

Project Notes

This project builds upon [CLT24] to extend Remark 3.1 and Section 4.3 to the analysis of deep neural networks (DNNs) and transformers.

1 Notations

\mathcal{A}	σ -algebra on \mathcal{Z} such that $\{z\} \in \mathcal{A}$ for any $z \in \mathcal{Z}$
$(\mathcal{Z}, \mathcal{A})$	Measurable space
$\mathcal{Z} \times \mathcal{Z}$	Cartesian product measurable space with σ -algebra $\mathcal{A} \times \mathcal{A}$
$\mathbb{P} : \mathcal{A} \rightarrow [0, \infty]$	Probability function with countably additivity, $\mathbb{P}(\emptyset) = 0$ and $\mathbb{P}(\mathcal{Z}) = 1$
$\mathcal{P}(\mathcal{Z})$	Space of all probabilities on \mathcal{Z}
$\mathbb{E}_{\mathbb{P}}[f(Z)] = \int_{\mathcal{Z}} f(z) d\mathbb{P}(z)$	Expectation of a measurable function f of a real-valued random variable Z on $(\mathcal{Z}, \mathcal{A}, \mathbb{P})$
$\delta_S : \mathcal{Z} \rightarrow \mathbb{R}$	Indicator function of a set $S \subset \mathcal{Z}$, $\delta_S(z) = 0$ if $z \in S$, and ∞ otherwise
$\chi_{\{\hat{z}\}} \in \mathcal{P}(\mathcal{Z})$	Point mass function (Dirac measure) at point $\hat{z} \in \mathcal{Z}$ as $\chi_{\{\hat{z}\}}(A) = 1$ if $\hat{z} \in A$, and 0 otherwise, for any measurable set $A \subset \mathcal{Z}$
$f \otimes g : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$	$(x, y) \rightarrow f(x) \cdot g(y)$ for any $(x, y) \in \mathcal{X} \times \mathcal{Y}$
$\langle x, y \rangle = \sum_{i=1}^n x_i y_i$	Inner product on \mathbb{R}^n for any $x, y \in \mathbb{R}^n$
$\ \cdot\ _{\mathbb{R}^n}$	An arbitrary norm on \mathbb{R}^n
$\ \cdot\ _{\mathbb{R}^n, *}$	Dual norm defined as $\ x\ _{\mathbb{R}^n, *} := \max_{y \in \mathbb{R}^n} \{\langle x, y \rangle \mid \ y\ _{\mathbb{R}^n} = 1\}$
$[A, B] \in \mathbb{R}^{n_1 \times (n_2 + n_3)}$	Horizontal concatenation of $A \in \mathbb{R}^{n_1 \times n_2}$ and $B \in \mathbb{R}^{n_1 \times n_3}$
$[A; C] \in \mathbb{R}^{(n_1 + n_3) \times n_2}$	Vertical concatenation of $A \in \mathbb{R}^{n_1 \times n_2}$ and $C \in \mathbb{R}^{n_3 \times n_2}$
sgn	Sign function as $\text{sgn}(t) = -1$ if $t < 0$, and $\text{sgn}(t) = 1$ otherwise
β	Decision variable from decision space \mathcal{B}
Z	Random variable in a given space \mathcal{Z} , with probability distribution \mathbb{P}_{true}
$\ell : \mathcal{Z} \times \mathcal{B} \rightarrow \mathbb{R}$	Loss function
$\mathbb{P}_N := \sum_{i=1}^N \mu_i \chi_{\{Z^{(i)}\}}$	Empirical distribution
$\mathcal{Z}_N := \{Z^{(1)}, \dots, Z^{(N)}\} \subset \mathcal{Z}$	Training dataset
$\{\mu_i\}_{i=1}^N$	Nonnegative weights satisfying $\sum_{i=1}^N \mu_i = 1$
$\mathfrak{M} \subset \mathcal{P}(\mathcal{Z})$	Ambiguity set
$d : \mathcal{Z} \times \mathcal{Z} \rightarrow [0, \infty]$	Extended nonnegative-valued function
$r \in [1, \infty)$	Exponent in \mathcal{W}
$\sigma(\mathcal{Z})$	Set of all measurable sets in \mathcal{Z}
$\Pi(\mathbb{P}, \mathbb{Q})$	Set of all joint probability distributions between \mathbb{P} and \mathbb{Q}
$\Pi(\mathbb{P}, \mathbb{Q}) = \{\pi \in \mathcal{P}(\mathcal{Z} \times \mathcal{Z}) \text{ such that } \forall A, B \in \sigma(\mathcal{Z}), \pi(A \times \mathcal{Z}) = \mathbb{P}(A), \pi(\mathcal{Z} \times B) = \mathbb{Q}(B)\}$	

$$\mathcal{W}_{d,r}(\mathbb{P}, \mathbb{Q}) := \left(\inf_{\pi \in \Pi(\mathbb{P}, \mathbb{Q})} \int_{\mathcal{Z} \times \mathcal{Z}} d^r(z', z) d\pi(z', z) \right)^{\frac{1}{r}} \quad (2)$$

$$\mathcal{S} := \sup_{\mathbb{P} : \mathcal{W}_{d,r}(\mathbb{P}, \mathbb{P}_N) \leq \delta} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \quad (4)$$

2 Remark 3.1

In [Theorem 3.2](#), it is required that the condition [\(A2\)](#) holds for any $i = 1, \dots, N$, with respect to the same Lipschitz constant $L_{\beta}^{\mathcal{Z}^N}$. To relax this condition, one might assume that Assumptions [\(A1\)](#) & [\(A2\)](#) hold at each $Z^{(i)}$ with a Lipschitz constant $L_{\beta}^{\{Z^{(i)}\}}$, for $i = 1, \dots, N$. Even though it might not guarantee that the lower bound and upper bound for \mathcal{S} coincide as in [Theorem 3.2](#), we show in [Appendix C](#) that one still has closed forms for the lower and upper bounds given by

$$\widehat{\mathcal{L}} = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + \sum_{i=1}^N \mu_i L_{\beta}^{\{Z^{(i)}\}} \delta,$$

$$\widehat{\mathcal{U}} = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + \max_{i=1, \dots, N} L_{\beta}^{\{Z^{(i)}\}} \delta.$$

2.1 Theorem 3.2

Let $\mathcal{Z}_N := \{Z^{(1)}, \dots, Z^{(N)}\} \subset \mathcal{Z}$ be a given dataset and $\mathbb{P}_N := \sum_{i=1}^N \mu_i \mathbf{X}_{\{Z^{(i)}\}} \in \mathcal{P}(\mathcal{Z})$ be the corresponding empirical distribution. In addition, let $d(\cdot, \cdot)$ be a cost function on $\mathcal{Z} \times \mathcal{Z}$ and $\delta \in (0, \infty)$ be a scalar. Suppose the loss function $\ell : \mathcal{Z} \times \mathcal{B} \rightarrow \mathbb{R}$ takes the form as

$$\ell : (z; \beta) \mapsto \psi_{\beta}(z),$$

where the function $\psi_{\beta} : \mathcal{Z} \rightarrow \mathbb{R}$ satisfies the following assumptions:

(A1) ψ_{β} is $(L_{\beta}^{\mathcal{Z}_N}, d)$ -Lipschitz at \mathcal{Z}_N with $L_{\beta}^{\mathcal{Z}_N} \in (0, \infty)$;

(A2) For any $\epsilon \in (0, L_{\beta}^{\mathcal{Z}_N})$ and each $Z^{(i)} \in \mathcal{Z}_N$, there exists $\tilde{Z}_{\epsilon}^{(i)} \in \mathcal{Z}$ such that $\delta \leq d(\tilde{Z}_{\epsilon}^{(i)}, Z^{(i)}) < \infty$ and

$$\psi_{\beta}(\tilde{Z}_{\epsilon}^{(i)}) - \psi_{\beta}(Z^{(i)}) \geq (L_{\beta}^{\mathcal{Z}_N} - \epsilon) d(\tilde{Z}_{\epsilon}^{(i)}, Z^{(i)}).$$

Then we have that $\mathcal{L} = \mathcal{S} = \mathcal{U}$ in [Theorem 3.1](#), that is,

$$\sup_{\mathbb{P} : \mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_N) \leq \delta} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + L_{\beta}^{\mathcal{Z}_N} \delta. \quad (7)$$

Proof. Since ψ_{β} is $(L_{\beta}^{\mathcal{Z}_N}, d)$ -Lipschitz at \mathcal{Z}_N , by [Theorem 3.1](#), we have that

$$\mathcal{L} \leq \mathcal{S} = \sup_{\mathbb{P} : \mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_N) \leq \delta} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \leq \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + L_{\beta}^{\mathcal{Z}_N} \delta =: \mathcal{U}.$$

Hence, in order to prove [\(7\)](#), it suffices to show that $\mathcal{L} \geq \mathcal{U}$.

Let $\epsilon \in (0, \min\{L_{\beta}^{\mathcal{Z}_N}, \delta L_{\beta}^{\mathcal{Z}_N}\})$ be an arbitrary scalar. By Assumption [\(A2\)](#), for any $Z^{(i)} \in \mathcal{Z}_N$, there exists $\tilde{Z}^{(i)} \in \mathcal{Z}$ such that $\delta \leq d(\tilde{Z}^{(i)}, Z^{(i)}) < \infty$ and

$$\psi_{\beta}(\tilde{Z}^{(i)}) - \psi_{\beta}(Z^{(i)}) \geq \left(L_{\beta}^{\mathcal{Z}_N} - \frac{\epsilon}{\delta} \right) d(\tilde{Z}^{(i)}, Z^{(i)}).$$

Let $\eta^{(i)} := \delta / d(\tilde{Z}^{(i)}, Z^{(i)}) \in (0, 1]$ and define

$$\tilde{\mathbb{P}}^{(i)} := \eta^{(i)} \mathbf{X}_{\{\tilde{Z}^{(i)}\}} + (1 - \eta^{(i)}) \mathbf{X}_{\{Z^{(i)}\}} \in \mathcal{P}(\mathcal{Z}).$$

Then we have

$$\mathcal{W}_{d,1}(\tilde{\mathbb{P}}^{(i)}, \chi_{\{Z^{(i)}\}}) = \eta^{(i)} d(\tilde{Z}^{(i)}, Z^{(i)}) + (1 - \eta^{(i)}) d(Z^{(i)}, Z^{(i)}) = \eta^{(i)} d(\tilde{Z}^{(i)}, Z^{(i)}) = \delta,$$

and

$$\begin{aligned} \mathbb{E}_{\tilde{\mathbb{P}}^{(i)}}[\ell(Z; \beta)] &= \eta^{(i)} \psi_\beta(\tilde{Z}^{(i)}) + (1 - \eta^{(i)}) \psi_\beta(Z^{(i)}) \\ &= \psi_\beta(Z^{(i)}) + \eta^{(i)} [\psi_\beta(\tilde{Z}^{(i)}) - \psi_\beta(Z^{(i)})] \\ &\geq \psi_\beta(Z^{(i)}) + \eta^{(i)} \left(L_\beta^{\mathcal{Z}_N} - \frac{\epsilon}{\delta} \right) d(\tilde{Z}^{(i)}, Z^{(i)}) \\ &= \ell(Z^{(i)}; \beta) + L_\beta^{\mathcal{Z}_N} \delta - \epsilon. \end{aligned}$$

Letting $\epsilon \rightarrow 0$, we get for all $i = 1, \dots, N$,

$$\mathcal{L}_i = \sup_{\mathbb{P} \in \mathcal{P}(\mathcal{Z})} \{ \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \mid \mathcal{W}_{d,1}(\mathbb{P}, \chi_{\{Z^{(i)}\}}) \leq \delta \} \geq \ell(Z^{(i)}; \beta) + L_\beta^{\mathcal{Z}_N} \delta.$$

Therefore, it holds that

$$\mathcal{L} = \sum_{i=1}^N \mu_i \mathcal{L}_i \geq \sum_{i=1}^N \mu_i \left(\ell(Z^{(i)}; \beta) + L_\beta^{\mathcal{Z}_N} \delta \right) = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + L_\beta^{\mathcal{Z}_N} \delta = \mathcal{U}.$$

□

2.2 Appendix C

Let $\mathcal{Z}_N := \{Z^{(1)}, \dots, Z^{(N)}\} \subset \mathcal{Z}$ be a given dataset and $\mathbb{P}_N := \sum_{i=1}^N \mu_i \chi_{\{Z^{(i)}\}} \in \mathcal{P}(\mathcal{Z})$ be the corresponding empirical distribution. In addition, let $d(\cdot, \cdot)$ be a cost function on $\mathcal{Z} \times \mathcal{Z}$ and $\delta \in (0, \infty)$ be a scalar. Suppose the loss function $\ell : \mathcal{Z} \times \mathcal{B} \rightarrow \mathbb{R}$ takes the form

$$\ell : (z; \beta) \mapsto \psi_\beta(z),$$

where the function $\psi_\beta : \mathcal{Z} \rightarrow \mathbb{R}$ satisfies the following assumptions:

(C1) ψ_β is $(L_\beta^{\{Z^{(i)}\}}, d)$ -Lipschitz at $\{Z^{(i)}\}$ with $L_\beta^{\{Z^{(i)}\}} \in (0, \infty)$ for each $1 \leq i \leq N$;

(C2) For any $\epsilon \in (0, \min_i L_\beta^{\{Z^{(i)}\}})$ and each $Z^{(i)} \in \mathcal{Z}_N$, there exists $\tilde{Z}_\epsilon^{(i)} \in \mathcal{Z}$ such that $\delta \leq d(\tilde{Z}_\epsilon^{(i)}, Z^{(i)}) < \infty$ and

$$\psi_\beta(\tilde{Z}_\epsilon^{(i)}) - \psi_\beta(Z^{(i)}) \geq (L_\beta^{\{Z^{(i)}\}} - \epsilon) d(\tilde{Z}_\epsilon^{(i)}, Z^{(i)}).$$

Then we have that $\hat{\mathcal{L}} \leq \mathcal{S} \leq \hat{\mathcal{U}}$, where

$$\hat{\mathcal{L}} = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + \sum_{i=1}^N \mu_i L_\beta^{\{Z^{(i)}\}} \delta,$$

$$\hat{\mathcal{U}} = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + \max_{i=1, \dots, N} L_\beta^{\{Z^{(i)}\}} \delta,$$

which means that

$$\hat{\mathcal{L}} = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + \sum_{i=1}^N \mu_i L_\beta^{\{Z^{(i)}\}} \delta \leq \sup_{\mathbb{P} : \mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_N) \leq \delta} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \leq \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + \max_{i=1, \dots, N} L_\beta^{\{Z^{(i)}\}} \delta = \hat{\mathcal{U}}.$$

Proof. Since ψ_β is $(L_\beta^{\{Z^{(i)}\}}, d)$ -Lipschitz at $\{Z^{(i)}\}$ for each $1 \leq i \leq N$, it implies that ψ_β is $(L_\beta^{\mathcal{Z}_N}, d)$ -Lipschitz at \mathcal{Z}_N , with

$$L_\beta^{\mathcal{Z}_N} = \max_{i=1, \dots, N} L_\beta^{\{Z^{(i)}\}}.$$

By Theorem 3.1, letting

$$\mathcal{L}_i := \sup_{\mathbb{P} \in \mathcal{P}(\mathcal{Z})} \{ \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \mid \mathcal{W}_{d,1}(\mathbb{P}, \chi_{\{Z^{(i)}\}}) \leq \delta \}, \quad i = 1, \dots, N,$$

we have

$$\sum_{i=1}^N \mu_i \mathcal{L}_i \leq \mathcal{S} = \sup_{\mathbb{P}: \mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_N) \leq \delta} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \leq \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + L_\beta^{\mathcal{Z}_N} \delta = \widehat{\mathcal{U}}.$$

Then by applying Theorem 3.2 to each \mathcal{L}_i , we obtain:

$$\mathcal{L}_i = \ell(Z^{(i)}; \beta) + L_\beta^{\{Z^{(i)}\}} \delta,$$

which means that

$$\sum_{i=1}^N \mu_i \mathcal{L}_i = \sum_{i=1}^N \mu_i \ell(Z^{(i)}; \beta) + \sum_{i=1}^N \mu_i L_\beta^{\{Z^{(i)}\}} \delta = \widehat{\mathcal{L}}.$$

□

2.3 Theorem 3.1

Let $\mathcal{Z}_N := \{Z^{(1)}, \dots, Z^{(N)}\} \subset \mathcal{Z}$ be a given dataset and $\mathbb{P}_N := \sum_{i=1}^N \mu_i \chi_{\{Z^{(i)}\}} \in \mathcal{P}(\mathcal{Z})$ be the corresponding empirical distribution. In addition, let $r \in [1, \infty)$ be a scalar and $d(\cdot, \cdot)$ be a cost function on $\mathcal{Z} \times \mathcal{Z}$. Suppose the loss function $\ell : \mathcal{Z} \times \mathcal{B} \rightarrow \mathbb{R}$ takes the form as

$$\ell : (z; \beta) \mapsto \psi_\beta^r(z), \quad \text{with} \quad \begin{cases} \psi_\beta : \mathcal{Z} \rightarrow \mathbb{R} & \text{if } r = 1, \\ \psi_\beta : \mathcal{Z} \rightarrow \mathbb{R}_+ & \text{if } r > 1. \end{cases}$$

Let \mathcal{S} be defined as in (4). Then the following statements hold for any $\delta \geq 0$.

(a) Let

$$\mathcal{L}_i := \sup_{\mathbb{P} \in \mathcal{P}(\mathcal{Z})} \{ \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \mid \mathcal{W}_{d,r}(\mathbb{P}, \chi_{\{Z^{(i)}\}}) \leq \delta \}, \quad \text{for } i = 1, \dots, N.$$

Then

$$\mathcal{S} \geq \mathcal{L} := \sum_{i=1}^N \mu_i \mathcal{L}_i \geq \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)].$$

(b) Suppose ψ_β is $(L_\beta^{\mathcal{Z}_N}, d)$ -Lipschitz at \mathcal{Z}_N with $L_\beta^{\mathcal{Z}_N} \in (0, \infty)$, then

$$\mathcal{S} \leq \mathcal{U} := \left((\mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)])^{1/r} + L_\beta^{\mathcal{Z}_N} \delta \right)^r.$$

(c) Suppose ψ_β is $(0, d)$ -Lipschitz at \mathcal{Z}_N , then

$$\mathcal{S} = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)].$$

Proof. (a) For any collection $\{\tilde{\mathbb{P}}^{(i)}\}_{i=1}^N \subseteq \mathcal{P}(\mathcal{Z})$ such that $\mathcal{W}_{d,r}(\tilde{\mathbb{P}}^{(i)}, \chi_{\{Z^{(i)}\}}) \leq \delta$ for all $i = 1, \dots, N$. It follows from Lemma 3.1 that for each $i = 1, \dots, N$,

$$\mathcal{W}_{d,r}(\tilde{\mathbb{P}}^{(i)}, \chi_{\{Z^{(i)}\}}) = \left(\int_{\mathcal{Z}} d^r(z, Z^{(i)}) d\tilde{\mathbb{P}}^{(i)}(z) \right)^{1/r} \leq \delta.$$

Define

$$\tilde{\mathbb{P}} := \sum_{i=1}^N \mu_i \tilde{\mathbb{P}}^{(i)}, \quad \tilde{\pi} := \sum_{i=1}^N \left(\mu_i \tilde{\mathbb{P}}^{(i)} \otimes \chi_{\{Z^{(i)}\}} \right). \quad (6)$$

Then $\tilde{\mathbb{P}} \in \mathcal{P}(\mathcal{Z})$, $\tilde{\pi} \in \mathcal{P}(\mathcal{Z} \times \mathcal{Z})$, and $\tilde{\pi} \in \Pi(\tilde{\mathbb{P}}, \mathbb{P}_N)$, since for any measurable sets $A, B \subset \mathcal{Z}$,

$$\begin{aligned} \tilde{\pi}(\mathcal{Z} \times B) &= \sum_{i=1}^N \mu_i \tilde{\mathbb{P}}^{(i)}(\mathcal{Z}) \chi_{\{Z^{(i)}\}}(B) = \sum_{i=1}^N \mu_i \chi_{\{Z^{(i)}\}}(B) = \mathbb{P}_N(B), \\ \tilde{\pi}(A \times \mathcal{Z}) &= \sum_{i=1}^N \mu_i \tilde{\mathbb{P}}^{(i)}(A) \chi_{\{Z^{(i)}\}}(\mathcal{Z}) = \sum_{i=1}^N \mu_i \tilde{\mathbb{P}}^{(i)}(A) = \tilde{\mathbb{P}}(A). \end{aligned}$$

Hence,

$$\begin{aligned} \mathcal{W}_{d,r}(\tilde{\mathbb{P}}, \mathbb{P}_N) &\leq \left(\int_{\mathcal{Z} \times \mathcal{Z}} d^r(\tilde{z}, z) d\tilde{\pi}(\tilde{z}, z) \right)^{1/r} = \left(\int_{\mathcal{Z} \times \mathcal{Z}} d^r(\tilde{z}, z) d \sum_{i=1}^N \left(\mu_i \tilde{\mathbb{P}}^{(i)}(\tilde{z}) \chi_{\{Z^{(i)}\}}(z) \right) \right)^{1/r} \\ &= \left(\sum_{i=1}^N \mu_i \int_{\mathcal{Z}} d^r(\tilde{z}, Z^{(i)}) d\tilde{\mathbb{P}}^{(i)}(\tilde{z}) \right)^{1/r} = \left(\sum_{i=1}^N \mu_i \left(\mathcal{W}_{d,r}(\tilde{\mathbb{P}}^{(i)}, \chi_{\{Z^{(i)}\}}) \right)^r \right)^{1/r} \leq \delta. \end{aligned}$$

Moreover, from (6) we have:

$$\mathbb{E}_{\tilde{\mathbb{P}}}[\ell(Z; \beta)] = \sum_{i=1}^N \mu_i \mathbb{E}_{\tilde{\mathbb{P}}^{(i)}}[\ell(Z; \beta)].$$

By taking the supremum over all possible $\{\tilde{\mathbb{P}}^{(i)}\}_{i=1}^N$ such that $\mathcal{W}_{d,r}(\tilde{\mathbb{P}}^{(i)}, \chi_{\{Z^{(i)}\}}) \leq \delta$ for all $i = 1, \dots, N$, we have

$$\begin{aligned} \mathcal{S} &= \sup_{\mathbb{P}: \mathcal{W}_{d,r}(\mathbb{P}, \mathbb{P}_N) \leq \delta} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \\ &\geq \sum_{i=1}^N \mu_i \sup_{\mathbb{P} \in \mathcal{P}(\mathcal{Z})} \{ \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \mid \mathcal{W}_{d,r}(\mathbb{P}, \chi_{\{Z^{(i)}\}}) \leq \delta \} = \sum_{i=1}^N \mu_i \mathcal{L}_i = \mathcal{L}. \end{aligned}$$

Besides, since $\mathcal{W}_{d,r}(\chi_{\{Z^{(i)}\}}, \chi_{\{Z^{(i)}\}}) = 0 \leq \delta$ by Lemma 3.1, we have that

$$\mathcal{L}_i = \sup_{\mathbb{P} \in \mathcal{P}(\mathcal{Z})} \{ \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \mid \mathcal{W}_{d,r}(\mathbb{P}, \chi_{\{Z^{(i)}\}}) \leq \delta \} \geq \mathbb{E}_{\chi_{\{Z^{(i)}\}}}[\ell(Z; \beta)] = \ell(Z^{(i)}; \beta),$$

and hence

$$\mathcal{L} = \sum_{i=1}^N \mu_i \mathcal{L}_i \geq \sum_{i=1}^N \mu_i \ell(Z^{(i)}; \beta) = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)].$$

(b) Let $\epsilon > 0$ be an arbitrary scalar. Fix any $\tilde{\mathbb{P}} \in \mathcal{P}(\mathcal{Z})$ such that $\mathcal{W}_{d,r}(\tilde{\mathbb{P}}, \mathbb{P}_N) \leq \delta$. Then by the definition of $\mathcal{W}_{d,r}(\cdot, \cdot)$, there exists $\tilde{\pi} \in \Pi(\tilde{\mathbb{P}}, \mathbb{P}_N)$ such that

$$\left(\int_{\mathcal{Z} \times \mathcal{Z}} d^r(\tilde{z}, z) d\tilde{\pi}(\tilde{z}, z) \right)^{1/r} \leq \delta + \frac{\epsilon}{L_{\beta}^{\mathcal{Z}_N}}.$$

Besides, by the definition of the loss function $\ell(\cdot, \cdot)$, we have

$$\begin{aligned}
(\mathbb{E}_{\tilde{\mathbb{P}}}[\ell(Z; \beta)])^{\frac{1}{r}} &= \left(\int_{\mathcal{Z}} \psi_{\beta}^r(\tilde{z}) d\tilde{\mathbb{P}}(\tilde{z}) \right)^{\frac{1}{r}} = \left(\int_{\mathcal{Z} \times \mathcal{Z}} \psi_{\beta}^r(\tilde{z}) d\tilde{\pi}(\tilde{z}, z) \right)^{\frac{1}{r}} \\
&= \left(\int_{\mathcal{Z} \times \mathcal{Z}} (\psi_{\beta}(z) + \psi_{\beta}(\tilde{z}) - \psi_{\beta}(z))^r d\tilde{\pi}(\tilde{z}, z) \right)^{\frac{1}{r}} \\
&\leq^{(*)} \left(\int_{\mathcal{Z} \times \mathcal{Z}} \psi_{\beta}^r(z) d\tilde{\pi}(\tilde{z}, z) \right)^{\frac{1}{r}} + \left(\int_{\mathcal{Z} \times \mathcal{Z}} |\psi_{\beta}(\tilde{z}) - \psi_{\beta}(z)|^r d\tilde{\pi}(\tilde{z}, z) \right)^{\frac{1}{r}} \\
&= \left(\int_{\mathcal{Z}} \psi_{\beta}^r(z) d\mathbb{P}_N(z) \right)^{\frac{1}{r}} + \left(\int_{\mathcal{Z} \times \mathcal{Z}} |\psi_{\beta}(\tilde{z}) - \psi_{\beta}(z)|^r d\tilde{\pi}(\tilde{z}, z) \right)^{\frac{1}{r}} \\
&= (\mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)])^{\frac{1}{r}} + \left(\int_{\mathcal{Z} \times \mathcal{Z}} |\psi_{\beta}(\tilde{z}) - \psi_{\beta}(z)|^r d\tilde{\pi}(\tilde{z}, z) \right)^{\frac{1}{r}},
\end{aligned}$$

where the inequality $(*)$ holds naturally if $r = 1$, and follows from the Minkowski inequality if $r > 1$. Since ψ_{β} is $(L_{\beta}^{\mathcal{Z}_N}, d)$ -Lipschitz at \mathcal{Z}_N , it holds that

$$(\mathbb{E}_{\tilde{\mathbb{P}}}[\ell(Z; \beta)])^{\frac{1}{r}} \leq (\mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)])^{\frac{1}{r}} + L_{\beta}^{\mathcal{Z}_N} \left(\int_{\mathcal{Z} \times \mathcal{Z}} d^r(\tilde{z}, z) d\tilde{\pi}(\tilde{z}, z) \right)^{\frac{1}{r}} \leq (\mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)])^{\frac{1}{r}} + L_{\beta}^{\mathcal{Z}_N} \delta + \epsilon.$$

This means that for any $\epsilon > 0$, we have

$$\mathcal{S}^{\frac{1}{r}} = \sup_{\mathbb{P} \in \mathcal{W}_{d,r}(\mathbb{P}, \mathbb{P}_N) \leq \delta} (\mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)])^{\frac{1}{r}} \leq (\mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)])^{\frac{1}{r}} + L_{\beta}^{\mathcal{Z}_N} \delta + \epsilon.$$

By letting $\epsilon \rightarrow 0$, we get the desired inequality.

(c) Since ψ_{β} is $(0, d)$ -Lipschitz at \mathcal{Z}_N , by the convention that $0 \cdot \infty = 0$, one has $\psi_{\beta}(z') = \psi_{\beta}(z)$ for any $z' \in \mathcal{Z}, z \in \mathcal{Z}_N$. In particular, $\psi_{\beta}(\tilde{z}) = \psi_{\beta}(z)$ for any $\tilde{z}, z \in \mathcal{Z}_N$. Therefore, $\psi_{\beta}(\cdot)$ is a constant function on \mathcal{Z} , and so is $\ell(\cdot; \beta)$. Thus, we have

$$\mathcal{S} = \sup_{\mathbb{P} \in \mathcal{W}_{d,r}(\mathbb{P}, \mathbb{P}_N) \leq \delta} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)].$$

□

2.4 Lemma 3.1

Given any distribution $\mathbb{P} \in \mathcal{P}(\mathcal{Z})$ and any point $\hat{z} \in \mathcal{Z}$, for any scalar $r \geq 1$ and any extended nonnegative-valued measurable function $d : \mathcal{Z} \times \mathcal{Z} \rightarrow [0, \infty]$, we have

$$\mathcal{W}_{d,r}(\mathbb{P}, \chi_{\{\hat{z}\}}) = \left(\int_{\mathcal{Z}} d^r(z, \hat{z}) d\mathbb{P}(z) \right)^{1/r}.$$

Proof. For any $\pi \in \Pi(\mathbb{P}, \chi_{\{\hat{z}\}})$, we have $\pi(A \times \mathcal{Z}) = \mathbb{P}(A)$, $\pi(\mathcal{Z} \times B) = \chi_{\{\hat{z}\}}(B)$ for any measurable sets $A, B \subset \mathcal{Z}$. In particular, it holds that

$$\pi(\mathcal{Z} \times (\mathcal{Z} \setminus \{\hat{z}\})) = \chi_{\{\hat{z}\}}(\mathcal{Z} \setminus \{\hat{z}\}) = 0. \tag{11}$$

This implies that for any measurable set $A \subset \mathcal{Z}$, $\pi(A \times (\mathcal{Z} \setminus \{\hat{z}\})) = 0$ and hence

$$\begin{aligned}
\pi(A \times \{\hat{z}\}) &= \pi(A \times \mathcal{Z}) - \pi(A \times (\mathcal{Z} \setminus \{\hat{z}\})) \\
&= \pi(A \times \mathcal{Z}) = \mathbb{P}(A).
\end{aligned}$$

Moreover, (11) also implies that

$$\int_{\mathcal{Z} \times (\mathcal{Z} \setminus \{\hat{z}\})} d^r(z', z) d\pi(z', z) = 0.$$

Therefore, one has that

$$\begin{aligned} \int_{\mathcal{Z} \times \mathcal{Z}} d^r(z', z) d\pi(z', z) &= \int_{\mathcal{Z} \times \{\hat{z}\}} d^r(z', z) d\pi(z', z) \\ &= \int_{\mathcal{Z}} d^r(z', \hat{z}) d\mathbb{P}(z'). \end{aligned}$$

□

2.5 Definition 3.1

The function $d(\cdot, \cdot)$ defined on $\mathcal{Z} \times \mathcal{Z}$ is called a cost function if it is extended nonnegative-valued, measurable, and vanishes whenever two arguments are the same, that is, for any $z', z \in \mathcal{Z}$, $d(z', z) \in [0, \infty]$ and $d(z, z) = 0$.

2.6 Definition 3.2

(Weak Lipschitz property). Given a function $f : \mathcal{Z} \rightarrow \mathbb{R}$, a cost function $d(\cdot, \cdot)$ on $\mathcal{Z} \times \mathcal{Z}$ and a subset $\mathcal{S} \subset \mathcal{Z}$, f is called $(L_f^{\mathcal{S}}, d)$ -Lipschitz at \mathcal{S} if for any $z \in \mathcal{S}$, $z' \in \mathcal{Z}$, one has

$$|f(z') - f(z)| \leq L_f^{\mathcal{S}} d(z', z),$$

where $L_f^{\mathcal{S}} \in [0, \infty)$ is a constant depending on f and \mathcal{S} .

3 Section 4.3

Apply our results to the cases where the cost function $d(\cdot, \cdot)$ is nonconvex, not positive definite, and the weak Lipschitz constant is not in the popular form of the norm of the regression vector β .

3.1 Example 4.4

(Ridge linear ordinary regression). For any $z' = (x', y'), z = (x, y) \in \mathbb{R}^n \times \mathbb{R}$, define $d(z', z) = \|z' - z\|_2 \|z' + z\|_2$. Given any $\delta > 0$, $\beta \in \mathbb{R}^n$ and any empirical distribution \mathbb{P}_N on $\mathbb{R}^n \times \mathbb{R}$, for $\mathfrak{M}_1 := \{\mathbb{P} \in \mathcal{P}(\mathcal{Z}) \mid \mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_N) \leq \delta\}$, we have

$$\sup_{\mathbb{P} \in \mathfrak{M}_1} \mathbb{E}_{\mathbb{P}}[(Y + \langle \beta, X \rangle)^2] = \mathbb{E}_{\mathbb{P}_N}[(Y + \langle \beta, X \rangle)^2] + \|\beta\|_2^2 \delta + \delta.$$

Proof. We first show that $\psi_{\beta}(z) := \langle [\beta; 1], z \rangle^2$ for any $z \in \mathbb{R}^{n+1}$ satisfies Assumption (A1) with $L_{\beta} := \|\beta\|_2^2 + 1$. For any $z', z \in \mathbb{R}^{n+1}$, we have

$$\begin{aligned} |\psi_{\beta}(z') - \psi_{\beta}(z)| &= |\langle [\beta; 1], z' \rangle^2 - \langle [\beta; 1], z \rangle^2| \\ &= |\langle [\beta; 1], z' - z \rangle \langle [\beta; 1], z' + z \rangle| \\ &\leq \|[\beta; 1]\|_2 \|z' - z\|_2 \cdot \|[\beta; 1]\|_2 \|z' + z\|_2 \\ &= (\|\beta\|_2^2 + 1) d(z', z). \end{aligned}$$

Hence, ψ_{β} is (L_{β}, d) -Lipschitz on \mathbb{R}^{n+1} .

Next, we show that ψ_{β} satisfies Assumption (A2). For any $z \in \mathbb{R}^{n+1}$ and $k > 0$, let $\tilde{z} := z + k\Delta$ with

$$\Delta := \frac{[\beta; 1]}{\|[\beta; 1]\|_2},$$

then $\|\tilde{z} - z\|_2 = \|k\Delta\|_2 = k$, $\|\tilde{z} + z\|_2 = \|2z + k\Delta\|_2$ and

$$d(\tilde{z}, z) = \|\tilde{z} - z\|_2 \|\tilde{z} + z\|_2 = k \|2z + k\Delta\|_2 \geq k |k - 2\|z\|_2| \rightarrow \infty \text{ as } k \rightarrow \infty.$$

On the other hand, we have

$$\frac{|\langle \Delta, \tilde{z} + z \rangle|}{\|\tilde{z} + z\|_2} \leq \|\Delta\|_2 = 1,$$

and

$$\frac{\langle \Delta, \tilde{z} + z \rangle}{\|\tilde{z} + z\|_2} = \frac{\langle \Delta, 2z + k\Delta \rangle}{\|2z + k\Delta\|_2} = \frac{\sum_{i=1}^{n+1} \Delta_i (2z_i/k + \Delta_i)}{\sqrt{\sum_{i=1}^{n+1} (2z_i/k + \Delta_i)^2}} \rightarrow 1, \text{ as } k \rightarrow \infty.$$

Thus, for the given δ and any $0 < \epsilon < L_\beta$, there exists a positive integer k_ϵ such that for

$$\tilde{z}_\epsilon = z + k_\epsilon \Delta,$$

one has

$$\begin{aligned} d(\tilde{z}_\epsilon, z) &= k_\epsilon \|\tilde{z}_\epsilon + z\|_2 \geq \delta, \\ \frac{\langle \Delta, \tilde{z}_\epsilon + z \rangle}{\|\tilde{z}_\epsilon + z\|_2} &\geq 1 - \frac{\epsilon}{\|[\beta; 1]\|_2^2}. \end{aligned}$$

This implies that

$$\begin{aligned} \psi_\beta(\tilde{z}_\epsilon) - \psi_\beta(z) &= \langle [\beta; 1], \tilde{z}_\epsilon - z \rangle \cdot \langle [\beta; 1], \tilde{z}_\epsilon + z \rangle \\ &= \|[\beta; 1]\|_2^2 \langle \Delta, k_\epsilon \Delta \rangle \langle \Delta, \tilde{z}_\epsilon + z \rangle \\ &\geq \|[\beta; 1]\|_2^2 k_\epsilon \left(1 - \frac{\epsilon}{\|[\beta; 1]\|_2^2}\right) \|\tilde{z}_\epsilon + z\|_2 \\ &= (\|[\beta; 1]\|_2^2 - \epsilon) k_\epsilon \|\tilde{z}_\epsilon + z\|_2 = (L_\beta - \epsilon) d(\tilde{z}_\epsilon, z). \end{aligned}$$

Therefore, it satisfies Assumption (A2). By Theorem 3.2. \square

4 Extension to DNN/Transformer

The main idea is that if a DNN or a Transformer's loss function is Lipschitz continuous (even just locally near the training data), WDRO theory provides upper/lower bound formulas for the worst-case loss, which is crucial for extending robust guarantees to high-dimensional models.

4.1 Literature Review

The notations used in the reviewed literature have been adapted to align with the notations in [CLT24].

4.1.1 [OSHL19]

Problem Statement Learn a language model \mathbb{P}_β based on sentences sampled from the training distribution $Z \sim \mathbb{P}_N$, such that \mathbb{P}_β performs well on unknown test distributions \mathbb{P}_{test} .

Language models \mathbb{P}_β are generally trained to approximate \mathbb{P}_N by minimizing the KL divergence $\text{KL}(\mathbb{P}_N \parallel \mathbb{P}_\beta)$ via maximum likelihood estimation (MLE),

$$\inf_{\beta} \mathbb{E}[-\log \mathbb{P}_\beta(Z)]$$

Applying DRO, we optimize a model for loss ℓ and an ambiguity set of potential test distributions \mathfrak{M} by minimizing the risk under the worst-case distribution in \mathfrak{M} ,

$$\sup_{\mathbb{P} \in \mathfrak{M}} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)]$$

The above worst-case objective does not depend on the unknown quantity \mathbb{P}_{test} . The objective also upper bounds the test risk for all $\mathbb{P}_{\text{test}} \in \mathfrak{M}$ as

$$\mathbb{E}_{\mathbb{P}_{\text{test}}}[\ell(Z; \beta)] \leq \sup_{\mathbb{P} \in \mathfrak{M}} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)],$$

so optimizing the above objective gives guarantees on test performance whenever $\mathbb{P}_{\text{test}} \in \mathfrak{M}$.

4.1.2 [SV19]

Background and Notations A function f is said to be Lipschitz continuous if there exists a constant $L > 0$ such that

$$\|f(x) - f(y)\|_2 \leq L\|x - y\|_2, \quad \forall x, y \in \mathbb{R}^n.$$

The smallest such L is called the Lipschitz constant of f , denoted $L(f)$. When f is differentiable, we have $L(f) = \sup_x \|D_x f\|_2$.

$f \circ g$ Composition of functions $f : \mathbb{R}^k \rightarrow \mathbb{R}^m$ and $g : \mathbb{R}^n \rightarrow \mathbb{R}^k$

$D_x f \in \mathbb{R}^{m \times n}$ The Jacobian matrix at $x \in \mathbb{R}^n$, for any differentiable function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$

$\nabla f(x) = (D_x f)^\top$ The gradient in the scalar case ($m = 1$)

$\text{diag}_{n,m}(x) \in \mathbb{R}^{n \times m}$ The rectangular diagonal matrix with entries of $x \in \mathbb{R}^{\min(n,m)}$ on the diagonal and zeros elsewhere (write $\text{diag}(x)$ when unambiguous)

Multi-Layer Perceptron (MLP) A K -layer MLP $f_{\text{MLP}} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is a function of the form:

$$f_{\text{MLP}}(x) = T_K \circ \rho_{K-1} \circ \cdots \circ \rho_1 \circ T_1(x),$$

where $T_k(x) = M_k x + b_k$ is an affine function and $\rho_k : x \mapsto (g_k(x_i))_{i \in \llbracket 1, n_k \rrbracket}$ is a non-linear activation function.

Computing the exact Lipschitz constant of a 2-layer MLP with ReLU activations is NP-hard.

Sequential Neural Networks and Lipschitz Bounds For an MLP, the Lipschitz constant has the following form:

$$L(f_{\text{MLP}}) = \sup_{x \in \mathbb{R}^n} \|M_K \text{diag}(g'_{K-1}(\theta_{K-1})) \cdots \text{diag}(g'_1(\theta_1)) M_1\|_2,$$

where $\theta_k = T_k \circ \rho_{k-1} \circ \cdots \circ \rho_1 \circ T_1(x)$ is the output after k layers.

The SeqLip algorithm approximates this by maximizing over all possible diagonal activations $\sigma_i \in [0, 1]^{n_i}$ and decomposing the expression via SVD. The resulting upper bound is:

$$\hat{L}_{\text{SL}} = \prod_{i=1}^{K-1} \max_{\sigma_i \in [0,1]^{n_i}} \left\| \tilde{\Sigma}_{i+1} V_{i+1}^\top \text{diag}(\sigma_i) U_i \tilde{\Sigma}_i \right\|_2,$$

where $\tilde{\Sigma}_i$ adjusts for boundary layers and U_i, V_i are singular vector matrices from M_i .

4.1.3 [BKM19]

The Robust Wasserstein Profile Function Given i.i.d. samples $\{\mathcal{W}_1, \dots, \mathcal{W}_n\}$ and an estimating equation:

$$\mathbb{E}[h(W, \theta_*)] = 0,$$

the RWP function is defined as:

$$R_n(\theta) := \inf \{D_c(\mathbb{P}, \mathbb{P}_n) : \mathbb{E}_{\mathbb{P}}[h(W, \theta)] = 0\},$$

where D_c is a transport cost (typically Wasserstein), and $c(u, w) = \|w - u\|_q^\rho$.

Asymptotic Behavior Under regularity assumptions (A1-A4), the scaled RWP function converges in distribution:

$$n^{\rho/2} R_n(\theta_*) \xrightarrow{D} \bar{R}(\rho),$$

where, for $\rho > 1$,

$$\bar{R}(\rho) := \max_{\zeta \in \mathbb{R}^r} \left\{ \rho \zeta^\top H - (\rho - 1) \mathbb{E} \left\| \zeta^\top D_w h(W, \theta_*) \right\|_p^{\rho/(\rho-1)} \right\},$$

and $H \sim \mathcal{N}(0, \text{Cov}[h(W, \theta_*)])$.

4.1.4 [SNVD20]

Introduction The key objective is to minimize the worst-case expected loss over a set of distributions \mathfrak{M} around the empirical distribution \mathbb{P}_N :

$$\min_{\beta} \sup_{\mathbb{P} \in \mathfrak{M}} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)]$$

To ensure tractability, consider a Lagrangian relaxation with Wasserstein cost $\mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_N) \leq \delta$ and introduce a penalty parameter $\gamma \geq 0$:

$$\begin{aligned} \min_{\beta} F(\beta) &= \min_{\beta} \sup_{\mathbb{P}} \{ \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] - \gamma \mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_N) \} \\ &= \min_{\beta} \mathbb{E}_{\mathbb{P}_N}[\phi_{\gamma}(Z; \beta)] \end{aligned}$$

where $\phi_{\gamma}(Z; \beta)$ is the robust surrogate loss defined as:

$$\phi_{\gamma}(z_0; \beta) := \sup_{z \in \mathcal{Z}} \{ \ell(z; \beta) - \gamma d(z_0, z) \}$$

Certified Robust Test Loss Bound Let \mathbb{P}_{test} denote the empirical distribution on a test set $\{Z_{\text{test}}^i\}_{i=1}^{N_{\text{test}}}$. The robust test-time loss under worst-case perturbations within Wasserstein radius δ satisfies:

$$\frac{1}{N_{\text{test}}} \sum_{i=1}^{N_{\text{test}}} \sup_{z: d(z, Z_{\text{test}}^i) \leq \delta} \{ \ell(z; \beta) \} \leq \sup_{\mathbb{P}: \mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_{\text{test}}) \leq \delta} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \leq \gamma \delta + \mathbb{E}_{\mathbb{P}_{\text{test}}}[\phi_{\gamma}(Z; \beta)]$$

This bound holds for all $\gamma, \delta \geq 0$. When γ is sufficiently large (so that the dual formulation is tight for small δ), this provides an efficient and certifiable upper bound on the worst-case test loss under Wasserstein perturbations.

4.1.5 [KKWP20]

Gradient-Based Approximation of DRO Objective Approximate the Wasserstein DRO worst-case risk by penalizing the expected norm of the gradient:

$$\sup_{\mathbb{P}: \mathcal{W}_{d,r}(\mathbb{P}, \mathbb{P}_N)} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)] \approx \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + \alpha_n \|\nabla_z \ell(Z; \beta)\|_{\mathbb{P}_N, r^*},$$

where the norm $\|\cdot\|_{\mathbb{P}_N, r^*}$ is defined as:

$$\|g\|_{\mathbb{P}_N, r^*} := \left(\int_{\mathcal{Z}} \|g(z)\|_*^{r^*} d\mathbb{P}_N(z) \right)^{1/r^*},$$

with $r^* := \frac{r}{r-1}$ denoting the Hölder conjugate of r . This surrogate loss avoids computing Lipschitz constants explicitly.

Theoretical Risk Consistency Assume ψ_{β} is differentiable and $\nabla_z \psi_{\beta} : \mathcal{Z} \rightarrow \mathbb{R}^d$ is (C_H, k) -Hölder continuous, i.e.,

$$\|\nabla_z \psi_{\beta}(z) - \nabla_z \psi_{\beta}(\tilde{z})\|_* \leq C_H \|z - \tilde{z}\|^k, \quad \forall z, \tilde{z} \in \mathcal{Z}.$$

Under smoothness assumptions (i.e., differentiability and Hölder continuity of gradients), the gradient-norm surrogate objective yields consistent minimizers, and the resulting estimator converges to the minimizer of the true worst-case risk.

4.1.6 [GFPC20]

Layerwise Composition of Lipschitz Constants A function $f : X \rightarrow Y$ is k -Lipschitz with respect to metrics D_X and D_Y if:

$$D_Y(f(\vec{x}_1), f(\vec{x}_2)) \leq k D_X(\vec{x}_1, \vec{x}_2), \quad \forall \vec{x}_1, \vec{x}_2 \in X.$$

For feedforward neural networks expressed as compositions of layers $f(\vec{x}) = (\phi_l \circ \dots \circ \phi_1)(\vec{x})$, the Lipschitz constant satisfies:

$$L(f) \leq \prod_{i=1}^l L(\phi_i).$$

4.1.7 [GCK20]

Problem Formulation Given a family \mathcal{F} of loss functions, a nominal distribution $\mathbb{Q} \in \mathcal{P}_r(\mathcal{Z})$, and a radius $\delta \geq 0$, the corresponding Wasserstein DRO problem is:

$$\min_{f \in \mathcal{F}} \sup_{\mathbb{P} \in \mathcal{P}(\mathcal{Z})} \{ \mathbb{E}_{Z \sim \mathbb{P}}[f(Z)] : \mathcal{W}_{d,r}(\mathbb{P}, \mathbb{Q}) \leq \delta \}.$$

When $\mathbb{Q} = \mathbb{P}_N$ is the empirical distribution, the dual formulation of the inner supremum is:

$$\begin{cases} \min_{\lambda \geq 0} \{ \lambda \delta^r + \mathbb{E}_{Z \sim \mathbb{Q}} [\sup_{\tilde{z} \in \mathcal{Z}} \{ f(\tilde{z}) - \lambda d(\tilde{z}, Z)^r \}] \}, & r \in (1, \infty), \\ \mathbb{E}_{Z \sim \mathbb{Q}} [\sup_{\tilde{z} \in \mathcal{Z}} \{ f(\tilde{z}) : d(\tilde{z}, Z) \leq \delta \}], & r = \infty. \end{cases}$$

The Wasserstein regularizer is defined as:

$$\mathcal{R}_{\mathbb{Q},r}(\delta; f) := \sup_{\mathbb{P} \in \mathcal{P}(\mathcal{Z})} \{ \mathbb{E}_{\mathbb{P}}[f(Z)] : \mathcal{W}_{d,r}(\mathbb{P}, \mathbb{Q}) \leq \delta \} - \mathbb{E}_{\mathbb{Q}}[f(Z)].$$

Theorem 1 (r -Wasserstein DRO)

(I) Let $r = \infty$. Assume Assumptions 1 and 2 hold. Then there exists $\bar{\delta} > 0$ such that for all $\delta < \bar{\delta}$ and $f \in \mathcal{F}$,

$$|\mathcal{R}_{\mathbb{P}_N, \infty}(\delta; f) - \delta| \|\nabla f\|_* \|_{\mathbb{P}_N, 1}| \leq \delta^2 \|H\|_{\mathbb{P}_N, 1} + M \mathbb{E}_{\mathbb{P}_N}[(\delta - d(z, \mathcal{D}_f))_+].$$

(II) Let $r \in (1, \infty)$, $\delta_N = \delta_0 / \sqrt{N}$, and assume Assumptions 1, 2, and 4 hold. Then there exist $\bar{\delta}, C_1, C_2 > 0$ such that for all $\delta_0 < \bar{\delta}$ and $f \in \mathcal{F}$,

$$|\mathcal{R}_{\mathbb{P}_N, r}(\delta_N; f) - \delta_N| \|\nabla f\|_* \|_{\mathbb{P}_N, r^*}| \leq \delta_N^{2 \wedge r} \left(\|H\|_{\mathbb{P}_N, \frac{r}{r-2}} \mathbf{1}_{\{r > 2\}} + C_1 \right) + M \mathbb{E}_{\mathbb{P}_N}[(C_2 \delta_N - d(z, \mathcal{D}_f))_+].$$

(III) Assume Assumption 3 holds. Let $t > 0$. Then there exists $\bar{\delta}, C > 0$ such that for all $\delta < \bar{\delta}$, with probability at least $1 - e^{-t}$, for every $f \in \mathcal{F}$,

$$\mathbb{E}_{\mathbb{P}_N}[(\delta - d(z, \mathcal{D}_f))_+] \leq C \delta^2 + 2 \delta \mathbb{E}_{\otimes}[\mathfrak{R}_N(\mathcal{I}_{\delta})] + \delta \sqrt{\frac{t}{2N}},$$

and

$$\mathbb{E}_{\mathbb{P}_N}[(\delta - d(z, \mathcal{D}_f))_+] \leq 2C \delta^2 + \frac{48\delta}{\sqrt{N}} \int_0^1 \sqrt{\log \mathcal{N}(\epsilon \delta; \mathcal{E}, \|\cdot\|_{\mathbb{P}_N, 2})} d\epsilon + \delta \sqrt{\frac{t}{2N}}.$$

Under the condition $\delta_N = O(1/\sqrt{N})$ and $\mathbb{E}_{\mathbb{P}_N}[(\delta_N - d(z, \mathcal{D}_f))_+] = O(1/N)$, it follows that:

$$\min_{f \in \mathcal{F}} \sup_{\mathbb{P} : \mathcal{W}_{d,r}(\mathbb{P}, \mathbb{P}_N) \leq \delta_N} \mathbb{E}_{\mathbb{P}}[f(Z)] = \min_{f \in \mathcal{F}} \{ \mathbb{E}_{\mathbb{P}_N}[f(Z)] + \delta_N \mathcal{V}_{\mathbb{P}_N, r^*}(f) \} + O_p(1/N).$$

Neural Network Example Let $\theta = (W_1, W_2)$, and define a two-layer neural network with leaky ReLU activation and softmax cross-entropy loss:

$$f_\theta(z) := \ell(W_2 \sigma(W_1 x), y), \quad z = (x, y) \in \mathcal{Z},$$

where ℓ is the cross-entropy loss and $\sigma(z) = z \cdot \mathbf{1}\{z \geq 0\} + az \cdot \mathbf{1}\{z < 0\}$. Assume $\|W_2\|_{\text{op}} \cdot \|W_1\|_{\text{op}} \leq 1$, $\mathcal{X} \subset \mathbb{R}^d$ compact, and that $\mathbb{P}_{\text{true}}^x$ has continuous density. Then for differentiable points:

$$\|\nabla f_\theta(z)\|_2 = \|\nabla \ell(W_2 \sigma(W_1 x), y) \cdot W_2 \cdot \sigma'(W_1 x) \cdot W_1\|_2.$$

Using Theorem 1 and Lemma EC.21, there exists $\bar{\delta}, C > 0$ such that for all $\delta < \bar{\delta}$, with probability at least $1 - e^{-t}$, for all $\theta \in \Theta$,

$$\left| \mathcal{R}_{\mathbb{P}_N, 2}(\delta_N; f_\theta) - \delta_N \|\nabla f_\theta\|_* \|_{\mathbb{P}_N, 2} \right| \leq C_1 \delta_N^2 + C_2 d_1 \sqrt{\frac{d}{N}} + \delta_N \sqrt{\frac{t}{2N}}.$$

4.1.8 [KPM21]

Theorem 3.1 The dot-product multi-head attention (DP-MHA) mapping is not Lipschitz with respect to any p -norm $\|\cdot\|_p$ for $p \in [1, \infty]$.

Bounding the Lipschitz Constant of L2 Attention To address this limitation, analyze an alternative attention mechanism based on L2 similarity. For a Transformer block with:

- N : input sequence length,
- D : embedding dimension,
- H : number of attention heads,
- $W^{Q,h}, W^{K,h}, W^{V,h}$: query, key, value projection matrices for head h ,
- W^O : output projection matrix,

Derive the following upper bound for the Lipschitz constant of the overall attention mapping F under the ℓ_2 -norm:

$$\text{Lip}_2(F) \leq \frac{\sqrt{N}}{\sqrt{D/H}} (4\phi^{-1}(N-1) + 1) \left(\sqrt{\sum_{h=1}^H \|W^{Q,h}\|_2^2 \|W^{V,h}\|_2^2} \right) \|W^O\|_2$$

They also provide a bound under the ℓ_∞ -norm:

$$\text{Lip}_\infty(F) \leq (4\phi^{-1}(N-1) + 1) \cdot \max_h (\|W^{Q,h}\|_\infty \|W^{V,h}\|_\infty) \cdot \|W^O\|_\infty$$

where $\phi(x) = x \exp(x+1)$ and ϕ^{-1} is its inverse (which grows sub-logarithmically as $\mathcal{O}(\log N - \log \log N)$).

Specifically, for large N , these bounds simplify to:

$$\text{Lip}_\infty(F) = \mathcal{O}(\log N), \quad \text{Lip}_2(F) = \mathcal{O}(\sqrt{N} \log N).$$

4.1.9 [ZYK+23]

Wasserstein DRO for CNN Classification. Propose a DRO framework for improving the generalization of CNNs on classification tasks under distribution shift. The goal is to minimize the worst-case expected loss over a Wasserstein ambiguity set $\mathfrak{M} := \{\mathbb{P} \in \mathcal{P}(\mathcal{Z}) \mid \mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_N) \leq \delta\}$:

$$\sup_{\mathbb{P} \in \mathfrak{M}} \mathbb{E}_{\mathbb{P}}[\ell(Z; \beta)],$$

where $\ell : \mathcal{Z} \times \mathcal{B} \rightarrow \mathbb{R}$ is the loss function and \mathbb{P}_N is the empirical distribution.

Since directly solving the min-max problem is intractable, reformulate the objective into a regularized empirical risk minimization problem. Specifically, when the constraint

$$\left(\sum_{m=1}^M \frac{\|W_m\|}{M} \right)^M \leq \left(\frac{\theta}{M} \right)^M, \quad \text{for } \theta = \sum_{m=1}^M \|W_m^*\|$$

is satisfied by an optimal hypothesis h^* , there exists a Lagrange multiplier $\tilde{\lambda} > 0$ such that h^* also solves the penalized problem:

$$\inf_{h \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^N \ell(h(x^i), y^i) + \tilde{\lambda} \sum_{m=1}^M \|W_m\|.$$

In the experimental setup, the CNN feature extractor is pretrained and fixed, and DRO is applied only to the final classification layer (i.e., $M = 1$), making \mathcal{H} a space of linear classifiers over frozen features. The regularization parameter λ is treated as a hyperparameter and selected empirically via validation.

4.1.10 [LGL⁺23]

Wasserstein Penalty for Fair Representation Learning. Propose a fairness-aware classification method that promotes statistical independence between learned feature representations and sensitive attributes using a Wasserstein penalty. Rather than formulating distributional robustness via ambiguity sets, incorporate the 1-Wasserstein distance as a regularization term into the objective:

$$\min_{\theta} \mathcal{L}_{\text{cls}}(f_{\theta}(x), y) + \lambda \cdot \mathcal{W}(P_{f(x)}, P_{f(x)|A}),$$

where f_{θ} is the feature extractor, A denotes the sensitive attribute, and \mathcal{W} is estimated using the Kantorovich–Rubinstein dual formulation.

4.1.11 [BHJO25]

First-Order W-DRO Fine-Tuning for Deep Neural Networks. Extend adversarial training to distributional threat models using Wasserstein DRO (W-DRO). Building on the sensitivity analysis of the inner adversary, derive a first-order approximation of the W-DRO objective and propose a two-step training method that can be applied to pretrained networks. The formulation,

$$\inf_{\theta} \left\{ \mathbb{E}_P[\mathcal{L}(f_{\theta}(x), y)] + \beta \sup_{\pi \in \Pi_2(P, \delta)} \mathbb{E}_{\pi}[\tilde{\mathcal{L}}(f_{\theta}(x), f_{\theta}(x'))] \right\},$$

captures both clean accuracy and distributional robustness via a Wasserstein ball.

4.2 Analysis

This section extends [CLT24]’s analysis to deep neural networks (DNNs), residual networks (ResNets), and transformer architectures.

Given any $\delta > 0$ and any empirical distribution \mathbb{P}_N on \mathcal{Z} , for $\mathfrak{M}_1 := \{\mathbb{P} \in \mathcal{P}(\mathcal{Z}) \mid \mathcal{W}_{d,1}(\mathbb{P}, \mathbb{P}_N) \leq \delta\}$, our target is as follows:

$$\inf_{\beta \in \mathcal{B}} \left\{ \sup_{\mathbb{P} \in \mathfrak{M}_1} \mathbb{E}_{\mathbb{P}}[\psi_{\beta}(Z)] \right\}.$$

Following [ZYK⁺23], the sub-problem in the inner part of the above target can be rewritten in the following form:

$$\begin{aligned} & \sup_{\pi \in \Pi(\mathbb{P}, \mathbb{P}_N)} \int_{\mathcal{Z} \times \mathcal{Z}} \psi_{\beta}(z') d\pi(z', z) \\ & \text{s.t.} \quad \int_{\mathcal{Z} \times \mathcal{Z}} d(z', z) d\pi(z', z) \leq \delta. \end{aligned}$$

Suppose $\mathcal{Z}_N := \{Z^{(1)}, \dots, Z^{(N)}\} \subset \mathcal{Z}$ is a given dataset and we define $\mathbb{P}_N := \sum_{i=1}^N \mu_i \mathbf{X}_{\{Z^{(i)}\}} \in \mathcal{P}(\mathcal{Z})$ as the corresponding empirical distribution then we have:

$$\mathbb{P}(z') = \pi(z', \mathcal{Z}_N) = \sum_{i=1}^N \pi(z', z = Z^{(i)}) = \sum_{i=1}^N \pi(z'|z = Z^{(i)}) \mathbb{P}_N(Z^{(i)}) = \sum_{i=1}^N \mathbb{P}^i(z') \mu_i$$

$$\pi(z', z) = \pi(z', z = Z^{(i)}) = \pi(z'|z = Z^{(i)}) \mathbb{P}_N(Z^{(i)}) = \mathbb{P}^i(z') \mu_i ,$$

where $\mathbb{P}^i(z') = \pi(z'|z = Z^{(i)})$. Using these two equations, we can rewrite the sub-problem as:

$$\begin{aligned} \sup_{\{\mathbb{P}^i\}_{i=1}^N} \quad & \sum_{i=1}^N \mu_i \int_{\mathcal{Z}} \psi_{\beta}(z') d\mathbb{P}^i(z') \\ \text{s.t.} \quad & \sum_{i=1}^N \mu_i \int_{\mathcal{Z}} d(z', Z^{(i)}) d\mathbb{P}^i(z') \leq \delta \\ & \int_{\mathcal{Z}} d\mathbb{P}^i(z') = 1, \forall i \in [N] . \end{aligned}$$

Considering the Lagrangian of the above, we have:

$$\begin{aligned} \mathcal{L}(\{P^i\}, \lambda, \{\eta_i\}) &= \sum_{i=1}^N \mu_i \int_{\mathcal{Z}} \psi_{\beta}(z') d\mathbb{P}^i(z') + \lambda \left[\delta - \sum_{i=1}^N \mu_i \int_{\mathcal{Z}} d(z', Z^{(i)}) d\mathbb{P}^i(z') \right] \\ &\quad + \sum_{i=1}^N \eta_i \left[1 - \int_{\mathcal{Z}} d\mathbb{P}^i(z') \right] \\ &= \lambda \delta + \sum_{i=1}^N \left\{ \eta_i + \int \left[\mu_i \psi_{\beta}(z') - \lambda \mu_i d(z', Z^{(i)}) - \eta_i \right] d\mathbb{P}^i(z') \right\} , \end{aligned}$$

where $\lambda \geq 0$ and η_i are dual variables of the constraints. For a fixed i define:

$$f_i^{\lambda, \eta_i}(z') := \mu_i \psi_{\beta}(z') - \lambda \mu_i d(z', Z^{(i)}) - \eta_i .$$

Because \mathbb{P}^i can put all its mass wherever f_i^{λ, η_i} is largest,

$$\sup_{\{\mathbb{P}^i\}_{i=1}^N} \int f_i^{\lambda, \eta_i}(z') d\mathbb{P}^i = \sup_{z' \in \mathcal{Z}} f_i^{\lambda, \eta_i}(z') .$$

Hence

$$\begin{aligned} \sup_{\{\mathbb{P}^i\}_{i=1}^N} \mathcal{L}(\{P^i\}, \lambda, \{\eta_i\}) &= \lambda \delta + \sum_{i=1}^N \left[\eta_i + \sup_{z' \in \mathcal{Z}} \left(\mu_i \psi_{\beta}(z') - \lambda \mu_i d(z', Z^{(i)}) - \eta_i \right) \right] \\ &= \lambda \delta + \sum_{i=1}^N \mu_i \sup_{z' \in \mathcal{Z}} \left[\psi_{\beta}(z') - \lambda d(z', Z^{(i)}) \right] . \end{aligned}$$

The dual problem is

$$\inf_{\lambda \geq 0} \left\{ \lambda \delta + \sum_{i=1}^N \mu_i \sup_{z' \in \mathcal{Z}} \left[\psi_{\beta}(z') - \lambda d(z', Z^{(i)}) \right] \right\} . \quad (\text{D})$$

Suppose ψ_{β} is $(L_{\beta}^{\mathcal{Z}_N}, d)$ -Lipschitz at \mathcal{Z}_N with $L_{\beta}^{\mathcal{Z}_N} \in (0, \infty)$ we have:

$$\psi_{\beta}(z') - \psi_{\beta}(z) \leq |\psi_{\beta}(z') - \psi_{\beta}(z)| \leq L_{\beta}^{\mathcal{Z}_N} d(z', z) \quad \forall z \in \mathcal{Z}_N, z' \in \mathcal{Z} .$$

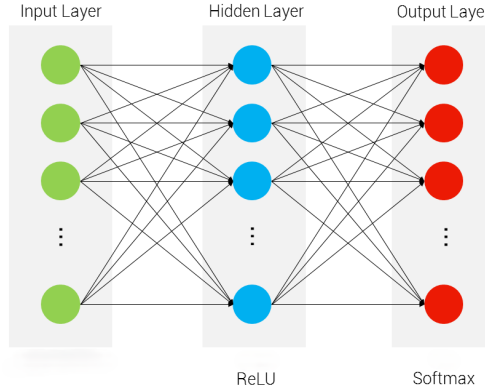
Using this assumption, we can approximate an upper bound for (D) as follows:

$$\begin{aligned}
(\text{D}) &\leq \inf_{\lambda \geq 0} \left\{ \lambda \delta + \sum_{i=1}^N \mu_i \sup_{z' \in \mathcal{Z}} \left[\psi_\beta(Z^{(i)}) + L_\beta^{\mathcal{Z}_N} d(z', Z^{(i)}) - \lambda d(z', Z^{(i)}) \right] \right\} \\
&= \inf_{\lambda \geq 0} \left\{ \lambda \delta + \sum_{i=1}^N \mu_i \sup_{z' \in \mathcal{Z}} \left[\psi_\beta(Z^{(i)}) + (L_\beta^{\mathcal{Z}_N} - \lambda) d(z', Z^{(i)}) \right] \right\} \\
&= L_\beta^{\mathcal{Z}_N} \delta + \sum_{i=1}^N \mu_i \psi_\beta(Z^{(i)}) = \mathbb{E}_{\mathbb{P}_N}[\ell(Z; \beta)] + L_\beta^{\mathcal{Z}_N} \delta .
\end{aligned}$$

4.2.1 DNN

Toy Case Following the example given in [GCK20], we consider a two-layer network in the context of a K -class classification problem with ReLU activation function σ :

$$\sigma(z) = \begin{cases} z, & z \geq 0 \\ 0, & z < 0 \end{cases}$$



Let $z' = (x', y')$, $z = (x, y) \in \mathcal{Z} = \mathcal{X} \times \mathcal{Y}$, where $\mathcal{X} \subset \mathbb{R}^n$ and \mathcal{Y} is a subset of the probability simplex in \mathbb{R}^K . Let $\beta = (W_1, W_2)$ where $W_1 \in \mathbb{R}^{n_1 \times n}$ and $W_2 \in \mathbb{R}^{K \times n_1}$ are weight matrices. Define the cost function d as:

$$d(z', z) = \|x' - x\|_2 + \kappa \mathbf{1}_{\{y' \neq y\}},$$

where κ is a positive constant, and define a two-layer ReLU network with cross-entropy loss as:

$$\psi_\beta(z) := \ell(W_2 \sigma(W_1 x), y) = - \sum_{i=1}^K y_i \log \left(\frac{e^{W_{2,i} \sigma(W_1 x)}}{\sum_{k=1}^K e^{W_{2,k} \sigma(W_1 x)}} \right),$$

where $W_{2,i}$ is the i -th row of W_2 . We shall prove that ψ_β satisfies assumption (C1) and (C2).

Rewrite ψ_β as follows:

$$\psi_\beta(z) = \log \left(\sum_{k=1}^K e^{W_{2,k} \sigma(W_1 x)} \right) - \sum_{i=1}^K y_i W_{2,i} \sigma(W_1 x) .$$

Using the gradient of ψ_β with respect to $\theta(x) := W_2 \sigma(W_1 x) \in \mathbb{R}^K$ and applying the mean-value theorem, we have:

$$\psi_\beta(z') - \psi_\beta(z) = \langle \nabla_\theta \ell(\theta + \tau(\theta' - \theta), y), \theta' - \theta \rangle, \quad \text{for some } \tau \in (0, 1).$$

Using the Cauchy-Schwarz inequality, we have:

$$|\psi_\beta(z') - \psi_\beta(z)| \leq \|\nabla_\theta \ell(\theta + \tau(\theta' - \theta), y)\|_2 \|\theta' - \theta\|_2 \leq \sup_\theta \{\|\nabla_\theta \ell(\theta, y)\|_2\} \|\theta' - \theta\|_2 .$$

We have:

$$\begin{aligned} \|\nabla_\theta \ell(\theta, y)\|_2 &= \|\text{softmax}(\theta) - y\|_2 \\ &= \sqrt{\|\text{softmax}(\theta)\|_2^2 + \|y\|_2^2 - 2\text{softmax}(\theta)^\top y} \\ &\leq \sqrt{1 + 1 - 0} = \sqrt{2} , \end{aligned}$$

where the inequality holds because both $\text{softmax}(\theta)$ and y are probability vectors. Hence

$$|\psi_\beta(z') - \psi_\beta(z)| \leq \sqrt{2} \|\theta' - \theta\|_2 = \sqrt{2} \|W_2 \sigma(W_1 x') - W_2 \sigma(W_1 x)\|_2 .$$

For $Z^{(i)} = (x^{(i)}, y^{(i)}) \in \mathcal{Z}_N$, we introduce assumption

(D1): no training point lies on a ReLU facet,

and let

$$D^{(i)} = \text{diag} \left(\mathbf{1}_{\{(W_1 x^{(i)})_j > 0\}} \right) \in \mathbb{R}^{n_1 \times n_1} ,$$

then for $z \in \{Z^{(i)}\}$

$$\theta(x) = W_2 D^{(i)} W_1 x ,$$

and the Jacobian is given by

$$J^{(i)} := \nabla_x \theta(x) = W_2 D^{(i)} W_1 .$$

For any z' that has x' in the same ReLU cell as $x^{(i)}$, we have:

$$\begin{aligned} |\psi_\beta(z') - \psi_\beta(z)| &\leq \sqrt{2} \|W_2 D^{(i)} W_1 x' - W_2 D^{(i)} W_1 x\|_2 = \sqrt{2} \|J^{(i)}(x' - x)\|_2 \\ &\leq \sqrt{2} \|J^{(i)}\|_2 \|x' - x\|_2 \\ &\leq \sqrt{2} \|J^{(i)}\|_2 d(z', z) . \end{aligned}$$

For any z' that has x' in a different ReLU cell as $x^{(i)}$, we define the straight path from $x^{(i)}$ to x' as

$$x(t) = x^{(i)} + t(x' - x^{(i)}), \quad t \in [0, 1]$$

and the hidden-unit pre-activations along the path as

$$h_j(t) := (W_1 x(t))_j, \quad \text{where each is an affine function of } t \text{ and } j \in [n_1].$$

For each hidden unit j with $h_j(0)h_j(1) < 0$, there exist a unique $t \in (0, 1)$ such that $h_j(t) = 0$. Collect all such t , then we can sort them as

$$0 = t_0 < t_1 < \dots < t_{m-1} < t_m = 1, \quad m - 1 \leq n_1 .$$

For every $k \in \{0, \dots, m - 1\}$ define

$$x^{(k)} := x(t_k), \quad \therefore \quad D^{(k)} = \text{diag} \left(\mathbf{1}_{\{(W_1 x^{(k)})_j > 0\}} \right) .$$

Because the activation mask is constant and equal to $D^{(k)}$ on the sub-segment $[x^{(k)}, x^{(k+1)}]$, we have:

$$\begin{aligned}
|\psi_\beta(z') - \psi_\beta(z)| &= \left| \sum_{k=0}^{m-1} [\psi_\beta((x^{(k+1)}, y)) - \psi_\beta((x^{(k)}, y))] \right| \\
&\leq \sum_{k=0}^{m-1} |\psi_\beta((x^{(k+1)}, y)) - \psi_\beta((x^{(k)}, y))| \\
&\leq \sqrt{2} \left(\max_{k \in \{0, \dots, m-1\}} \|J^{(k)}\|_2 \right) \sum_{k=0}^{m-1} \|x^{(k+1)} - x^{(k)}\|_2 \stackrel{(*)}{\leq} L_{(i)} \|x' - x^{(i)}\|_2 \\
&\leq L_{(i)} d(z', z),
\end{aligned}$$

where

$$\begin{aligned}
L_{(i)} &:= \sqrt{2} \left(\max_{D \in \mathcal{D}_{(i)}} \|W_2 D W_1\|_2 \right), \\
\mathcal{D}_{(i)} &:= \left\{ D \mid \exists x \in \mathbb{R}^n, \exists 0 \leq t_1 < t_2 \leq 1 : x(t) = x^{(i)} + t(x - x^{(i)}) \in \mathcal{C}_D \forall t \in [t_1, t_2] \right\}, \\
\mathcal{C}_D &:= \{x : D W_1 x > 0, (I - D) W_1 x < 0\}, \\
(*) : \sum_{k=0}^{m-1} \|x^{(k+1)} - x^{(k)}\|_2 &= \sum_{k=0}^{m-1} \|(t_{k+1} - t_k)(x' - x^{(i)})\|_2 = \sum_{k=0}^{m-1} (t_{k+1} - t_k) \|x' - x^{(i)}\|_2 = \|x' - x^{(i)}\|_2
\end{aligned}$$

Therefore, ψ_β satisfies Assumption (C1) with $L_\beta^{\{Z^{(i)}\}} = L_{(i)}$. Let

$$L := \sqrt{2} \max_{D \in \mathcal{D}} \|W_2 D W_1\|_2, \quad \mathcal{D} := \{D(x) \mid x \in \mathbb{R}^n\},$$

where $D(x) = \text{diag}(\mathbf{1}_{W_1 x > 0})$ is the usual ReLU mask. Fix an arbitrary $D \in \mathcal{D}$. By definition there exists a point $x^D \in \mathbb{R}^n$ that strictly satisfies the inequalities of that mask:

$$D W_1 x^D > 0, \quad (I - D) W_1 x^D < 0.$$

Because the inequalities are strict, the cell $\mathcal{C}_D := \{x : D W_1 x > 0, (I - D) W_1 x < 0\}$ is an open set that contains x^D . By continuity, there is an $\varepsilon > 0$ such that every point within Euclidean distance ε of x^D still lies in \mathcal{C}_D . Now consider the straight segment joining the reference point $x^{(i)}$ to x^D :

$$x(t) = x^{(i)} + t(x^D - x^{(i)}), \quad t \in [0, 1].$$

Choose $t_1 := 1 - \frac{\varepsilon}{\|x^{(i)} - x^D\|_2}$ and $t_2 := 1$. For every $t' \in [t_1, t_2]$ we have

$$\|x(t') - x^D\|_2 = \|x^{(i)} + t'(x^D - x^{(i)}) - x^D\|_2 \leq (1 - t_1) \|x^{(i)} - x^D\|_2 \leq \varepsilon,$$

hence $x(t') \in \mathcal{C}_D$. That means the mask stays constant and equal to D on the entire sub-segment $[t_1, t_2]$. Therefore $D \in \mathcal{D}_{(i)}$. Because the choice of D was arbitrary, we have shown the opposite inclusion $\mathcal{D} \subseteq \mathcal{D}_{(i)}$. The other direction $\mathcal{D}_{(i)} \subseteq \mathcal{D}$ is immediate from the definitions, so

$$\mathcal{D}_{(i)} = \mathcal{D} \quad \therefore \quad L_{(i)} = L.$$

Hence ψ_β satisfies Assumption (A1) on the whole input space with

$$L_\beta^{Z_N} = L = \sqrt{2} \max_{D \in \mathcal{D}} \|W_2 D W_1\|_2$$

Next, we show that ψ_β satisfies Assumption (A2). Let

$$D^* := \arg \max_{D \in \mathcal{D}} \|W_2 D W_1\|_2, \quad J^* := W_2 D^* W_1, \quad \|J^*\|_2 = L/\sqrt{2}.$$

For the strict ReLU cell

$$\mathcal{C}^* = \{x : D^*W_1x > 0, (I - D^*)W_1x < 0\},$$

write its recession cone

$$\text{rec}(\mathcal{C}^*) = \{u \neq 0 : D^*W_1u \geq 0, (I - D^*)W_1u \leq 0\}.$$

Denote

$$\Omega := \text{int}(\text{rec}(\mathcal{C}^*)),$$

$$V := J^*(\Omega) \subset \mathbb{R}^K,$$

$$S_*^{K-1} := \{z : \|z\|_2 = \|J^*\|_2\}, \quad V_* := V \cap S_*^{K-1}.$$

We introduce an assumption:

(D2) Fix the training label $c \in \{1, \dots, K\}$, there exists $j_+ \neq c$ and a unit vector $u \in \Omega$, such that

$$J^*u = w := \frac{\|J^*\|_2}{\sqrt{2}}(e_{j_+} - e_c), \quad \|w\|_2 = \|J^*\|_2, \quad w \in V_*$$

with e_j being the j -th canonical basis vector.

We have,

$$w_{j_+} - w_c := (e_{j_+} - e_c)^\top w = \frac{\|J^*\|_2}{\sqrt{2}} (e_{j_+} - e_c)^\top (e_{j_+} - e_c) = L$$

Because $u \in \Omega$, each coordinate of $W_1(x^{(i)} + tu)$ moves strictly toward the sign prescribed by D^* . For every j put

$$t_j := \max\left\{0, -\frac{(W_1x^{(i)})_j}{(W_1u)_j}\right\},$$

each denominator is non-zero and finite, hence $t_j < \infty$. Define the first hit time

$$\tau := \max_j t_j + \eta,$$

where η is an infinitesimal amount and set

$$x^* := x^{(i)} + \tau u \in \mathcal{C}^*, \quad z^* := (x^*, y^{(i)}).$$

By Assumption (A1), we have

$$\psi_\beta(z^*) - \psi_\beta(Z^{(i)}) \geq -L\tau.$$

For $t \geq 0$, stay on the ray

$$x(t) = x^* + tu, \quad z(t) = (x(t), y^{(i)}),$$

which never leaves the strict cell \mathcal{C}^* (u is in its recession cone). Inside that cell, the directional derivative of the loss in direction u is

$$\dot{\psi}_\beta(z(t)) := u^\top \nabla_x \psi_\beta(z(t)) = w^\top (\text{softmax} \theta(t) - y^{(i)}).$$

Using the Cauchy-Schwarz inequality, we have for all $t \geq 0$

$$\left| \dot{\psi}_\beta(z(t)) \right| \leq \|w\|_2 \|\text{softmax} \theta(t) - y^{(i)}\|_2 \leq \sqrt{2} \|J^*\|_2 = L \quad \therefore \quad \dot{\psi}_\beta(z(t)) \geq -L.$$

Because $w_{j_+} - w_c > 0$, $\theta_{j_+}(t) - \theta_c(t) = (\theta_{j_+}^{(i)} - \theta_c^{(i)}) + t(w_{j_+} - w_c) \rightarrow \infty$ as $t \rightarrow \infty$ hence, $\text{softmax}_{j_+} \rightarrow 1$, $\text{softmax}_c \rightarrow 0$ as $t \rightarrow \infty$. Because the label vector $y^{(i)}$ is one-hot with a 1 in position c ,

$$\dot{\psi}_\beta(z(t)) = w_{j_+} [\text{softmax}_{j_+}(\theta(t))] + w_c [\text{softmax}_c(\theta(t)) - 1] + \sum_{k \notin \{j_+, c\}} w_k \text{softmax}_k(\theta(t)).$$

Therefore $\dot{\psi}_\beta(z(t)) \rightarrow w_{j_+} - w_c$ as $t \rightarrow \infty$. Fix an accuracy level $0 < \varepsilon < L$ where $L = \sqrt{2} \|J^*\|_2$. By continuity, there exist $t_\varepsilon > 0$ such that

$$\dot{\psi}_\beta(z(t)) \geq L - \varepsilon/2 \quad \forall t \geq t_\varepsilon.$$

For any $T > t_\varepsilon$, using the mean-value theorem, we have:

$$\begin{aligned} \psi_\beta(z(T)) - \psi_\beta(Z^{(i)}) &= [\psi_\beta(z(T)) - \psi_\beta(z(t_\varepsilon))] + [\psi_\beta(z(t_\varepsilon)) - \psi_\beta(z^*)] + [\psi_\beta(z^*) - \psi_\beta(Z^{(i)})] \\ &\geq (L - \varepsilon/2)(T - t_\varepsilon) - L t_\varepsilon - L \tau \\ &= (L - \varepsilon)(T + \tau) + \varepsilon(T/2 + t_\varepsilon/2 + \tau) - 2L(t_\varepsilon + \tau). \end{aligned}$$

By choosing $T \geq \frac{4L(t_\varepsilon + \tau)}{\varepsilon} - t_\varepsilon - 2\tau + \delta$, we have

$$\psi_\beta(z(T)) - \psi_\beta(Z^{(i)}) \geq (L - \varepsilon)(T + \tau)$$

Finally, define the witness

$$\tilde{Z}_\varepsilon^{(i)} := (x^* + T u, y^{(i)}),$$

where the distance is

$$d(\tilde{Z}_\varepsilon^{(i)}, Z^{(i)}) = \|x^* + T u - x^{(i)}\|_2 = \|x^{(i)} + \tau u + T u - x^{(i)}\|_2 = (\tau + T)\|u\|_2 = \tau + T \geq \delta.$$

Then we have:

$$\psi_\beta(\tilde{Z}_\varepsilon^{(i)}) - \psi_\beta(Z^{(i)}) \geq (L - \varepsilon) d(\tilde{Z}_\varepsilon^{(i)}, Z^{(i)}).$$

All in all, Assumption (A2) holds under Assumptions (D1 & D2). Therefore, by Theorem 3.2,

$$\sup_{\mathbb{P}: W_{d,1}(\mathbb{P}, \mathbb{P}_N) \leq \delta} \mathbb{E}_{\mathbb{P}}[\psi_\beta(Z)] = \mathbb{E}_{\mathbb{P}_N}[\psi_\beta(Z)] + L \delta$$

General Case Fix an integer $H \geq 1$. We consider an $(H + 1)$ -layer ReLU network with parameters

$$\beta = (W_1, \dots, W_{H+1}), \quad W_\ell \in \mathbb{R}^{n_\ell \times n_{\ell-1}} \quad (n_0 = n, n_{H+1} = K),$$

and define

$$x_0 = x, \quad x_\ell = \sigma(W_\ell x_{\ell-1}) \quad (\ell = 1, \dots, H), \quad \theta(x) = W_{H+1} x_H.$$

The loss is

$$\psi_\beta(z) = \ell(\theta(x), y) = - \sum_{k=1}^K y_k \log \frac{e^{\theta_k(x)}}{\sum_{j=1}^K e^{\theta_j(x)}}.$$

On each strict ReLU cell, we freeze the activation masks

$$D_\ell(x) = \text{diag}(\mathbf{1}_{\{W_\ell x_{\ell-1} > 0\}}), \quad \ell = 1, \dots, H,$$

so that

$$J(x) = \nabla_x \theta(x) = W_{H+1} D_H(x) W_H \cdots D_1(x) W_1$$

is constant on that cell.

Let $Z^{(i)} = (x^{(i)}, y^{(i)})$ be any training sample, and let $\mathcal{D}_{(i)}$ be the collection of all mask-tuples (D_1, \dots, D_H) that arise along the straight segment from $x^{(i)}$ to any x' . Then, exactly as in the two-layer case, splitting into sub-segments, each lying inside one cell, and applying the mean-value theorem plus $\|\nabla_\theta \ell\|_2 \leq \sqrt{2}$ gives

$$|\psi_\beta(z') - \psi_\beta(z)| \leq \sqrt{2} \max_{(D_1, \dots, D_H) \in \mathcal{D}_{(i)}} \|W_{H+1} D_H \cdots D_1 W_1\|_2 \|x' - x\|_2 \leq L_{(i)} d(z', z),$$

where

$$L_{(i)} := \sqrt{2} \max_{(D_1, \dots, D_H) \in \mathcal{D}_{(i)}} \|W_{H+1} D_H \cdots D_1 W_1\|_2.$$

A standard “ ε -ball” argument then shows $\mathcal{D}_{(i)}$ exhausts all global mask-tuples \mathcal{D} , so in fact

$$L_{\beta}^{Z_N} = L := \sqrt{2} \max_{(D_1, \dots, D_H) \in \mathcal{D}} \|W_{H+1} D_H \cdots D_1 W_1\|_2$$

and Assumption (A1) holds on the whole input space.

Let (D_1^*, \dots, D_H^*) attain the maximum defining L , and set

$$J^* = W_{H+1} D_H^* W_H \cdots D_1^* W_1, \quad \|J^*\|_2 = \frac{L}{\sqrt{2}}.$$

Denote the corresponding strict cell $\mathcal{C}^* = \{x : D_\ell^* W_\ell x_{\ell-1} > 0, (I - D_\ell^*) W_\ell x_{\ell-1} < 0 \ \forall \ell\}$ and its recession cone $\text{rec}(\mathcal{C}^*)$. Under the assumptions

(D1) $x^{(i)}$ not on any ReLU facet,

(D2) \exists unit vector $u \in \text{int}(\text{rec}(\mathcal{C}^*))$ with $J^* u = \frac{\|J^*\|_2}{\sqrt{2}}(e_{j_+} - e_c)$,

the ray $x(t) = x^* + t u$ (starting from some $x^* \in \mathcal{C}^*$) keeps all masks frozen and makes the directional derivative $\dot{\psi}_\beta(z(t)) \rightarrow L$. Integrating as before yields, for any $0 < \varepsilon < L$, a witness $\tilde{Z}_\varepsilon^{(i)}$ such that

$$\psi_\beta(\tilde{Z}_\varepsilon^{(i)}) - \psi_\beta(Z^{(i)}) \geq (L - \varepsilon) d(\tilde{Z}_\varepsilon^{(i)}, Z^{(i)}),$$

so Assumption (A2) holds under (D1 & D2).

By Theorem 3.2, combining (A1) and (A2) gives the formula

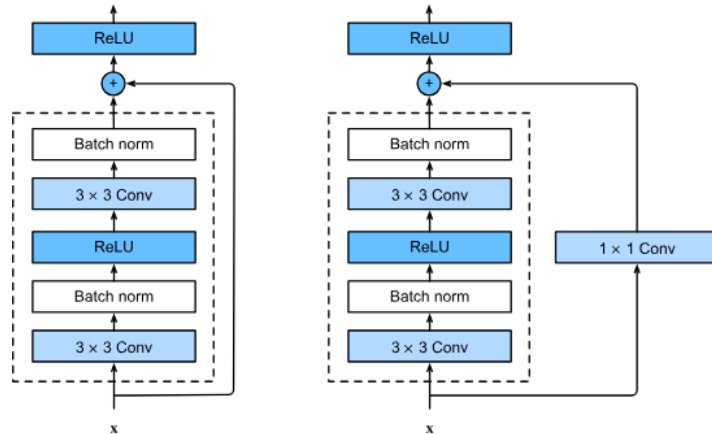
$$\sup_{P: W_{d,1}(P, P_N) \leq \delta} \mathbb{E}_P[\psi_\beta(Z)] = \mathbb{E}_{P_N}[\psi_\beta(Z)] + L \delta.$$

4.2.2 ResNet

Toy Case Let $s \in \mathbb{N}$ be the stride of the first 3×3 convolution. Assume, for simplicity, that s divides both H and W . Then

$$x^b \in \mathbb{R}^{d_{\text{in}}}, \quad z^b \in \mathbb{R}^{d_{\text{out}}}, \\ d_{\text{in}} = C_{\text{in}} H W, \quad d_{\text{out}} = C_{\text{out}} \frac{H}{s} \frac{W}{s},$$

and, in typical ResNet implementations, the channel dimension expands in proportion to the stride, e.g. $C_{\text{out}} = s C_{\text{in}}$ (this choice is not required for the analysis; any $C_{\text{out}} \geq 1$ works).



For our analysis, each “3×3 Conv → BN” pair is absorbed into a single matrix:

$$W_1 \in \mathbb{R}^{d_{\text{mid}} \times d_{\text{in}}}, \quad W_2 \in \mathbb{R}^{d_{\text{out}} \times d_{\text{mid}}},$$

where W_1 incorporates stride s and W_2 has stride 1. The skip path is a 1×1 projection

$$P \in \mathbb{R}^{d_{\text{out}} \times d_{\text{in}}},$$

which defaults to the identity map whenever $d_{\text{out}} = d_{\text{in}}$ (in practice, this is the case $s = 1$ and $C_{\text{out}} = C_{\text{in}}$). With ReLU masks $D_1 = \text{diag}(\mathbf{1}_{W_1 x^b > 0})$, define

$$\mathcal{F}(x^b) = W_2 W_1 D_1 x^b.$$

$$z^b = P x^b + \mathcal{F}(x^b), \quad \tilde{z}^b := \sigma(z^b).$$

For a single-block toy analysis we identify $\tilde{z}^b \equiv z^b$. Holding D_1 fixed,

$$\nabla_{x^b} z^b = P + W_2 D_2 W_1 D_1.$$

General Case

4.2.3 Transformer

Toy Case

General Case

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