) holds for any \( j \). Note that we have the following inequality by Lemma C.4:

\[
\|\theta^{(j)} - \theta^{(0)} - (Z)^{-1}b/\sqrt{m}\|_2 \leq (1 - \eta m \lambda^2)^j \sqrt{t/(m \lambda)}.
\] (C.14)

Using (C.12) and (C.14), we have

\[
\|\theta^{(j)} - \theta^{(0)} - Z^{-1}b/\sqrt{m}\|_2 \leq (1 - \eta m \lambda^2)^j \sqrt{t/(m \lambda)} + C_5 m^{-2/3} \sqrt{\log m} L^{7/2} \lambda^{-5/3}(1 + \sqrt{t/\lambda}).
\]

This completes the proof.

\[\Box\]

C.3. Proof of Lemma B.3

In this section we prove Lemma B.3.

Proof of Lemma B.3. Set \( \tau = 2\sqrt{t/(m \lambda)} \). By Lemma B.2 we have that \( \|\theta_t - \theta_0\|_2 \leq \tau \) for \( i \in [t] \). \( \|Z_i\|_2 \) can be bounded as follows.

\[
\|Z_i\|_2 = \left\| \lambda I + \frac{t}{m} g(x_{i,a}; \theta_{i-1}) g(x_{i,a}; \theta_{i-1})^\top \right\|_2 \\
\leq \lambda + \left\| \lambda I + \frac{t}{m} g(x_{i,a}; \theta_{i-1}) g(x_{i,a}; \theta_{i-1})^\top \right\|_2 \\
\leq \lambda + \sum_{i=1}^t \left\| g(x_{i,a}; \theta_{i-1}) \right\|_2^2 / m \\
\leq \lambda + C_0 t L,
\]

where \( C_0 > 0 \) is a constant, the first inequality holds due to the fact that \( \|aa^\top\| = \|a\|_2^2 \), the second inequality holds due to Lemma B.6 with the fact that \( \|\theta_t - \theta_0\|_2 \leq \tau \). We bound \( \|Z_t - \tilde{Z}_t\|_2 \) as follows. We have

\[
\|Z_t - \tilde{Z}_t\|_F = \left\| \sum_{i=1}^t \left( g(x_{i,a}; \theta_0) g(x_{i,a}; \theta_0)^\top - g(x_{i,a}; \theta_i) g(x_{i,a}; \theta_i)^\top \right) \right\|_F \\
\leq \sum_{i=1}^t \left\| g(x_{i,a}; \theta_0) g(x_{i,a}; \theta_0)^\top - g(x_{i,a}; \theta_i) g(x_{i,a}; \theta_i)^\top \right\|_F / m \\
\leq \sum_{i=1}^t \left( \left\| g(x_{i,a}; \theta_0) \right\|_2 + \left\| g(x_{i,a}; \theta_i) \right\|_2 \right) \left\| g(x_{i,a}; \theta_0) - g(x_{i,a}; \theta_i) \right\|_2 / m,
\]

(C.15)

where the first inequality holds due to triangle inequality, the second inequality holds the fact that \( \|aa^\top - bb^\top\|_F \leq (\|a\|_2 + \|b\|_2) \|a - b\|_2 \) for any vectors \( a, b \). To bound (C.15), we have

\[
\left\| g(x_{i,a}; \theta_0) \right\|_2, \left\| g(x_{i,a}; \theta_i) \right\|_2 \leq C_1 \sqrt{m L},
\]

(C.16)

where \( C_1 > 0 \) is a constant, the inequality holds due to Lemma B.6 with the fact that \( \|\theta_t - \theta_0\|_2 \leq \tau \). We also have

\[
\left\| g(x_{i,a}; \theta_0) - g(x_{i,a}; \theta_i) \right\|_2 \leq C_2 \sqrt{\log m} \sqrt{L^3} \left\| g(x_j; \theta_0) \right\|_2 \leq C_3 \sqrt{m} \log m \sqrt{L^3},
\]

(C.17)

where \( C_2, C_3 > 0 \) are constants, the first inequality holds due to Lemma B.5 with the fact that \( \|\theta_t - \theta_0\|_2 \leq \tau \), the second inequality holds due to Lemma B.6. Substituting (C.16) and (C.17) into (C.15), we have

\[
\|Z_t - \tilde{Z}_t\|_F \leq C_4 t \sqrt{\log m} \sqrt{L^4},
\]

where \( C_4 > 0 \) is a constant. We now bound \( \log \det \tilde{Z}_t - \log \det Z_t \). It is easy to verify that \( Z_t = \lambda I + \tilde{J} \tilde{J}^\top, \tilde{Z}_t = \lambda I + JJ^\top \), where

\[
\tilde{J} = \left( g(x_{1,a}; \theta_0), \ldots, g(x_{t,a}; \theta_0) \right) / \sqrt{m},
\]

\[
J = \left( g(x_{1,a}; \theta_0), \ldots, g(x_{t,a}; \theta_{t-1}) \right) / \sqrt{m}.
\]
We have the following inequalities:
\[
\log \frac{\det(Z_t)}{\det(\lambda I)} - \log \frac{\det(Z_k)}{\det(\lambda I)} = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + JJ^\top / \lambda) = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + J^\top J / \lambda) \\
\leq \langle I + J^\top J / \lambda \rangle^{-1} J^\top J - J^\top J \rangle
\]
where the second equality holds due to the fact that \( \log \det(I + AA^\top) = \det(I + A^\top A) \), the first inequality holds due to the fact that \( \log(1 + x) \leq x \) for any \( x > 0 \). We have the following inequalities:
\[
\log \frac{\det(Z_t)}{\det(\lambda I)} - \log \frac{\det(Z_k)}{\det(\lambda I)} = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + JJ^\top / \lambda) = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + J^\top J / \lambda) \\
\leq \langle I + J^\top J / \lambda \rangle^{-1} J^\top J - J^\top J \rangle
\]
where the second equality holds due to the fact that \( \log \det(I + AA^\top) = \det(I + A^\top A) \), the first inequality holds due to the fact that \( \log(1 + x) \leq x \) for any \( x > 0 \). We have the following inequalities:
\[
\log \frac{\det(Z_t)}{\det(\lambda I)} - \log \frac{\det(Z_k)}{\det(\lambda I)} = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + JJ^\top / \lambda) = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + J^\top J / \lambda) \\
\leq \langle I + J^\top J / \lambda \rangle^{-1} J^\top J - J^\top J \rangle
\]
where the second equality holds due to the fact that \( \log \det(I + AA^\top) = \det(I + A^\top A) \), the first inequality holds due to the fact that \( \log(1 + x) \leq x \) for any \( x > 0 \). We have the following inequalities:
\[
\log \frac{\det(Z_t)}{\det(\lambda I)} - \log \frac{\det(Z_k)}{\det(\lambda I)} = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + JJ^\top / \lambda) = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + J^\top J / \lambda) \\
\leq \langle I + J^\top J / \lambda \rangle^{-1} J^\top J - J^\top J \rangle
\]
where the second equality holds due to the fact that \( \log \det(I + AA^\top) = \det(I + A^\top A) \), the first inequality holds due to the fact that \( \log(1 + x) \leq x \) for any \( x > 0 \).

\[
\det(I + \bar{J}^\top / \lambda) - \log \det(I + J^\top J / \lambda) \\
\leq \langle I + J^\top J / \lambda \rangle^{-1} J^\top J - J^\top J \rangle
\]
where the second equality holds due to the fact that \( \log \det(I + AA^\top) = \det(I + A^\top A) \), the first inequality holds due to the fact that \( \log(1 + x) \leq x \) for any \( x > 0 \).

\[
\log \frac{\det(Z_t)}{\det(\lambda I)} - \log \frac{\det(Z_k)}{\det(\lambda I)} = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + JJ^\top / \lambda) = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + J^\top J / \lambda) \\
\leq \langle I + J^\top J / \lambda \rangle^{-1} J^\top J - J^\top J \rangle
\]
where the second equality holds due to the fact that \( \log \det(I + AA^\top) = \det(I + A^\top A) \), the first inequality holds due to the fact that \( \log(1 + x) \leq x \) for any \( x > 0 \).

\[
\log \frac{\det(Z_t)}{\det(\lambda I)} - \log \frac{\det(Z_k)}{\det(\lambda I)} = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + JJ^\top / \lambda) = \log \det(I + \bar{J}^\top / \lambda) - \log \det(I + J^\top J / \lambda) \\
\leq \langle I + J^\top J / \lambda \rangle^{-1} J^\top J - J^\top J \rangle
\]
where the second equality holds due to the fact that \( \log \det(I + AA^\top) = \det(I + A^\top A) \), the first inequality holds due to the fact that \( \log(1 + x) \leq x \) for any \( x > 0 \).
where $C_2, C_3 > 0$ are constants, the first inequality holds due to Lemma B.5 with the assumption that $\|\theta^{(j)} - \theta^{(0)}\|_2 \leq \tau$, the second inequality holds due to (D.1).

We also have
\[
\|f^{(s)} - f^{(j)} - [J^{(j)}]^{\top} (\theta^{(s)} - \theta^{(j)})\|_2 \\
\quad \leq \max_{i \in [t]} \sqrt{\frac{I}{f(x_i,a_i;\theta^{(s)}) - f(x_i,a_i;\theta^{(j)})}} \leq \langle \nabla L_\tau, \theta' - \theta \rangle + \|e\|_2 + \frac{m\lambda}{2} \|\theta' - \theta\|_2^2 \\
\quad \leq C_4 \tau^{4/3} L^3 \sqrt{tm \log m},
\]
where $C_4 > 0$ is a constant, the first inequality holds due to Lemma B.4 with the assumption that $\|\theta^{(j)} - \theta^{(0)}\|_2 \leq \tau$, the second inequality holds due to Lemma B.4 with the assumption that $\|\theta^{(0)}\|_2 \leq \tau$, $\|\theta^{(s)} - \theta^{(0)}\|_2 \leq \tau$.

For $\|y\|_2$, we have $\|y\|_2 \leq \sqrt{t} \max_{1 \leq i \leq t} |r(x_i,a_i)| \leq \sqrt{t}$. This completes our proof. \(\square\)

D.2. Proof of Lemma C.3

Proof of Lemma C.3. It can be verified that $\tau$ satisfies the conditions of Lemma C.2, thus Lemma C.2 holds. Recall that the loss function $L$ is defined as
\[
L(\theta) = \frac{1}{2} \|f(\theta) - y\|^2 + \frac{m\lambda}{2} \|\theta - \theta^{(0)}\|^2.
\]
We define $J(\theta)$ and $f(\theta)$ as follows:
\[
J(\theta) = \left( g(x_{1,a_1};\theta), \ldots, g(x_{t,a_t};\theta) \right) \in \mathbb{R}^{(md + m^2(L-2) + m) \times t},
\]
\[
f(\theta) = (f(x_{1,a_1};\theta), \ldots, f(x_{t,a_t};\theta))^\top \in \mathbb{R}^{t \times 1}.
\]
Suppose $\|\theta - \theta^{(0)}\|_2 \leq \tau$. Then by the fact that $\|\cdot\|^2_2/2$ is 1-strongly convex and 1-smooth, we have the following inequalities:
\[
L(\theta') - L(\theta) \\
\quad \leq \langle f(\theta) - y, f(\theta') - f(\theta) \rangle + \frac{1}{2} \|f(\theta') - f(\theta)\|_2^2 + m\lambda(\theta - \theta^{(0)}, \theta' - \theta) + \frac{m\lambda}{2} \|\theta' - \theta\|_2^2 \\
\quad = \langle f(\theta) - y, [J(\theta)]^\top (\theta' - \theta) + e \rangle + \frac{1}{2} \|J(\theta)[J(\theta)]^\top (\theta' - \theta) + e\|_2^2 \\
\quad \quad + m\lambda(\theta - \theta^{(0)}, \theta' - \theta) + \frac{m\lambda}{2} \|\theta' - \theta\|_2^2 \\
\quad = \langle J(\theta)(f(\theta) - y) + m\lambda(\theta - \theta^{(0)}), \theta' - \theta \rangle + \langle f(\theta) - y, e \rangle \\
\quad \quad + \frac{1}{2} \|J(\theta)[J(\theta)]^\top (\theta' - \theta) + e\|_2^2 + m\lambda \|\theta' - \theta\|_2^2 \\
\quad = \langle \nabla L(\theta), \theta' - \theta \rangle + \langle f(\theta) - y, e \rangle + \frac{1}{2} \|J(\theta)[J(\theta)]^\top (\theta' - \theta) + e\|_2 \\
\quad \quad \quad + \frac{m\lambda}{2} \|\theta' - \theta\|_2^2, \quad \text{(D.3)}
\]
where $e = f(\theta') - f(\theta) - J(\theta)^\top (\theta' - \theta)$. $I_1$ can be bounded as follows:
\[
I_1 \leq \|f(\theta) - y\|_2 \|e\|_2 + \|J(\theta)\|^2_2 \|\theta' - \theta\|^2_2 + \|e\|^2_2 + \frac{m\lambda}{2} \|\theta' - \theta\|^2_2 \\
\quad \leq C_1 \left( (m\lambda + tmL) \|\theta' - \theta\|^2_2 \right) + \|f(\theta) - y\|_2 \|e\|_2 + \|e\|^2_2, \quad \text{(D.4)}
\]
where the first inequality holds due to Cauchy-Schwarz inequality, the second inequality holds due to the fact that $\|J(\theta)\|_2 \leq C_2 \sqrt{tmL}$ with $\|\theta - \theta^{(0)}\|_2 \leq \tau$ by (C.5) in Lemma C.2. Substituting (D.4) into (D.3), we obtain
\[
L(\theta') - L(\theta) \leq \langle \nabla L(\theta), \theta' - \theta \rangle + C_1 \left( (m\lambda + tmL) \|\theta' - \theta\|^2_2 \right) + \|f(\theta) - y\|_2 \|e\|_2 + \|e\|^2_2. \quad \text{(D.5)}
\]
Taking $\theta' = \theta - \eta \nabla L(\theta)$, then by (D.5), we have
\[
L(\theta - \eta \nabla L(\theta)) - L(\theta) \leq -\eta \|\nabla L(\theta)\|^2 [1 - C_1 (m\lambda + tmL)\eta] + \|f(\theta) - y\|_2 \|e\|_2 + \|e\|^2_2. \tag{D.6}
\]
By the 1-strongly convexity of $\|\cdot\|^2$, we further have
\[
L(\theta') - L(\theta)
\geq \langle f(\theta) - y, f'(\theta') - f'(\theta) \rangle + m\lambda \langle \theta' - \theta^{(0)}, \theta' - \theta \rangle + \frac{m\lambda}{2} \|\theta' - \theta\|^2 \\
= \langle f(\theta) - y, [J(\theta)]^T (\theta' - \theta) + e \rangle + m\lambda \langle \theta' - \theta^{(0)}, \theta' - \theta \rangle + \frac{m\lambda}{2} \|\theta' - \theta\|^2 \\
= \langle \nabla L(\theta), \theta' - \theta \rangle + \frac{m\lambda}{2} \|\theta' - \theta\|^2 + \langle f(\theta) - y, e \rangle \\
\geq \langle \nabla L(\theta), \theta' - \theta \rangle + \frac{m\lambda}{2} \|\theta' - \theta\|^2 - \|f(\theta) - y\|_2 \|e\|_2 \\
\geq -\frac{\|\nabla L(\theta)\|^2_2}{2m\lambda} - \|f(\theta) - y\|_2 \|e\|_2, \tag{D.7}
\]
where the second inequality holds due to Cauchy-Schwarz inequality, the last inequality holds due to the fact that $\langle a, x \rangle + c\|x\|^2 \geq -\|a\|^2/(4c)$ for any vectors $a, x$ and $c > 0$. Substituting (D.7) into (D.6), we obtain
\[
L(\theta - \eta \nabla L(\theta)) - L(\theta)
\leq 2m\lambda\eta [1 - C_1 (m\lambda + tmL)\eta] [L(\theta') - L(\theta) + \|f(\theta) - y\|^2 \|e\|^2_2 + \|f(\theta) - y\|^2 \|e\|^2_2 + \|e\|^2_2] \\
\leq 2m\lambda\eta [L(\theta') - L(\theta) + \|f(\theta) - y\|^2 \|e\|^2_2 + \|f(\theta) - y\|^2 \|e\|^2_2 + \|e\|^2_2] \\
\leq 2m\lambda\eta [L(\theta') - L(\theta) + \|f(\theta) - y\|^2 \|e\|^2_2 / 8 + 2\|e\|^2_2] + m\lambda\eta \|f(\theta) - y\|^2 \|e\|^2_2 / (m\lambda\eta) + \|e\|^2_2 \\
\leq 2m\lambda\eta [L(\theta') - L(\theta) / 2] + \|e\|^2_2 (1 + 2m\lambda + 2/(m\lambda)) \tag{D.8},
\]
where the second inequality holds due to the choice of $\eta$, third inequality holds due to Young's inequality, fourth inequality holds due to the fact that $\|f(\theta) - y\|^2 \|e\|^2 \leq 2L(\theta)$. Now taking $\theta = \theta^{(j)}$ and $\theta' = \theta^{(0)}$, rearranging (D.8), with the fact that $\theta^{(j+1)} = \theta^{(j)} - \eta \nabla L(\theta^{(j)})$, we have
\[
L(\theta^{(j+1)}) - L(\theta^{(0)})
\leq (1 - m\lambda\eta / 2) [L(\theta^{(j)}) - L(\theta^{(0)})] + m\lambda\eta / 2L(\theta^{(0)}) + \|e\|^2_2 (1 + 2m\lambda + 2/(m\lambda)) \\
\leq (1 - m\lambda\eta / 2) [L(\theta^{(j)}) - L(\theta^{(0)})] + m\lambda\eta / 2 \cdot t + m\lambda\eta / 2 \cdot t \\
\leq (1 - m\lambda\eta / 2) [L(\theta^{(j)}) - L(\theta^{(0)})] + m\lambda\eta \cdot t \tag{D.9},
\]
where the second inequality holds due to the fact that $L(\theta^{(0)}) = \|f(\theta^{(0)}) - y\|^2 / 2 = \|y\|^2 / 2 \leq t$, and
\[
(1 + 2m\lambda + 2/(m\lambda)) \|e\|^2_2 \leq 3/(m\lambda\eta) \cdot C_2^2 \eta^{8/3} L^6 t m \log m \leq t m\lambda/2, \tag{D.10}
\]
where the first inequality holds due to (C.5) in Lemma C.2, the second inequality holds due to the choice of $\tau$. Recursively applying (D.9) for $u$ times, we have
\[
L(\theta^{(j+1)}) - L(\theta^{(0)}) \leq \frac{m\lambda\eta t}{m\lambda\eta / 2} = 2t,
\]
which implies that $\|f^{(j+1)} - y\|_2 \leq 2\sqrt{t}$. This completes our proof. \qed

D.3. Proof of Lemma C.4

In this section we prove Lemma C.4.

Proof of Lemma C.4. It can be verified that $\tau$ satisfies the conditions of Lemma C.2, thus Lemma C.2 holds. It is worth noting that $\theta^{(j)}$ is the sequence generated by applying gradient descent on the following problem:
\[
\min_{\theta} \tilde{L}(\theta) = \frac{1}{2} \| [J(\theta)]^T (\theta - \theta^{(0)}) - y\|^2 + \frac{m\lambda}{2} \|\theta - \theta^{(0)}\|^2.
\]
Then \( \| \theta^{(0)} - \tilde{\theta}^{(j)} \|_2 \) can be bounded as

\[
m\lambda \frac{1}{2} \| \theta^{(0)} - \tilde{\theta}^{(j)} \|_2^2 \leq \frac{1}{2} \| J^{(0)} \top (\tilde{\theta}^{(j)} - \theta^{(0)}) - y \|_2^2 + \frac{m\lambda}{2} \| \tilde{\theta}^{(j)} - \theta^{(0)} \|_2^2 \leq \frac{1}{2} \| J^{(0)} \top (\tilde{\theta}^{(0)} - \theta^{(0)}) - y \|_2^2 + \frac{m\lambda}{2} \| \tilde{\theta}^{(0)} - \theta^{(0)} \|_2^2 \leq \frac{1}{2} \| J^{(0)} \top (\tilde{\theta}^{(0)} - \theta^{(0)}) - y \|_2^2 + \frac{m\lambda}{2} \| \tilde{\theta}^{(0)} - \theta^{(0)} \|_2^2 \leq t/2,
\]

where the first inequality holds trivially, the second inequality holds due to the monotonic decreasing property brought by gradient descent, the third inequality holds due to (C.6) in Lemma C.2. It is easy to verify that \( \tilde{L} \) is a \( m\lambda \)-strongly convex and function and \( C_1 tmL + m\lambda \)-smooth function, since

\[
\nabla^2 \tilde{L} \preceq (\| J^{(0)} \|_2^2 + m\lambda) I \preceq C_1 tmL + m\lambda
\]

where the first inequality holds due to the definition of \( \tilde{L} \), the second inequality holds due to (C.3) in Lemma C.2. Since we choose \( \eta \leq C_2 (tmL + m\lambda)^{-1} \) for some small enough \( C_2 > 0 \), then by standard results of gradient descent on ridge linear regression, \( \tilde{\theta}^{(j)} \) converges to \( \theta^{(0)} + (\tilde{Z}^{-1}) b / \sqrt{m} \) with the convergence rate

\[
\| \tilde{\theta}^{(j)} - \theta^{(0)} - \tilde{Z}^{-1} b / \sqrt{m} \|_2^2 \leq (1 - \eta m\lambda)^j \cdot \frac{2}{m\lambda} \tilde{L}(\theta^{(0)}) - \tilde{L}(\theta^{(0)} + \tilde{Z}^{-1} b / \sqrt{m}) \leq \frac{2(1 - \eta m\lambda)^j \cdot \| y \|_2^2}{m\lambda} \leq (1 - \eta m\lambda)^j t,
\]

where the first inequality holds due to the convergence result for gradient descent and the fact that \( \theta^{(0)} + (\tilde{Z}^{-1}) b / \sqrt{m} \) is the minimal solution to \( L \), the second inequality holds since \( \tilde{L} \geq 0 \), the last inequality holds due to Lemma C.2.

\[\square\]

**E. A Variant of NeuralUCB**

In this section, we present a variant of NeuralUCB called NeuralUCB\(_0\). Compared with Algorithm 1, The main differences between NeuralUCB and NeuralUCB\(_0\) are as follows: NeuralUCB uses gradient descent to train a deep neural network to learn the reward function \( h(x) \) based on observed contexts and rewards. In contrast, NeuralUCB\(_0\) uses matrix inversions to obtain parameters in closed forms. At each round, NeuralUCB uses the current DNN parameters (\( \theta_t \)) to compute an upper confidence bound. In contrast, NeuralUCB\(_0\) computes the UCB using the initial parameters (\( \theta_0 \)).
Algorithm 3 NeuralUCB

1: **Input:** number of rounds $T$, regularization parameter $\lambda$, exploration parameter $\nu$, confidence parameter $\delta$, norm parameter $S$, network width $m$, network depth $L$

2: **Initialization:** Generate each entry of $W_l$ independently from $N(0, 2/m)$ for $1 \leq l \leq L - 1$, and each entry of $W_L$ independently from $N(0, 1/m)$. Define $\phi(x) = g(x, \theta_0)/\sqrt{m}$, where $\theta_0 = [\text{vec}(W_1)^\top, \ldots, \text{vec}(W_L)^\top]^\top \in \mathbb{R}^p$

3: $Z_0 = \lambda I$, $b_0 = 0$

4: for $t = 1, \ldots, T$ do

5: Observe $\{x_t,a\}_{a=1}^K$ and compute

$$\left(a_t, \bar{\theta}_{t,a_t}\right) = \arg\max_{a \in [K], \theta \in C_{t-1}} \langle \phi(x_{t,a_t}), \theta - \theta_0 \rangle \quad (E.1)$$

6: Play $a_t$ and receive reward $r_{t,a_t}$

7: Compute

$$Z_t = Z_{t-1} + \phi(x_{t,a_t})\phi(x_{t,a_t})^\top \in \mathbb{R}^{p \times p}, \quad b_t = b_{t-1} + r_{t,a_t}\phi(x_{t,a_t}) \in \mathbb{R}^p$$

8: Compute $\theta_t = Z_t^{-1}b_t + \theta_0 \in \mathbb{R}^p$

9: Construct $C_t$ as

$$C_t = \{\theta : \|\theta - \theta\|_{Z_t} \leq \gamma_t\}, \quad \text{where} \quad \gamma_t = \nu \sqrt{\log \frac{\det Z_t}{\det \lambda I} - 2 \log \delta + \sqrt{\lambda S}} \quad (E.2)$$

10: end for