

## A Auxiliary Lemmas

In this section, we introduce auxiliary lemmas used in our analysis. The first one is Hoeffding's inequality.

**Lemma A** (Hoeffding's inequality). *Let  $Z_1, \dots, Z_s$  be i.i.d. random variables to  $[-a, a]$  for  $a > 0$ . Denote by  $A_s$  the sample average  $\sum_{i=1}^s Z_i/s$ . Then, for any  $\epsilon > 0$ , we get*

$$\mathbb{P}[A_s + \epsilon \leq \mathbb{E}[A_s]] \leq \exp\left(-\frac{\epsilon^2 s}{2a^2}\right).$$

Note that this statement can be reinterpreted as follows: it follows that for  $\delta \in (0, 1)$  with probability at least  $1 - \delta$

$$A_s + a\sqrt{\frac{2}{s} \log \frac{1}{\delta}} \geq \mathbb{E}[A_s].$$

We next introduce the uniform bound by Rademacher complexity. For a set  $\mathcal{G}$  of functions from  $\mathcal{Z}$  to  $[-a, a]$  and a dataset  $S = \{z_i\}_{i=1}^s \subset \mathcal{Z}$ , we denote empirical Rademacher complexity by  $\hat{\mathfrak{R}}_S(\mathcal{G})$  and denote Rademacher complexity by  $\mathfrak{R}_s(\mathcal{G})$ ; let  $\sigma = (\sigma_i)_{i=1}^s$  be i.i.d random variables taking  $-1$  or  $1$  with equal probability and let  $S$  be distributed according to a distribution  $\mu^s$ ,

$$\hat{\mathfrak{R}}_S(\mathcal{G}) = \mathbb{E}_\sigma \left[ \sup_{f \in \mathcal{G}} \frac{1}{s} \sum_{i=1}^s \sigma_i f(x_i) \right], \quad \mathfrak{R}_s(\mathcal{G}) = \mathbb{E}_{\mu^s} [\hat{\mathfrak{R}}_S(\mathcal{G})].$$

**Lemma B.** *Let  $Z_1, \dots, Z_s$  be i.i.d random variables to  $\mathcal{Z}$ . Denote by  $A_s(f)$  the sample average  $\sum_{i=1}^s f(Z_i)/s$ . Then, for any  $\delta \in (0, 1)$ , we get with probability at least  $1 - \delta$  over the choice of  $S$ ,*

$$\sup_{f \in \mathcal{G}} |A_s(f) - \mathbb{E}[A_s(f)]| \leq 2\mathfrak{R}_s(\mathcal{G}) + a\sqrt{\frac{2}{s} \log \frac{2}{\delta}}.$$

When a function class is VC-class (for the definite see [vdVW96]), its Rademacher complexity is uniformly bounded as in the following lemma which can be easily shown by Dudley's integral bound [Dud99] and the bound on the covering number by VC-dimension (pseudo-dimension) [vdVW96].

**Lemma C.** *Let  $\mathcal{G}$  be VC-class. Then, there exists positive value  $M$  depending on  $\mathcal{G}$  such that  $\mathfrak{R}_s(\mathcal{G}) \leq M/\sqrt{m}$ .*

The following lemma is useful in estimating Rademacher complexity.

**Lemma D.** (i) *Let  $h_i : \mathbb{R} \rightarrow \mathbb{R}$  ( $i \in \{1, \dots, s\}$ ) be  $L$ -Lipschitz functions. Then it follows that*

$$\mathbb{E}_\sigma \left[ \sup_{f \in \mathcal{G}} \sum_{i=1}^s \sigma_i h_i \circ f(x_i) \right] \leq L \mathbb{E}_\sigma \left[ \sup_{f \in \mathcal{G}} \sum_{i=1}^s \sigma_i \circ f(x_i) \right].$$

(ii) *We denote by  $\text{conv}(\mathcal{G})$  the convex hull of  $\mathcal{G}$ . Then, we have  $\hat{\mathfrak{R}}_S(\text{conv}(\mathcal{G})) = \hat{\mathfrak{R}}_S(\mathcal{G})$ .*

The following lemma gives the generalization bound by the margin distribution, which is originally derived by [KP02]. Let  $\mathcal{G}$  be the set of predictors;  $\mathcal{G} \subset \{f : \mathcal{X} \rightarrow \mathbb{R}^c\}$  and denote  $\Pi\mathcal{G} = \{f_y(\cdot) : \mathcal{X} \rightarrow \mathbb{R}^c \mid f \in \mathcal{G}, y \in \mathcal{Y}\}$ , then the following holds.

**Lemma E.** *Fix  $\delta > 0$ . Then, for  $\forall \rho > 0$ , with probability at least  $1 - \rho$  over the random choice of  $S$  from  $\nu^n$ , we have  $\forall f \in \mathcal{G}$ ,*

$$\mathbb{P}_\nu[m_f(X, Y) \leq 0] \leq \mathbb{P}_{\nu_n}[m_f(X, Y) \leq \delta] + \frac{2c^2}{\delta} \mathfrak{R}_n(\Pi\mathcal{G}) + \sqrt{\frac{1}{2n} \log \frac{1}{\rho}}.$$

## B Proofs

In this section, we provide missing proofs in the paper.

## B.1 Proofs of Section 3 and 4

We first prove Proposition 1 that states Lipschitz smoothness of the risk function.

*Proof of Proposition 1.* Because  $l(z, y, w)$  is  $\mathcal{C}^2$ -function with respect to  $z, w$ , there exist semi-positive definite matrices  $A_{x,y}^{\phi,\psi}, B_{x,y}^{\phi,\psi}$  such that

$$\begin{aligned} l(\psi(x), y, w_\phi) &= l(\phi(x), y, w_\phi) + \partial_z l(\phi(x), y, w_\phi)^\top (\psi(x) - \phi(x)) \\ &\quad + \frac{1}{2} (\psi(x) - \phi(x))^\top A_{x,y}^{\phi,\psi} (\psi(x) - \phi(x)), \end{aligned} \quad (1)$$

$$\begin{aligned} l(\psi(x), y, w_\phi) + \frac{\lambda}{2} \|w_\phi\|_2^2 &= l(\psi(x), y, w_\psi) + \frac{\lambda}{2} \|w_\psi\|_2^2 \\ &\quad + (\partial_w l(\psi(x), y, w_\psi) + \lambda w_\psi)^\top (w_\phi - w_\psi) \\ &\quad + \frac{1}{2} (w_\phi - w_\psi)^\top B_{x,y}^{\phi,\psi} (w_\phi - w_\psi). \end{aligned} \quad (2)$$

By Assumption 1, we find spectral norms of  $A_{x,y}^{\phi,\psi}$  is uniformly bounded with respect to  $x, y, \phi, \psi$ , hence eigen-values are also uniformly bounded. In particular, since  $\frac{\lambda}{2} \|w_\phi\|_2^2 \leq \mathcal{R}(\phi, w_\phi) \leq \mathcal{R}(\phi, 0) \leq l_0$ , we see  $-A_{c_\lambda} I \preceq A_{x,y}^{\phi,\psi} \preceq A_{c_\lambda} I$ .

By taking the expectation  $\mathbb{E}_\nu$  of the equality (1), we get

$$\mathcal{R}(\psi, w_\phi) = \mathcal{R}(\phi, w_\phi) + \langle \nabla_\phi \mathcal{R}(\phi), \psi - \phi \rangle_{L_2^d(\nu_X)} + \frac{1}{2} \mathbb{E}_\nu [(\psi(x) - \phi(x))^\top A_{x,y}^{\phi,\psi} (\psi(x) - \phi(x))] \quad (3)$$

and by taking the expectation  $\mathbb{E}_\nu$  of the equality (2), we get

$$\mathcal{R}(\psi, w_\phi) = \mathcal{R}(\psi, w_\psi) + \frac{1}{2} (w_\phi - w_\psi)^\top \mathbb{E}_\nu [B_{x,y}^{\phi,\psi}] (w_\phi - w_\psi), \quad (4)$$

where we used  $\partial_w \mathcal{R}(\psi, w_\psi) = 0$ . By combining equalities (3) and (4), we have

$$\mathcal{R}(\psi) = \mathcal{R}(\phi) + \langle \nabla_\phi \mathcal{R}(\phi), \psi - \phi \rangle_{L_2^d(\nu_X)} + H_\phi(\psi),$$

where

$$H_\phi(\psi) = \frac{1}{2} \mathbb{E}_\nu [(\psi(x) - \phi(x))^\top A_{x,y}^{\phi,\psi} (\psi(x) - \phi(x))] - \frac{1}{2} (w_\phi - w_\psi)^\top \mathbb{E}_\nu [B_{x,y}^{\phi,\psi}] (w_\phi - w_\psi).$$

By the uniformly boundedness of  $A_{x,y}^{\phi,\psi}$  and the semi-positivity of  $B_{x,y}^{\phi,\psi}$ , we find  $H_\phi(\psi) \leq \frac{A_{c_\lambda}}{2} \|\phi - \psi\|_{L_2^d(\nu_X)}^2$ .

The other cases can be shown in the same manner, thus, we finish the proof.  $\square$

We next show the consistency of functional gradient norms.

*Proof of Proposition 2.* We now prove the first inequality. Note that the integrand of  $y'$ -th element of  $\nabla_f \mathcal{L}(f)(x)$  for multiclass logistic loss can be written as

$$\partial_{\zeta_{y'}} l(f(x), y) = -\mathbf{1}[y = y'] + \frac{\exp(f_{y'}(x))}{\sum_{\bar{y} \in \mathcal{Y}} \exp(f_{\bar{y}}(x))}.$$

Therefore, we get

$$\begin{aligned} \|\nabla_f \mathcal{L}(f)\|_{L_1^c(\nu_X)} &= \mathbb{E}_{\nu_X} \|\nabla_f \mathcal{L}(f)(X)\|_2 \\ &= \mathbb{E}_{\nu_X} \|\mathbb{E}_{\nu(Y|X)} [\partial_\zeta(f(X), Y)]\|_2 \\ &= \mathbb{E}_{\nu_X} \left[ \sqrt{\sum_{y' \in \mathcal{Y}} (\mathbb{E}_{\nu(Y|X)} [\partial_{\zeta_{y'}}(f(X), Y)])^2} \right] \\ &\geq \frac{1}{\sqrt{c}} \sum_{y' \in \mathcal{Y}} \mathbb{E}_{\nu_X} \left[ \left| \mathbb{E}_{\nu(Y|X)} [\partial_{\zeta_{y'}}(f(X), Y)] \right| \right] \end{aligned}$$

$$\begin{aligned}
 &= \frac{1}{\sqrt{c}} \sum_{y' \in \mathcal{Y}} \mathbb{E}_{\nu_X} \left[ \left[ \nu(y'|X) \left( -1 + \frac{\exp(f_{y'}(X))}{\sum_{\bar{y} \in \mathcal{Y}} \exp(f_{\bar{y}}(X))} \right) + \sum_{y \neq y'} \nu(y|X) \frac{\exp(f_{y'}(X))}{\sum_{\bar{y} \in \mathcal{Y}} \exp(f_{\bar{y}}(X))} \right] \right] \\
 &= \frac{1}{\sqrt{c}} \sum_{y' \in \mathcal{Y}} \mathbb{E}_{\nu_X} \left[ \left[ \nu(y'|X) \left( -1 + \frac{\exp(f_{y'}(X))}{\sum_{\bar{y} \in \mathcal{Y}} \exp(f_{\bar{y}}(X))} \right) + (1 - \nu(y'|X)) \frac{\exp(f_{y'}(X))}{\sum_{\bar{y} \in \mathcal{Y}} \exp(f_{\bar{y}}(X))} \right] \right] \\
 &= \frac{1}{\sqrt{c}} \sum_{y' \in \mathcal{Y}} \mathbb{E}_{\nu_X} \left[ \left[ -\nu(y'|X) + \frac{\exp(f_{y'}(X))}{\sum_{\bar{y} \in \mathcal{Y}} \exp(f_{\bar{y}}(X))} \right] \right] \\
 &= \frac{1}{\sqrt{c}} \sum_{y' \in \mathcal{Y}} \| -\nu(y'|\cdot) + p_f(y'|\cdot) \|_{L_1(\nu_X)},
 \end{aligned}$$

where for the first inequality we used  $(\sum_{i=1}^c a_i)^2 \leq c \sum_{i=1}^c a_i^2$ . Noting that the second inequality in Proposition 2 can be shown in the same way by replacing  $\nu$  by  $\nu_n$ , we finish the proof.  $\square$

We here give the proof of the following inequality concerning choice of embedding introduced in section 4.

$$\|T_{k_t, n} \partial_\phi \mathcal{R}_n(\phi_t, w_{t+1})\|_{k_t}^2 \geq \frac{1}{d} \|\partial_\phi \mathcal{R}_n(\phi_t, w_{t+1})\|_{L_1^d(\nu_{n, X})}^2 \quad (5)$$

*Proof of (5).* For notational simplicity, we denote by  $G_t = \partial_\phi \mathcal{R}_n(\phi_t, w_{t+1})(\cdot)$  and by  $G_t^i$  the  $i$ -th element of  $G_t$ . Then, we get

$$\begin{aligned}
 \|T_{k_t, n}(G_t / \|G_t(\cdot)\|_2)\|_{k_t}^2 &= \langle G_t, T_{k_t, n}(G_t / \|G_t(\cdot)\|_2) \rangle_{L_2^d(\nu_{n, X})} \\
 &= \mathbb{E}_{(X, X') \sim \nu_{n, X}^2} [G_t(X)^\top G_t(X') G_t(X')^\top G_t(X) / (\|G_t(X)\|_2 \|G_t(X')\|_2)] \\
 &= \sum_{i, j=1}^d (\mathbb{E}_{\nu_{n, X}} [G_t^i(X) G_t^j(X) / \|G_t(X)\|_2])^2 \\
 &\geq \sum_{i=1}^d (\mathbb{E}_{\nu_{n, X}} [G_t^i(X)^2] / \|G_t(X)\|_2)^2 \\
 &\geq \frac{1}{d} \mathbb{E}_{\nu_{n, X}} [\|G_t(X)\|_2^2] = \frac{1}{d} \|G_t\|_{L_1^d(\nu_{n, X})}^2,
 \end{aligned}$$

where we used  $(\sum_{i=1}^c a_i)^2 \leq c \sum_{i=1}^c a_i^2$ .  $\square$

## B. 2 Empirical risk minimization and generalization bound

In this section, we give the proof of convergence of Algorithm 1 for the empirical risk minimization. We here briefly introduce the kernel function that provides useful bound in our analysis. A kernel function  $k$  is a symmetric function  $\mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  such that for arbitrary  $s \in \mathbb{N}$  and points  $\forall (x_i)_{i=1}^s$ , a matrix  $(k(x_i, x_j))_{i, j=1}^s$  is positive semi-definite. This kernel defines a reproducing kernel Hilbert space  $\mathcal{H}_k$  of functions on  $\mathcal{X}$ , which has two characteristic properties: (i) for  $\forall x \in \mathcal{X}$ , a function  $k(x, \cdot) : \mathcal{X} \rightarrow \mathbb{R}$  is an element of  $\mathcal{H}_k$ , (ii) for  $\forall f \in \mathcal{H}_k$  and  $\forall x \in \mathcal{X}$ ,  $f(x) = \langle f, k(x, \cdot) \rangle_{\mathcal{H}_k}$ , where  $\langle \cdot, \cdot \rangle_{\mathcal{H}_k}$  is the inner-product in  $\mathcal{H}_k$ . These properties are very important and the latter one is called reproducing property. We extend the inner-product into the product space  $\mathcal{H}_k^d$  in a straightforward way, i.e.,  $\langle f, g \rangle_{\mathcal{H}_k^d} = \sum_{i=1}^d \langle f^i, g^i \rangle_{\mathcal{H}_k}$ .

The following proposition is useful in our analysis. The first property mean that the notation  $\|T_{k_t, n} \nabla \mathcal{R}_n(\phi_t)\|_{k_t}$  provided in the paper is nothing but the norm of  $T_{k_t, n} \nabla \mathcal{R}_n(\phi_t)$  by the inner-product  $\langle \cdot, \cdot \rangle_{\mathcal{H}_{k_t}^d}$ .

**Proposition A.** *For a kernel function  $k$ , the following hold.*

- $\langle f, g \rangle_{L_2(\nu_X)} = \langle T_k f, g \rangle_{\mathcal{H}_k^d}$  for  $f \in L_2^d(\nu_X)$ ,  $g \in \mathcal{H}_k^d$  where  $T_k f = \mathbb{E}_{\nu_X} [f(X) k(X, \cdot)]$ ,  
 $\langle f, g \rangle_{L_2(\nu_{n, X})} = \langle T_{k, n} f, g \rangle_{\mathcal{H}_k^d}$  for  $f \in L_2^d(\nu_{n, X})$ ,  $g \in \mathcal{H}_k^d$  where  $T_{k, n} f = \mathbb{E}_{\nu_{n, X}} [f(X) k(X, \cdot)]$ ,
- $\|f\|_{L_2(\nu_X)}^2 \leq \mathbb{E}_{\nu_X} [k(X, X)] \|f\|_{\mathcal{H}_k^d}^2$  for  $f \in \mathcal{H}_k^d$ ,  
 $\|f\|_{L_2(\nu_{n, X})}^2 \leq \mathbb{E}_{\nu_{n, X}} [k(X, X)] \|f\|_{\mathcal{H}_k^d}^2$  for  $f \in \mathcal{H}_k^d$ .

*Proof.* We show only the case of  $\nu_X$  because we can prove the other case in the same manner. For  $f \in L_2(\nu_X)$ ,  $g \in \mathcal{H}_k^d$ , we get the first property by using reproducing property,

$$\langle f, g \rangle_{L_2(\nu_X)} = \mathbb{E}_{\nu_X} [f(X) \top \langle g, k(X, \cdot) \rangle_{\mathcal{H}_k^d}] = \langle g, T_k f \rangle_{\mathcal{H}_k^d}.$$

We next show the second property as follows. For  $\forall f \in \mathcal{H}_k^d$ , we get

$$\begin{aligned} \|f\|_{L_2(\nu_X)}^2 &= \mathbb{E}_{\nu_X} \|f(X)\|_2^2 \\ &= \mathbb{E}_{\nu_X} \|\langle f(\cdot), k(X, \cdot) \rangle_{\mathcal{H}_k^d}\|_2^2 \\ &\leq \mathbb{E}_{\nu_X} \|k(X, \cdot)\|_{\mathcal{H}_k}^2 \|f\|_{\mathcal{H}_k^d}^2 \\ &= \mathbb{E}_{\nu_X} [k(X, X)] \|f\|_{\mathcal{H}_k^d}^2. \end{aligned}$$

□

We give the proof of Theorem 1 concerning the convergence of functional gradient norms.

*Proof of Theorem 1.* When  $\eta \leq \frac{1}{A_{c_\lambda} K}$ , we have from Proposition 1 and Proposition A,

$$\mathcal{R}_n(\phi_{t+1}, w_{t+2}) \leq \mathcal{R}_n(\phi_t, w_{t+1}) - \frac{\eta}{2} \|T_{k_t, n} \partial_\phi \mathcal{R}_n(\phi_t, w_{t+1})\|_{k_t}^2.$$

By Summing this inequality over  $t \in \{0, \dots, T-1\}$  and dividing by  $T$ , we get

$$\frac{1}{T} \sum_{t=0}^{T-1} \|T_{k_t, n} \partial_\phi \mathcal{R}_n(\phi_t, w_{t+1})\|_{k_t}^2 \leq \frac{2}{\eta T} \mathcal{R}_n(\phi_0, w_0), \quad (6)$$

where we used  $\mathcal{R}_n \geq 0$  and  $\mathcal{R}_n(\phi_0, w_1) \leq \mathcal{R}_n(\phi_0, w_0)$ .

On the other hand, since  $\partial_z l(z, y, w) = \partial_z l(w^\top z, y) = w \partial_\zeta l(w^\top z, y)$ , it follows that

$$\begin{aligned} \partial_\phi \mathcal{R}(\phi, w)(x) &= \mathbb{E}_{\nu(Y|x)} [\partial_z l(\phi(x), y, w)] \\ &= \mathbb{E}_{\nu(Y|x)} [w \partial_\zeta l(w^\top \phi(x), y)] \\ &= w \nabla_f \mathcal{L}(w^\top \phi)(x). \end{aligned}$$

Thus, by the assumption on  $(w_t^\top w_t)_{t=0}^{T_0}$ , we get for  $t \in \{0, \dots, T-1\}$

$$\begin{aligned} \|\partial_\phi \mathcal{R}(\phi_t, w_{t+1})\|_{L_2^d(\nu_X)}^2 &= \mathbb{E}_{\nu_X} [\|\nabla_f \mathcal{L}(w_{t+1}^\top \phi_t)(X)^\top w_{t+1}^\top w_{t+1} \nabla_f \mathcal{L}(w_{t+1}^\top \phi_t)(X)\|_2^2] \\ &\geq \sigma^2 \mathbb{E}_{\nu_X} [\|\nabla_f \mathcal{L}(w_{t+1}^\top \phi_t)(X)\|_2^2] \\ &= \sigma^2 \|\nabla_f \mathcal{L}(w_{t+1}^\top \phi_t)\|_{L_2^d(\nu_X)}^2. \end{aligned} \quad (7)$$

Combining inequalities (6) (7) and Assumption 2, we get

$$\min_{t \in [T]} \|\nabla_f \mathcal{L}(w_{t+1}^\top \phi_t)\|_{L_p^c(\nu_X)}^q \leq \frac{1}{T} \sum_{t=0}^{T-1} \|\nabla_f \mathcal{L}(w_{t+1}^\top \phi_t)\|_{L_p^c(\nu_X)}^q \leq \frac{2}{\eta \gamma \sigma^q T} \mathcal{R}_n(\phi_0, w_0) + \frac{\epsilon}{\sigma^q}.$$

Since  $p \geq 1$ , we observe  $\|\nabla_f \mathcal{L}(w_{t+1}^\top \phi_t)\|_{L_1^c(\nu_X)} \leq \|\nabla_f \mathcal{L}(w_{t+1}^\top \phi_t)\|_{L_p^c(\nu_X)}$  and we finish the proof. □

We next show Theorem 2 that gives the generalization bound by the margin distribution. To do that, we give an upper-bound on the margin distribution by the functional gradient norm.

**Proposition B.** For  $\forall \delta > 0$ , the following bound holds.

$$\mathbb{P}_{\nu_n} [m_f(X, Y) \leq \delta] \leq \left(1 + \frac{1}{\exp(-\delta)}\right) \sqrt{c} \|\nabla_f \mathcal{L}_n(f)\|_{L_1^c(\nu_{n, X})}$$

*Proof.* If  $m_f(x, y) \leq \delta$ , then, we see

$$\sum_{y' \neq y} \exp(f_{y'}(x) - f_y(x)) \geq \exp\left(\max_{y' \neq y} f_{y'}(x) - f_y(x)\right) = \exp(-m_f(x, y)) \geq \exp(-\delta).$$

This implies,

$$p_f(y|x) = \frac{1}{1 + \sum_{y' \neq y} \exp(f_{y'}(x) - f_y(x))} \leq \frac{1}{1 + \exp(-\delta)}.$$

Thus, we get by Markov inequality and Proposition 2,

$$\begin{aligned} \mathbb{P}_{\nu_n}[m_f(X, Y) \leq \delta] &\leq \mathbb{P}_{\nu_n}\left[p_f(Y|X) \leq \frac{1}{1 + \exp(-\delta)}\right] \\ &= \mathbb{P}_{\nu_n}\left[1 - p_f(Y|X) \geq \frac{\exp(-\delta)}{1 + \exp(-\delta)}\right] \\ &\leq \left(1 + \frac{1}{\exp(-\delta)}\right) \mathbb{E}_{\nu_n}[1 - p_f(Y|X)] \\ &\leq \left(1 + \frac{1}{\exp(-\delta)}\right) \mathbb{E}_{\nu_n}[\nu_n(Y|X) - p_f(Y|X)] \\ &= \left(1 + \frac{1}{\exp(-\delta)}\right) \sum_{y \in \mathcal{Y}} \|\nu_n(y|\cdot) - p_f(y|\cdot)\|_{L_1(\nu_{n,X})} \\ &\leq \left(1 + \frac{1}{\exp(-\delta)}\right) \sqrt{c} \|\nabla_f \mathcal{L}_n(f)\|_{L_1^c(\nu_{n,X})}. \end{aligned}$$

□

We prove here Theorem 2.

*Proof of Theorem 2.* To proof the theorem, we give the network structure. Note that the connection at the  $t$ -th layer is as follows.

$$\phi_{t+1}(x) = \phi_t(x) - \eta D_t \sigma(C_t \phi_t(x)).$$

We define recursively the family of functions  $\mathcal{H}_t$  and  $\hat{\mathcal{H}}_t$  where each neuron belong: We denote by  $P_j \in \mathbb{R}^d$  the projection vector to  $j$ -th coordinate.

$$\begin{aligned} \mathcal{H}_0 &\stackrel{\text{def}}{=} \{P_j : \mathcal{X} \rightarrow \mathbb{R} \mid j \in \{1, \dots, d\}\}, \\ \hat{\mathcal{H}}_t &\stackrel{\text{def}}{=} \{\sigma(c_t^\top \phi_t) : \mathcal{X} \rightarrow \mathbb{R} \mid \phi_t \in \mathcal{H}_t^d, c_{t-1} \in \mathbb{R}^d, \|c_{t-1}\|_1 \leq \Lambda\}, \\ \mathcal{H}_{t+1} &\stackrel{\text{def}}{=} \{\phi_t^j - \eta d_t^\top \psi_t : \mathcal{X} \rightarrow \mathbb{R} \mid \phi_t^j \in \mathcal{H}_t, \psi_t \in \hat{\mathcal{H}}_t^d, d_t \in \mathbb{R}^d, \|d_t\|_1 \leq \Lambda'\}. \end{aligned}$$

Then, the family of predictors of  $y \in \mathcal{Y}$  can be written as

$$\mathcal{G}_{T-1,y} \stackrel{\text{def}}{=} \{w_y^\top \phi_{T-1} : \mathcal{X} \rightarrow \mathbb{R} \mid \phi \in \mathcal{H}_{T-1}^d, w_y \in \mathbb{R}^d, \|w_y\|_1 \leq \Lambda_w\}.$$

Note that  $\mathcal{G}_{T-1} = \{(f_y)_{y \in \mathcal{Y}} \mid f_y \in \mathcal{G}_{T-1,y}, y \in \mathcal{Y}\}$ .

From these relationships and Lemma D, we get

$$\begin{aligned} \hat{\mathfrak{R}}_S(\mathcal{H}_t) &\leq \hat{\mathfrak{R}}_S(\mathcal{H}_{t-1}) + \eta \Lambda' \hat{\mathfrak{R}}_S(\hat{\mathcal{H}}_{t-1}) \\ &\leq (1 + \eta \Lambda' \Lambda L_\sigma) \hat{\mathfrak{R}}_S(\mathcal{H}_{t-1}), \\ \hat{\mathfrak{R}}_S(\mathcal{G}_{T-1,y}) &\leq \Lambda_w \hat{\mathfrak{R}}_S(\mathcal{H}_{T-1}). \end{aligned}$$

The Rademacher complexity of  $\mathcal{H}_0$  is obtained as follows. Since  $\|P_j\|_2 = 1$ , we have

$$\hat{\mathfrak{R}}_S(\mathcal{H}_0) = \frac{1}{n} \mathbb{E}_{(\sigma_i)_{i=1}^n} \left[ \sup_{j \in \{1, \dots, d\}} \sum_{i=1}^n \sigma_i P_j x_i \right]$$

$$\begin{aligned}
 &\leq \frac{1}{n} \mathbb{E}_{(\sigma_i)_{i=1}^n} \left[ \sup_{j \in \{1, \dots, d\}} \|P_j\|_2 \left\| \sum_{i=1}^n \sigma_i x_i \right\|_2 \right] \\
 &= \frac{1}{n} \mathbb{E}_{(\sigma_i)_{i=1}^n} \left[ \left\| \sum_{i=1}^n \sigma_i x_i \right\|_2 \right] \\
 &\leq \frac{1}{n} \left( \mathbb{E}_{(\sigma_i)_{i=1}^n} \left[ \left\| \sum_{i=1}^n \sigma_i x_i \right\|_2^2 \right] \right)^{\frac{1}{2}} \\
 &= \frac{1}{n} \left( \sum_{i=1}^n \|x_i\|_2^2 \right)^{\frac{1}{2}} \leq \frac{\Lambda_\infty}{\sqrt{n}},
 \end{aligned}$$

where we used the independence of  $\sigma_i$  when taking the expectation.

We set  $\Pi \mathcal{G}_{T-1} = \{f_y(\cdot) : \mathcal{X} \rightarrow \mathbb{R} \mid f \in \mathcal{G}_{T-1}, y \in \mathcal{Y}\}$ . Noting that  $\hat{\mathfrak{R}}_S(\Pi \mathcal{G}_{T-1}) \leq \sum_{y \in \mathcal{Y}} \hat{\mathfrak{R}}_S(\mathcal{G}_{T-1, y})$ , we get

$$\hat{\mathfrak{R}}_S(\Pi \mathcal{G}_{T-1}) \leq c \Lambda_w \Lambda_\infty (1 + \eta \Lambda \Lambda' L_\sigma)^{T-1} / \sqrt{n}.$$

Thus, we can finish the proof by applying Proposition B and Lemma E.  $\square$

### B.3 Sample-splitting technique

In this subsection, we provide proofs for the convergence analysis of the sample-splitting variant of the method for the expected risk minimization. We first give the statistical error bound on the gap between the empirical and expected functional gradients.

*Proof of Proposition 3.* For the probability measure  $\nu$ , we denote by  $\phi_\# \nu$  the push-forward measure  $(\phi, id)_\# \nu$ , namely,  $(\phi, id)_\# \nu$  is the measure that the random variable  $(\phi(X), Y)$  follows. We also define  $\phi_\# \nu_m$  in the same manner. Then, we get

$$\begin{aligned}
 &\|T_k \partial_\phi \mathcal{R}(\phi, w_0) - T_{k,m} \partial_\phi \mathcal{R}_m(\phi, w_0)\|_{L_2^d(\mu)} \\
 &= \sqrt{\mathbb{E}_{X' \sim \mu} \|\mathbb{E}_\nu[\partial_{z_j} l(\phi(X), Y, w_0) k(X, X')] - \mathbb{E}_{\nu_m}[\partial_{z_j} l(\phi(X), Y, w_0) k(X, X')]\|_2^2} \\
 &= \sqrt{\sum_{j=1}^d \mathbb{E}_{X' \sim \mu} |(\mathbb{E}_\nu[\partial_{z_j} l(\phi(X), Y, w_0) \iota(\phi(X))]) - \mathbb{E}_{\nu_m}[\partial_{z_j} l(\phi(X), Y, w_0) \iota(\phi(X))])^\top \iota(\phi(X'))|^2} \\
 &\leq \sqrt{K \sum_{j=1}^d \|\mathbb{E}_\nu[\partial_{z_j} l(\phi(X), Y, w_0) \iota(\phi(X))]) - \mathbb{E}_{\nu_m}[\partial_{z_j} l(\phi(X), Y, w_0) \iota(\phi(X))]\|_2^2} \\
 &\leq \sqrt{K \sum_{j=1}^d \sum_{i=1}^D |\mathbb{E}_{\phi_\# \nu}[\partial_{z_j} l(X, Y, w_0) \iota^i(X)] - \mathbb{E}_{\phi_\# \nu_m}[\partial_{z_j} l(X, Y, w_0) \iota^i(X)]|^2}. \tag{8}
 \end{aligned}$$

To derive an uniform bound on (8), we estimate Rademacher complexity of

$$\mathcal{G}_{ij} \stackrel{def}{=} \{\partial_{z_j} l(x, y, w_0) \iota^i(x) : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R} \mid \iota^i \in \mathcal{F}^i\}.$$

For  $(x_l, y_l)_{l=1}^m \subset \mathcal{X} \times \mathcal{Y}$ , we set  $h_l(r) = r \partial_{z_j} l(x_l, y_l, w_0)$ . Since,  $|\partial_{z_j} l(x_l, y_l, w_0)| \leq \beta_{\|w_0\|_2}$  by Assumption 3,  $h_l$  is  $\beta_{\|w_0\|_2}$ -Lipschitz continuous. Thus, from Lemma C and Lemma D, there exists  $M$  such that for all  $i \in \{1, \dots, D\}$ ,  $j \in \{1, \dots, d\}$ ,

$$\hat{\mathfrak{R}}_m(\mathcal{G}_{ij}) = \mathbb{E}_\sigma \left[ \sup_{\iota^i \in \mathcal{F}^i} \sum_{l=1}^m \sigma_l h_l(\iota^i(x_l)) \right]$$

$$\begin{aligned} &\leq \beta_{\|w_0\|_2} \mathbb{E}_\sigma \left[ \sup_{i^i \in \mathcal{F}^i} \sum_{l=1}^m \sigma_l \iota^i(x_l) \right] \\ &\leq \beta_{\|w_0\|_2} \frac{M}{\sqrt{m}}. \end{aligned}$$

Therefore, by applying Lemma B with  $\delta = \frac{\rho}{dD}$  for  $\forall i, j$  simultaneously, it follows that with probability at least  $1 - \rho$  for  $\forall i, j$

$$\sup_{i^i \in \mathcal{F}^i} |\mathbb{E}_{\phi_i \nu} [\partial_{z_j} l(X, Y, w_0) \iota^i(X)] - \mathbb{E}_{\phi_i \nu_m} [\partial_{z_j} l(X, Y, w_0) \iota^i(X)]| \leq \frac{\beta_{\|w_0\|_2}}{\sqrt{m}} \left( 2M + \sqrt{2K \log \frac{2dD}{\rho}} \right). \quad (9)$$

Putting (9) into (8), we get with probability at least  $1 - \rho$

$$\sup_{i \in \mathcal{F}} \|T_k \partial_\phi \mathcal{R}(\phi, w_0) - T_{k,m} \partial_\phi \mathcal{R}_m(\phi, w_0)\|_{L_2^d(\mu)} \leq \beta_{\|w_0\|_2} \sqrt{\frac{KdD}{m}} \left( 2M + \sqrt{2K \log \frac{2dD}{\rho}} \right).$$

□

We here prove Theorem 3 by using statistical guarantees of empirical functional gradients.

*Proof of Theorem 3.* For notational simplicity, we set  $m \leftarrow \lfloor n/T \rfloor$  and  $\delta \leftarrow \rho/T$ . We first note that

$$\begin{aligned} \langle \partial_\phi \mathcal{R}(\phi_t, w_0), T_{k_t, m} \partial_\phi \mathcal{R}_m(\phi_t, w_0) \rangle_{L_2^d(\nu_X)} &= \frac{1}{m} \sum_{j=1}^m \mathbb{E}_{\nu_X} [\partial_\phi \mathcal{R}(\phi_t, w_0)(X)^\top \partial_\phi \mathcal{R}_m(\phi_t, w_0)(x_j) k_t(X, x_j)] \\ &= \frac{1}{m} \sum_{j=1}^m T_{k_t} \partial_\phi \mathcal{R}(\phi_t, w_0)(x_j)^\top \partial_\phi \mathcal{R}_m(\phi_t, w_0)(x_j) \\ &= \langle T_{k_t} \partial_\phi \mathcal{R}(\phi_t, w_0), \partial_\phi \mathcal{R}_m(\phi_t, w_0) \rangle_{L_2^d(\nu_{m, X})}. \end{aligned}$$

Noting that  $\|\partial_z l(\phi_t(x_j), y_j, w_0)\|_2 \leq \beta_{\|w_0\|_2}$  by Assumption 1, and applying Proposition 3 for all  $t \in \{0, \dots, T-1\}$  independently, it follows that with probability at least  $1 - T\delta$  (i.e.,  $1 - \rho$ ) for  $\forall t \in \{0, \dots, T-1\}$

$$\begin{aligned} &\left| \langle \partial_\phi \mathcal{R}(\phi_t, w_0), T_{k_t, m} \partial_\phi \mathcal{R}_m(\phi_t, w_0) \rangle_{L_2^d(\nu_X)} - \langle T_{k_t, m} \partial_\phi \mathcal{R}_m(\phi_t, w_0), \partial_\phi \mathcal{R}_m(\phi_t, w_0) \rangle_{L_2^d(\nu_{m, X})} \right| \\ &\leq \|T_{k_t} \partial_\phi \mathcal{R}(\phi_t, w_0) - T_{k_t, m} \partial_\phi \mathcal{R}_m(\phi_t, w_0)\|_{L_2^d(\nu_{m, X})} \|\partial_\phi \mathcal{R}_m(\phi_t, w_0)\|_{L_2^d(\nu_{m, X})} \\ &\leq \beta_{\|w_0\|_2} \epsilon(m, \delta). \end{aligned} \quad (10)$$

We next give the following bound.

$$\|T_{k_t} \partial_\phi \mathcal{R}_m(\phi_t, w_0)\|_{L_2^d(\nu_X)}^2 = \mathbb{E}_{\nu_X} \left\| \frac{1}{m} \sum_{j=1}^m \partial_z l(\phi_t(x_i), y_i, w_0) k_t(x_i, X) \right\|_2^2 \leq \beta_{\|w_0\|_2}^2 K^2. \quad (11)$$

On the other hand, we get by Proposition 1

$$\mathcal{R}(\phi_{t+1}, w_0) \leq \mathcal{R}(\phi_t, w_0) - \eta \langle \partial_\phi \mathcal{R}(\phi_t, w_0), T_{k_t, m} \partial_\phi \mathcal{R}_m(\phi_t, w_0) \rangle_{L_2^d(\nu_X)} + \frac{\eta^2 A_{\|w_0\|_2}}{2} \|T_{k_t} \partial_\phi \mathcal{R}_m(\phi_t, w_0)\|_{L_2^d(\nu_X)}^2. \quad (12)$$

Combining inequalities (10), (11), and (12), we have with probability at least  $1 - T\delta$  for  $t \in \{0, \dots, T-1\}$ ,

$$\mathcal{R}(\phi_{t+1}, w_0) \leq \mathcal{R}(\phi_t, w_0) - \eta \|T_{k_t, m} \partial_\phi \mathcal{R}_m(\phi_t, w_0)\|_{k_t}^2 + \eta \beta_{\|w_0\|_2} \epsilon(m, \delta) + \frac{\eta^2 \beta_{\|w_0\|_2}^2 K^2 A_{\|w_0\|_2}}{2}.$$

By Summing this inequality over  $t \in \{0, \dots, T-1\}$  and dividing by  $T$ , we get with probability  $1 - T\delta$

$$\frac{1}{T} \sum_{t=0}^{T-1} \|T_{k_t, m} \partial_\phi \mathcal{R}_m(\phi_t, w_0)\|_{k_t}^2 \leq \frac{\mathcal{R}(\phi_0, w_0)}{\eta T} + \beta_{\|w_0\|_2} \epsilon(m, \delta) + \frac{\eta \beta_{\|w_0\|_2}^2 K^2 A_{\|w_0\|_2}}{2}.$$

Thus by Assumption 2 and the assumption on  $w_0^\top w_0$ , we get

$$\frac{1}{T} \sum_{t=0}^{T-1} \|\nabla_f \mathcal{L}_m(w_0^\top \phi_t)\|_{L_p^d(\nu_{m, X})}^q \leq \frac{1}{\gamma \sigma^q} \left\{ \frac{\mathcal{R}(\phi_0, w_0)}{\eta T} + \beta_{\|w_0\|_2} \epsilon(m, \delta) + \frac{\eta \beta_{\|w_0\|_2}^2 K^2 A_{\|w_0\|_2}}{2} + \gamma \epsilon \right\}. \quad (13)$$

To clarify the relationship between  $\|\nabla_f \mathcal{L}_m(f)\|_{L_1^c(\nu_{m, X})}$  and  $\|\nabla_f \mathcal{L}(f)\|_{L_1^c(\nu_X)}$ , we take an expectation of the former term with respect to samples  $(X_j, Y_j)_{j=1}^m \sim \nu^m$ . Since  $\|\partial_\zeta l(\zeta, y)\|_2 \leq B$ , we obtain

$$\begin{aligned} \mathbb{E}_{(X_j, Y_j)_{j=1}^m \sim \nu^m} \|\nabla_f \mathcal{L}_m(f)\|_{L_1^c(\nu_{m, X})} &= \mathbb{E}_{(X, Y) \sim \nu_m} \|\partial_\zeta l(f(X), Y)\|_2 \\ &\geq \frac{1}{B} \mathbb{E}_{(X, Y) \sim \nu_m} \|\partial_\zeta l(f(X), Y)\|_2^2 \\ &\geq \frac{1}{B} \mathbb{E}_{\nu_{m, X}} \|\mathbb{E}_{\nu(Y|X)} [\partial_\zeta l(f(X), Y)]\|_2^2 \\ &= \frac{1}{B} \mathbb{E}_{\nu_{m, X}} \|\nabla_f \mathcal{L}(f)(X)\|_2^2 \\ &= \frac{1}{B} \|\nabla_f \mathcal{L}(f)\|_{L_2^c(\nu_X)}^2. \end{aligned}$$

Hence, applying Hoeffding's inequality with  $\delta \leftarrow \rho/T$  to  $\mathbb{E}_{(X_j, Y_j)_{j=1}^m \sim \nu^m} \|\nabla_f \mathcal{L}_m(w_0^\top \phi_t)\|_{L_1^c(\nu_{m, X})}$  for all  $t \in \{0, \dots, T-1\}$  independently, we find that with probability  $1 - T\delta$  for  $\forall t \in \{0, \dots, T-1\}$ ,

$$\|\nabla_f \mathcal{L}_m(w_0^\top \phi_t)\|_{L_1^c(\nu_{m, X})} + B \sqrt{\frac{2}{m} \log \frac{1}{\delta}} \geq \mathbb{E}_{\sim \nu^m} \|\nabla_f \mathcal{L}_m(w_0^\top \phi_t)\|_{L_1^c(\nu_{m, X})} \geq \frac{1}{B} \|\nabla_f \mathcal{L}(w_0^\top \phi_t)\|_{L_1^c(\nu_X)}^2, \quad (14)$$

where we used for the last inequality  $\|\cdot\|_{L_2^c(\nu_X)}^2 \geq \|\cdot\|_{L_1^c(\nu_X)}^2$ .

We set  $t_* = \arg \min_{t \in \{0, \dots, T-1\}} \|\nabla_f \mathcal{L}_m(w_0^\top \phi_t)\|_{L_p^d(\nu_{m, X})}$ . Combining inequalities (13) and (14) and noting  $p \geq 1$ , we get with probability at least  $1 - 2T\delta$ ,

$$\frac{1}{B} \|\nabla_f \mathcal{L}(w_0^\top \phi_{t_*})\|_{L_1^c(\nu_X)}^2 \leq B \sqrt{\frac{2}{m} \log \frac{1}{\delta}} + \frac{1}{\gamma^{1/q} \sigma} \left\{ \frac{\mathcal{R}(\phi_0, w_0)}{\eta T} + \beta_{\|w_0\|_2} \epsilon(m, \delta) + \frac{\eta \beta_{\|w_0\|_2}^2 K^2 A_{\|w_0\|_2}}{2} + \gamma \epsilon \right\}^{\frac{1}{q}}.$$

Noting that  $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$  for  $a, b > 0$ , we finally obtain

$$\|\nabla_f \mathcal{L}(w_0^\top \phi_{t_*})\|_{L_1^c(\nu_X)} \leq B \left( \frac{2}{m} \log \frac{1}{\delta} \right)^{\frac{1}{4}} + \sqrt{\frac{B}{\gamma^{1/q} \sigma}} \left\{ \frac{\mathcal{R}(\phi_0, w_0)}{\eta T} + \beta_{\|w_0\|_2} \epsilon(m, \delta) + \frac{\eta \beta_{\|w_0\|_2}^2 K^2 A_{\|w_0\|_2}}{2} + \gamma \epsilon \right\}^{\frac{1}{2q}}.$$

Recalling that  $m \leftarrow \lfloor n/T \rfloor$  and  $\delta \leftarrow \rho/T$ , the proof is finished.  $\square$

## References

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