Bounds on Deep Neural Network Partial Derivatives with Respect to Parameters

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Abstract

Deep neural networks (DNNs) have emerged as a powerful tool with a growing body of literature exploring Lyapunov-based approaches for real-time system identification and control. These methods depend on establishing bounds for the second partial derivatives of DNNs with respect to their parameters, a requirement often assumed but rarely addressed explicitly. This paper provides rigorous mathematical formulations of polynomial bounds on both the first and second partial derivatives of DNNs with respect to their parameters. We present lemmas that characterize these bounds for fully-connected DNNs, while accommodating various classes of activation function including sigmoidal and ReLU-like functions. Our analysis yields closed-form expressions that enable precise stability guarantees for Lyapunov-based deep neural networks (Lb-DNNs). Furthermore, we extend our results to bound the higher-order terms in first-order Taylor approximations of DNNs, providing important tools for convergence analysis in gradient-based learning algorithms. The developed theoretical framework develops explicit, computable expressions, for previously assumed bounds, thereby strengthening the mathematical foundation of neural network applications in safety-critical control systems.

1 Introduction

The integration of deep learning techniques into control systems has emerged as a promising research direction, with numerous recent studies exploring Lyapunov-based deep learning approaches for real-time system identification and control [1–10]. An important component of these approaches involves Lyapunov-based stability analysis, which is based on the existence of known bounds for the second partial derivatives of deep neural networks (DNNs) with respect to their parameters. Despite the theoretical significance of these bounds, their explicit mathematical formulation has remained largely unaddressed in the literature.

This paper addresses this gap by deriving rigorous mathematical lemmas that establish explicit polynomial bounds on both first and second partial derivatives of fully-connected DNNs with respect to their parameters. These results provide the theoretical foundation necessary for guaranteeing stability in Lyapunov-based deep learning control systems, transforming previously assumed bounds into computable expressions.

For completeness, we present a detailed description of the deep neural network architecture commonly employed in Lyapunov-based deep learning results. While our analysis focuses on this standard fully-connected feedforward DNN architecture, we note that the methodologies and results developed herein can be readily extended to accommodate various neural network architectures.

2 Preliminaries on Deep Neural Networks

Given some matrix $A \triangleq [a_{i,j}] \in \mathbb{R}^{n \times m}$, where $a_{i,j}$ denotes the element in the i^{th} row and j^{th} column of A, the vectorization operator is defined as $\operatorname{vec}(A) \triangleq [a_{1,1},\ldots,a_{n,1},\ldots,a_{1,m},\ldots,a_{n,m}]^{\top} \in \mathbb{R}^{nm}$. In the following development, we consider a fully-connected deep neural network (DNN) $\Phi : \mathbb{R}^{L_{\text{in}}} \times \mathbb{R}^p \to \mathbb{R}^{L_{\text{out}}}$ with $k \in \mathbb{Z}_{>0}$ hidden layers, input size $L_{\text{in}} \in \mathbb{Z}_{>0}$, output size $L_{\text{out}} \in \mathbb{Z}_{>0}$, and total number of parameters $p \in \mathbb{Z}_{>0}$, where the parameters include weights and bias terms. Let $\sigma \in \mathbb{R}^{L_{\text{in}}}$ denote the DNN input and $\theta \in \mathbb{R}^p$ denote the concatenated vector of DNN parameters. Then, a fully-connected feedforward DNN $\Phi(\sigma,\theta)$ is defined using a recursive relation $\Phi_j \in \mathbb{R}^{L_{j+1}}$ given by

$$\Phi_{j} \triangleq \begin{cases}
V_{j}^{\top} \phi_{j} \left(\Phi_{j-1}\right), & j \in \{1, \dots, k\}, \\
V_{j}^{\top} \sigma_{a}, & j = 0,
\end{cases}$$
(1)

where $\Phi(\sigma,\theta) = \Phi_k$, and $\sigma_a \triangleq \begin{bmatrix} \sigma^\top & 1 \end{bmatrix}^\top$ denotes the augmented input that accounts for the bias terms, $V_j \in \mathbb{R}^{L_j \times L_{j+1}}$ denotes the matrix of weights and biases, and $L_j \in \mathbb{Z}_{>0}$ denotes the number of neurons in the j^{th} layer for all $j \in \{0,\dots,k\}$ with $L_0 \triangleq L_{\text{in}} + 1$ and $L_{k+1} \triangleq L_{\text{out}}$. The vector of smooth activation functions is denoted by $\phi_j : \mathbb{R}^{L_j} \to \mathbb{R}^{L_j}$ for all $j \in \{1,\dots,k\}$. The activation functions at each layer are represented as $\phi_j \triangleq \begin{bmatrix} \varsigma_{j,1} & \dots & \varsigma_{j,L_j-1} & 1 \end{bmatrix}^\top$, where $\varsigma_{j,i} : \mathbb{R} \to \mathbb{R}$ denotes the activation function at the i^{th} node of the j^{th} layer. For the DNN architecture in (1), the vector of DNN weights is defined as $\theta \triangleq \begin{bmatrix} \operatorname{vec}(V_0)^\top & \dots & \operatorname{vec}(V_k)^\top \end{bmatrix}^\top$ with size $p = \sum_{j=0}^k L_j L_{j+1}$. The Jacobian of the activation function vector at the j^{th} layer is denoted by $\phi'_j : \mathbb{R}^{L_j} \to \mathbb{R}^{L_j \times L_j}$ and is defined as $\phi'_j(y) \triangleq \frac{\partial}{\partial y} \phi_j(y)$. Specifically, ϕ'_j evaluates as $\phi'_j = \operatorname{diag}\left(\left[\varsigma'_{j,1} & \dots & \varsigma'_{j,L_j-1} & 0\right]^\top\right)$, where $\varsigma'_{j,i}(\zeta) \triangleq \frac{\partial}{\partial \zeta} \varsigma_{j,i}(\zeta)$, and $\operatorname{diag}(\cdot)$ represents the diagonalization operation which returns a diagonal matrix with the elements of its input vector arranged along the diagonal. The Jacobian of the DNN with respect to the weights is denoted by $\frac{\partial}{\partial \theta} \Phi(\sigma,\theta)$ is represented as

$$\frac{\partial}{\partial \theta} \Phi(\sigma, \theta) = \begin{bmatrix} \frac{\partial \Phi(\sigma, \theta)}{\partial \text{vec}(V_0)}, & \frac{\partial \Phi(\sigma, \theta)}{\partial \text{vec}(V_1)}, & \dots, & \frac{\partial \Phi(\sigma, \theta)}{\partial \text{vec}(V_k)} \end{bmatrix} \in \mathbb{R}^{n \times p},$$

where $\frac{\partial \Phi(\sigma,\theta)}{\partial \text{vec}(V_1)} \in \mathbb{R}^{n \times L_j L_{j+1}}$. Then, applying the property $\frac{\partial}{\partial \text{vec}(B)} \text{vec}(ABC) = C^{\top} \otimes A$ to the DNN architecture in (1) yields

$$\frac{\partial \Phi\left(\sigma,\theta\right)}{\partial \text{vec}(V_j)} = \left(\prod_{l=j+1}^{\widehat{k}} V_l^{\top} \phi_l'\left(\Phi_{l-1}\right)\right) \left(I_{L_{j+1}} \otimes \varphi_j^{\top}\right),\tag{2}$$

where φ_j is a shorthand notation defined as $\varphi_0 \triangleq \sigma_a$ and $\varphi_j \triangleq \phi_j (\Phi_{j-1})$ for all $j \in \{1, \dots, k\}$. In (2), the notation $\prod_{p=1}^{\infty} A_p = I$ if a > m, and \otimes denotes the Kronecker product. To facilitate the subsequent development and analysis, the following assumption is made regarding the activation functions of the DNN

Assumption 1. For each $j \in \{0, ..., k\}$, the activation function ϕ_j , its Jacobian ϕ'_j , and Hessian $\phi''_j(y) \triangleq \frac{\partial^2}{\partial y^2} \phi_j(y)$ are bounded as

$$\|\phi_{j}(y)\| \leq \mathfrak{a}_{1} \|y\| + \mathfrak{a}_{0},$$

$$\|\phi'_{j}(y)\| \leq \mathfrak{b}_{0},$$

$$\|\phi''_{j}(y)\| \leq \mathfrak{c}_{0},$$
(3)

respectively, where $\mathfrak{a}_0, \mathfrak{a}_1, \mathfrak{b}_0, \mathfrak{c}_0 \in \mathbb{R}_{>0}$ are known constants.

Remark 1. Most activation functions used in practice satisfy Assumption 1. Specifically, sigmoidal activation functions (e.g., logistic function, hyperbolic tangent etc.) have $\|\phi_j(y)\|$, $\|\phi_j'(y)\|$, and $\|\phi_j''(y)\|$ bounded uniformly by constants. Smooth approximations of rectified linear unit (ReLUs) such as Swish grow linearly, and hence satisfy the bound $\|\phi_j(y)\| \le \mathfrak{a}_1 \|y\| + \mathfrak{a}_0$ of Assumption 1.

3 Bounding Analysis for DNN Layers and Partial Derivatives

The objective is to obtain polynomial bounds on the DNN layers and their first and second partial derivatives with respect to θ . In this section, Lemma 1 provides a bound on any arbitrary DNN layer, and Lemmas 2 and 3 provides on bounds on the first and second partial derivatives of the DNN layers with respect to θ , respectively.

Lemma 1. For the DNN architecture described in (1), the output of the j^{th} layer of the DNN, Φ_j , is bounded as

$$\|\Phi_j\| \le \mathfrak{a}_1^j \|\sigma_a\| \prod_{i=0}^j \|V_i\| + \mathfrak{a}_0 \sum_{i=1}^j \left(\mathfrak{a}_1^{j-i} \prod_{l=i}^j \|V_l\| \right),$$
 (4)

for all $j \in \{0, ..., k\}$, and the corresponding activation $\phi_j(\Phi_{j-1})$ is bounded as

$$\|\phi_j\left(\Phi_{j-1}\right)\| \le \mathfrak{a}_1^j \|\sigma_a\| \prod_{i=0}^{j-1} \|V_i\| + \mathfrak{a}_0 \sum_{i=1}^{j-1} \left(\mathfrak{a}_1^{j-i} \prod_{l=i}^{j-1} \|V_l\|\right) + \mathfrak{a}_0, \tag{5}$$

for all $j \in \{1, ..., k\}$. Furthermore, if the bound $||V_j|| \leq \bar{\theta}$ is applied for all $j \in \{0, ..., k\}$, it follows that $||\Phi_j|| \leq \mathfrak{a}_1^j \bar{\theta}^{j+1} ||\sigma_a|| + \mathfrak{a}_0 \sum_{i=1}^j \mathfrak{a}_1^{j-i} \bar{\theta}^{j-i+1}$. In addition, if the activation functions are uniformly bounded by constants, i.e., $\mathfrak{a}_1 = 0$ in Assumption 1, then the bound is further simplified to $||\Phi_0|| \leq \bar{\theta} ||\sigma_a||$ and $||\Phi_j|| \leq \mathfrak{a}_0 \bar{\theta}$ for all $j \in \{1, ..., k\}$.

Proof. Consider the base case of (4) when j=0 for mathematical induction. Substituting j=0 into (1) yields $\Phi_0 = V_0^\top \sigma_a$, which is bounded as

$$\|\Phi_0\| \leq \|V_0\| \|\sigma_a\|$$
.

Substituting j = 0 into (2) also yields $\|\Phi_0\| \le \|\sigma_a\| \|V_0\|$. Hence, (2) holds for the base case. Assume for induction that the bound in (4) holds for $\|\Phi_{j-1}\|$ for all $j \in \{1, \ldots, k\}$, i.e.,

$$\|\Phi_{j-1}\| \le \mathfrak{a}_1^{j-1} \|\sigma_a\| \prod_{i=0}^{j-1} \|V_i\| + \mathfrak{a}_0 \sum_{i=1}^{j-1} \left(\mathfrak{a}_1^{j-i-1} \prod_{l=i}^{j-1} \|V_l\| \right). \tag{6}$$

Recall from (1) that $\Phi_j = V_j^{\top} \phi_j(\Phi_{j-1})$ for all $j \in \{1, \dots, k\}$. Therefore, it follows that

$$\|\Phi_{j}\| \le \|V_{j}\| \|\phi_{j}(\Phi_{j-1})\|. \tag{7}$$

Applying (3) to the term $\|\phi_j(\Phi_{j-1})\|$ and substituting the inductive assumption from (6) yields (5). Substituting (5) into (7) yields (2). Hence, by mathematical induction, (4) and (5) hold for all $j \in \{1,\ldots,k\}$.

Furthermore, if the bound $\|V_j\| \leq \bar{\theta}$ is applied for all $j \in \{0, \dots, k\}$, it follows that $\|\Phi_j\| \leq \mathfrak{a}_1^j \bar{\theta}^{j+1} \|\sigma_a\| + \mathfrak{a}_0 \sum_{i=1}^j \mathfrak{a}_1^{j-i} \bar{\theta}^{j-i+1}$. In addition, if the activation functions are uniformly bounded by constants, i.e., $\mathfrak{a}_1 = 0$ in Assumption 1, then it follows that $\|\Phi_j\| \leq \|V_j\| \|\phi_j(\Phi_{j-1})\| \leq \|V_j\| \mathfrak{a}_0 \leq \bar{\theta}\mathfrak{a}_0$ for all $j \in \{1, \dots, k\}$.

Lemma 2. For the DNN architecture described in (1), the Jacobian of the w^{th} layer with respect to the j^{th} layer weights is bounded as

$$\left\| \frac{\partial \Phi_{w}}{\partial \text{vec}(V_{j})} \right\| \leq \begin{cases} \mathfrak{b}_{0}^{w-j} \left(\prod_{l=j+1}^{w} \|V_{l}\| \right) \left(\mathfrak{a}_{1}^{j} \|\sigma_{a}\| \prod_{i=0}^{j-1} \|V_{i}\| \right) \\ +\mathfrak{a}_{0} \sum_{i=1}^{j-1} \left(\mathfrak{a}_{1}^{j-i} \prod_{l=i}^{j-1} \|V_{l}\| \right) + \mathfrak{a}_{0} \right), & w \leq j, \\ 0, & j > w, \end{cases}$$
(8)

for all $w, j \in \{0, ..., k\}$. Furthermore, if the bound $||V_j|| \leq \bar{\theta}$ holds for all $j \in \{0, ..., k\}$, then the Jacobian $\frac{\partial \Phi(\sigma, \theta)}{\partial \theta}$ is bounded as

$$\left\| \frac{\partial \Phi \left(\sigma, \theta \right)}{\partial \theta} \right\| \leq \mathfrak{b}_{0}^{k} \bar{\theta}^{k} \left\| \sigma_{a} \right\| + \sum_{j=1}^{k} \left(\mathfrak{b}_{0}^{k-j} \bar{\theta}^{k-j} \left(\mathfrak{a}_{1}^{j} \left\| \sigma_{a} \right\| \bar{\theta}^{j+1} + \mathfrak{a}_{0} \sum_{i=1}^{j-1} \left(\mathfrak{a}_{1}^{j-i} \bar{\theta}^{j-i-1} \right) + \mathfrak{a}_{0} \right) \right). \tag{9}$$

In addition, if the activations are uniformly bounded by constants, i.e., $\mathfrak{a}_1 = 0$ in Assumption 1, then the Jacobian bound reduces to

$$\left\| \frac{\partial \Phi \left(\sigma, \theta \right)}{\partial \theta} \right\| \le \mathfrak{b}_0^k \bar{\theta}^k \left\| \sigma_a \right\| + \mathfrak{a}_0 \sum_{j=1}^k \mathfrak{b}_0^{k-j} \bar{\theta}^{k-j}. \tag{10}$$

Proof. Replacing k with w in (2) yields

$$\frac{\partial \Phi_{w}}{\partial \text{vec}(V_{j})} = \begin{cases} \left(\prod_{l=j+1}^{w} V_{l}^{\top} \phi_{l}'(\Phi_{l-1})\right) \left(I_{L_{j+1}} \otimes \varphi_{j}\right), & w \geq j, \\ 0, & j > w, \end{cases}$$
(11)

where $\frac{\partial \Phi_w}{\partial \text{vec}(V_j)} = 0$ if j > w because the outputs of the inner layers do not depend on the outer layer weights. Taking the norm on both sides of (11), and applying the Cauchy-Schwarz inequality and Lemma 1 to the resulting expression yields

$$\left\| \frac{\partial \Phi_{w}}{\partial \text{vec}(V_{j})} \right\| \leq \begin{cases} \mathfrak{b}_{0}^{w-j} \left(\prod_{l=j+1}^{w} \|V_{l}\| \right) \left(\mathfrak{a}_{1}^{j} \|\sigma_{a}\| \prod_{i=0}^{j-1} \|V_{i}\| \right. \\ + \mathfrak{a}_{0} \sum_{i=1}^{j-1} \left(\mathfrak{a}_{1}^{j-i} \prod_{l=i}^{j-1} \|V_{l}\| \right) + \mathfrak{a}_{0} \right), & w \geq j, \\ 0, & j > w. \end{cases}$$

Furthermore, using the triangle inequality, the Jacobian is bounded as $\left\|\frac{\partial \Phi(\sigma,\theta)}{\partial \theta}\right\| \leq \left\|\frac{\partial \Phi_k}{\partial \text{vec}(V_0)}\right\| + \left\|\frac{\partial \Phi_k}{\partial \text{vec}(V_1)}\right\| + \ldots + \left\|\frac{\partial \Phi_k}{\partial \text{vec}(V_k)}\right\|$. Therefore,

$$\left\| \frac{\partial \Phi \left(\sigma, \theta \right)}{\partial \theta} \right\| \leq \mathfrak{b}_{0}^{k} \left(\prod_{l=1}^{k} \| V_{l} \| \right) \| \sigma_{a} \| + \sum_{j=1}^{k} \left(\mathfrak{b}_{0}^{j-k} \left(\prod_{l=j+1}^{k} \| V_{l} \| \right) \left(\mathfrak{a}_{1}^{j} \| \sigma_{a} \| \prod_{i=0}^{j-1} \| V_{i} \| \right) + \mathfrak{a}_{0} \sum_{i=1}^{j-1} \left(\mathfrak{a}_{1}^{j-i} \prod_{l=i}^{j-1} \| V_{l} \| \right) + \mathfrak{a}_{0} \right) \right).$$

As a result, applying the bound $||V_j|| \leq \bar{\theta}$ is applied for all $j \in \{0, \dots, k\}$ yields

$$\left\|\frac{\partial\Phi\left(\sigma,\theta\right)}{\partial\theta}\right\| \hspace{2mm} \leq \hspace{2mm} \mathfrak{b}_{0}^{k}\bar{\theta}^{k}\left\|\sigma_{a}\right\| + \sum_{j=1}^{k}\left(\mathfrak{b}_{0}^{k-j}\bar{\theta}^{k-j}\left(\mathfrak{a}_{1}^{j}\left\|\sigma_{a}\right\|\bar{\theta}^{j+1} + \mathfrak{a}_{0}\sum_{i=1}^{j-1}\left(\mathfrak{a}_{1}^{j-i}\bar{\theta}^{j-i-1}\right) + \mathfrak{a}_{0}\right)\right).$$

Furthermore, if the activation functions are uniformly bounded by constants, i.e., $\mathfrak{a}_1 = 0$ in Assumption (1), then the bound is further simplified as

$$\left\| \frac{\partial \Phi\left(\sigma,\theta\right)}{\partial \theta} \right\| \leq \mathfrak{b}_{0}^{k} \bar{\theta}^{k} \left\| \sigma_{a} \right\| + \mathfrak{a}_{0} \sum_{i=1}^{k} \mathfrak{b}_{0}^{k-j} \bar{\theta}^{k-j}.$$

Lemma 3. For the DNN architecture described in (1), the second partial derivative term $\frac{\partial^2 \Phi_w}{\partial \text{vec}(V_q) \partial \text{vec}(V_j)}$ is bounded according to

$$\left\| \frac{\partial^2 \Phi_w}{\partial \text{vec} (V_q) \partial \text{vec} (V_j)} \right\| \leq \mathcal{R}_{w,q,j} \mathcal{Q}_j \mathcal{Q}_q + \mathcal{T}_{w,j} \mathcal{Q}_j,$$

where $Q_j \triangleq \mathfrak{a}_1^j \|\sigma_a\| \prod_{i=0}^{j-1} \|V_i\| + \mathfrak{a}_0 \sum_{i=1}^{j-1} \left(\mathfrak{a}_1^{j-i} \prod_{l=i}^{j-1} \|V_l\|\right) + \mathfrak{a}_0$, Q_q is obtained by replacing j with q in the expression for Q_j , $\mathcal{T}_{w,j} \triangleq \mathfrak{b}_0^{w-j+1} \left(\prod_{l=j+1}^w \|V_l\|\right)$, and

$$\mathcal{R}_{w,q,j} \triangleq \begin{cases} \left(\sum_{h=1}^{w-q} \mathfrak{c}_0 \mathfrak{b}_0^{2w-q-j-h-1} \left(\prod_{l=q+1}^{w-h} \|V_l\|\right)\right) \left(\prod_{l=j+1}^{w} \|V_l\|\right), & j \leq q \leq w, \\ \mathcal{R}_{w,j,q}, & q \leq j \leq w, \end{cases}$$

for all $j,q \leq w \leq k$, implying that $\frac{\partial^2 \Phi_w}{\partial \text{vec}(V_q)\partial \text{vec}(V_j)}$ is bounded by a quadratic polynomial in terms of $\|\sigma_a\|$. Furthermore, consider the bound $\|V_j\| \leq \bar{\theta}$ for all $j \in \{0,\ldots,k\}$. Then, the terms Q_j , $\mathcal{T}_{w,j}$, and $\mathcal{R}_{w,j,q}$ reduce to $Q_j = \mathfrak{a}_1^j \bar{\theta}^j \|\sigma_a\| + \sum_{i=1}^{j-1} \left(\mathfrak{a}_1^{j-i} \bar{\theta}^{j-i}\right) + \mathfrak{a}_0$, $\mathcal{T}_{w,j} = \mathfrak{b}_0^{w-j+1} \bar{\theta}^{w-j}$, and $\mathcal{R}_{w,q,j} = \sum_{h=1}^{w-q} \mathfrak{c}_0 \mathfrak{b}_0^{2w-q-j-h-1} \bar{\theta}^{2w-h-q-j}$. Furthermore, if the activation functions are uniformly bounded by constants, i.e., $\mathfrak{a}_1 = 0$ in Assumption 1, then Q_j reduces to $Q_0 = \|\sigma_a\|$ and $Q_j = \sum_{i=1}^{j-1} \left(\mathfrak{a}_1^{j-i} \bar{\theta}^{j-i}\right) + \mathfrak{a}_0$ for all $j \geq 1$.

Proof. For the ease of subsequent exposition, we consider scalar outputs for Φ_w . This reduction does not compromise generality because the bounds apply element-wise for the vector case. The second partial derivative term $\frac{\partial^2 \Phi_w}{\partial \text{vec}(V_q) \partial \text{vec}(V_j)}$ is expressed as

$$\frac{\partial \Phi_{w}}{\partial \text{vec}(V_{q}) \partial \text{vec}(V_{j})} = \frac{\partial}{\partial \text{vec}(V_{q})} \left(\frac{\partial}{\partial \text{vec}(V_{j})} V_{w}^{\top} \varphi_{w} \right)
= \begin{cases} \frac{\partial}{\partial \text{vec}(V_{q})} \left(\prod_{l=j+1}^{w} V_{l}^{\top} \phi_{l}'(\Phi_{l-1}) \right) \left(I_{L_{j+1}} \otimes \varphi_{j}^{\top} \right), & w \geq j, \\ 0, & j > w. \end{cases} (12)$$

Due to the symmetry of Hessian matrices, it follows that $\frac{\partial \Phi_w}{\partial \text{vec}(V_q)\partial \text{vec}(V_j)} = \frac{\partial \Phi_w}{\partial \text{vec}(V_j)\partial \text{vec}(V_q)}$. Without loss of generality, consider the case $w \geq q \geq j$. Such consideration does not affect generality because, if q < j, then the analysis can be performed by exchanging q and j. Applying the product rule and chain rule to (12) yields

$$\begin{split} \frac{\partial \Phi_{w}}{\partial \text{vec}\left(V_{q}\right) \text{vec}\left(V_{j}\right)} &= & \left(V_{w}^{\intercal}\left(\phi_{w}^{\prime\prime}\left(\Phi_{w-1}\right) \frac{\partial \Phi_{w-1}}{\partial \text{vec}\left(V_{q}\right)}\right) V_{w-1}^{\intercal}\phi_{w-1}^{\prime}\left(\Phi_{w-2}\right) \dots V_{j+1}^{\intercal}\phi_{j+1}^{\prime}\left(\Phi_{j}\right)\right) \left(I_{L_{j+1}} \otimes \varphi_{j}^{\intercal}\right) \\ &+ \left(V_{w}^{\intercal}\phi_{w}^{\prime}\left(\Phi_{w-1}\right) V_{w-1}^{\intercal}\left(\phi_{w-1}^{\prime\prime}\left(\Phi_{w-2}\right) \frac{\partial \Phi_{w-2}}{\partial \text{vec}\left(V_{q}\right)}\right) \dots V_{j+1}^{\intercal}\phi_{j+1}^{\prime}\left(\Phi_{j}\right)\right) \left(I_{L_{j+1}} \otimes \varphi_{j}^{\intercal}\right) \\ &\vdots \\ &+ \left(V_{w}^{\intercal}\phi_{w}^{\prime}\left(\Phi_{w-1}\right) \dots V_{q+1}^{\intercal}\left(\phi_{q+1}^{\prime\prime}\left(\Phi_{q}\right) \frac{\partial \Phi_{q}}{\partial \text{vec}\left(V_{q}\right)}\right) V_{q}^{\intercal}\phi_{q}^{\prime}\left(\Phi_{q-1}\right) \dots V_{j+1}^{\intercal}\phi_{j+1}^{\prime}\left(\Phi_{j}\right)\right) \left(I_{L_{j+1}} \otimes \varphi_{j}^{\intercal}\right) \\ &+ \left(V_{w}^{\intercal}\phi_{w}^{\prime}\left(\Phi_{w-1}\right) \dots \left(I_{L_{q+1}} \otimes \phi_{q}^{\prime}\right(\Phi_{q-1})\right) \dots V_{j+1}^{\intercal}\phi_{j+1}^{\prime}\left(\Phi_{j}\right)\right) \left(I_{L_{j+1}} \otimes \varphi_{j}^{\intercal}\right). \end{split}$$

Taking norms and applying the triangle inequality yields

$$\left\| \frac{\partial \Phi_{w}}{\partial \text{vec} (V_{q}) \text{ vec} \left(V_{j}\right)} \right\| \leq \|V_{w}\| \|\phi_{w}^{\prime \prime} \left(\Phi_{w-1}\right)\| \|\frac{\partial \Phi_{w-1}}{\partial \text{vec} (V_{q})} \| \|V_{w-1}\| \|\phi_{w-1}^{\prime} \left(\Phi_{w-2}\right)\| \cdots \|V_{j+1}\| \|\phi_{j+1}^{\prime} \left(\Phi_{j}\right)\| \|\varphi_{j}\|$$

$$+ \|V_{w}\| \|\phi_{w}^{\prime} \left(\Phi_{w-1}\right)\| \|V_{w-1}\| \|\phi_{w-1}^{\prime \prime} \left(\Phi_{w-2}\right)\| \|\frac{\partial \Phi_{w-2}}{\partial \text{vec} (V_{q})} \| \cdots \|V_{j+1}\| \|\phi_{j+1}^{\prime} \left(\Phi_{j}\right)\| \|\varphi_{j}\|$$

$$\vdots$$

$$+ \|V_{w}\| \|\phi_{w}^{\prime} \left(\Phi_{w-1}\right)\| \cdots \|V_{q+1}\| \|\phi_{q+1}^{\prime \prime} \left(\Phi_{q}\right)\| \|\frac{\partial \Phi_{q}}{\partial \text{vec} (V_{q})} \| \|V_{q}\| \|\phi_{q}^{\prime} \left(\Phi_{q-1}\right)\| \cdots \|V_{j+1}\| \|\phi_{j+1}^{\prime} \left(\Phi_{j}\right)\| \|\varphi_{j}\|$$

$$+ \|V_{w}\| \|\phi_{w}^{\prime} \left(\Phi_{w-1}\right)\| \cdots \|\phi_{q}^{\prime} \left(\Phi_{q-1}\right)\| \cdots \|V_{j+1}\| \|\phi_{j+1}^{\prime} \left(\Phi_{j}\right)\| \|\varphi_{j}\| .$$

$$(13)$$

We express the bounds from Lemma 2 using the definition of Q_j as $\left\| \frac{\partial \Phi_w}{\partial \text{vec}(V_j)} \right\| \leq \mathfrak{b}_0^{w-j} \left(\prod_{l=j+1}^w \|V_l\| \right) Q_j$ and $\left\| \frac{\partial \Phi_w}{\partial \text{vec}(V_q)} \right\| \leq \mathfrak{b}_0^{w-q} \left(\prod_{l=q+1}^w \|V_l\| \right) Q_q$, respectively. Applying these bounds to (13) yields

$$\begin{split} \left\| \frac{\partial \Phi_{w}}{\partial \text{vec} \left(V_{q} \right) \text{vec} \left(V_{j} \right)} \right\| & \leq & \mathfrak{c}_{0} \mathfrak{b}_{0}^{w-j-1} \left(\prod_{l=j+1}^{w} \left\| V_{l} \right\| \right) \mathcal{Q}_{j} \left(\mathfrak{b}_{0}^{w-q-1} \left(\prod_{l=q+1}^{w-1} \left\| V_{l} \right\| \right) \mathcal{Q}_{q} \right) \\ & + \mathfrak{c}_{0} \mathfrak{b}_{0}^{w-j-1} \left(\prod_{l=j+1}^{w} \left\| V_{l} \right\| \right) \mathcal{Q}_{j} \left(\mathfrak{b}_{0}^{w-q-2} \left(\prod_{l=q+1}^{w-2} \left\| V_{l} \right\| \right) \mathcal{Q}_{q} \right) \\ & \vdots \\ & + \mathfrak{c}_{0} \mathfrak{b}_{0}^{w-j-1} \left(\prod_{l=j+1}^{w} \left\| V_{l} \right\| \right) \mathcal{Q}_{j} \left(\mathfrak{b}_{0}^{0} \left(\prod_{l=q+1}^{q} \left\| V_{l} \right\| \right) \mathcal{Q}_{q} \right) \\ & + \mathfrak{b}_{0}^{w-j+1} \left(\prod_{l=j+1}^{w} \left\| V_{l} \right\| \right) \mathcal{Q}_{j}. \end{split}$$

Factoring like terms yields

$$\left\| \frac{\partial^2 \Phi_w}{\partial \text{vec}(V_q) \, \partial \text{vec}(V_j)} \right\| \le \mathcal{R}_{w,q,j} \mathcal{Q}_j \mathcal{Q}_q + \mathcal{T}_{w,j} \mathcal{Q}_j.$$

Because the terms Q_j and Q_q are linear in $\|\sigma_a\|$, it follows that the bound on $\left\|\frac{\partial^2 \Phi_w}{\partial \text{vec}(V_q)\partial \text{vec}(V_j)}\right\|$ is quadratic in $\|\sigma_a\|$.

4 Bounds on Higher-Order Terms in First-Order Taylor Series Approximation

The bounds obtained in the previous section can be used to compute analytical bounds on the first-order Taylor series approximation of $\theta \mapsto \Phi\left(\sigma,\theta\right)$. To this end, consider a compact convex set of admissible DNN parameters given by $\Theta \subset \mathbb{R}^p$. Additionally, consider any arbitrary elements $\theta^*, \hat{\theta} \in \Theta$, and let $\tilde{\theta} \triangleq \theta^* - \hat{\theta} \in \mathbb{R}^p$ denote their difference. Furthermore, let $\Phi^{(i)}$ denote the i^{th} element of Φ for all $i \in \{1, \dots, n\}$. Then performing a first-order application of Taylor's theorem [11, Theorem 4.7] element-wise to Φ yields

$$\Phi(\sigma, \theta^*) - \Phi\left(\sigma, \hat{\theta}\right) = \frac{\partial \Phi\left(\sigma, \hat{\theta}\right)}{\partial \hat{\theta}} \tilde{\theta} + R\left(\sigma, \tilde{\theta}\right), \tag{14}$$

where $R: \mathbb{R}^{2n} \times \mathbb{R}^p \to \mathbb{R}^n$ denotes the Lagrange remainder term given by

$$R\left(\sigma,\tilde{\theta}\right) = \frac{1}{2} \left[\tilde{\theta}^{\top} \frac{\partial^{2} \Phi^{(1)}}{\partial \hat{\theta}^{2}} \left(\sigma, \theta^{*} + \varpi_{1}\left(\hat{\theta}\right) \tilde{\theta}\right) \tilde{\theta}, \dots, \tilde{\theta}^{\top} \frac{\partial^{2} \Phi^{(n)}}{\partial \hat{\theta}^{2}} \left(\sigma, \theta^{*} + \varpi_{n}\left(\hat{\theta}\right) \tilde{\theta}\right) \tilde{\theta}\right]^{\top},$$

where $\varpi_i : \mathbb{R}^p \to [0,1]$ denote unknown functions parameterizing a convex combination of θ^* and $\hat{\theta}$ for all $i \in \{1,\ldots,n\}$. The following theorem provides a polynomial bound on the Lagrange remainder term.

Theorem 1. There exists a polynomial function $\rho_0 : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ of the form $\rho_0 (\|\sigma\|) = a_2 \|\sigma\|^2 + a_1 \|\sigma\|^1 + a_0$ with constants $a_2, a_1, a_0 \in \mathbb{R}_{> 0}$ such that the Lagrange remainder term is bounded as $\|R(\sigma, \tilde{\theta})\| \leq \rho_0 (\|\sigma\|) \|\tilde{\theta}\|^2$.

Proof. Using the triangle inequality, it follows that

$$\left\| R\left(\sigma, \tilde{\theta}\right) \right\| \leq \frac{\left\| \tilde{\theta} \right\|^{2}}{2} \left(\left\| \frac{\partial^{2} \Phi^{(1)}}{\partial \hat{\theta}^{2}} \left(\sigma, \theta^{*} + \varpi_{1} \left(\hat{\theta}\right) \tilde{\theta}\right) \right\| + \ldots + \left\| \frac{\partial^{2} \Phi^{(n)}}{\partial \hat{\theta}^{2}} \left(\sigma, \theta^{*} + \varpi_{n} \left(\hat{\theta}\right) \tilde{\theta}\right) \right\| \right). \tag{15}$$

Due to the facts that Θ is a convex set, $\varpi_i\left(\hat{\theta}\right) \in [0,1]$, and $\theta^*, \hat{\theta} \in \Theta$, it follows that $\theta^* + \varpi_i\left(\hat{\theta}\right) \tilde{\theta} \in \Theta$ for all $i \in \{1,\ldots,n\}$ and $\hat{\theta} \in \Theta$. Because ϖ_i is unknown, the term $\left\|\frac{\partial^2 \Phi^{(i)}}{\partial \hat{\theta}^2}\left(\sigma, \theta^* + \varpi_i\left(\hat{\theta}\right) \tilde{\theta}\right)\right\|$ is bounded in the following analysis considering the worst case bound in which $\left\|\theta^* + \varpi_i\left(\hat{\theta}\right) \tilde{\theta}\right\| \leq \bar{\theta}$ for all $i \in \{1,\ldots,n\}$. To this end, a bound is developed on $\frac{\partial^2 \Phi^{(i)}}{\partial \hat{\theta}^2}\left(\sigma,\theta\right)$ considering an arbitrary $\|\theta\| \leq \bar{\theta}$. The Hessian matrix $\frac{\partial^2 \Phi^{(i)}}{\partial \theta^2}\left(\sigma,\theta\right)$ is comprised of blocks of the form $\frac{\partial \Phi^{(i)}(\sigma,\theta)}{\partial \operatorname{vec}(V_q)\partial \operatorname{vec}(V_j)}$ for all $q \in \{1,\ldots,k\}$ and $i \in \{1,\ldots,n\}$. Therefore, using (15), the Lagrange remainder can be bounded as

$$\left\| R\left(\sigma, \tilde{\theta}\right) \right\| \leq \frac{\left\| \tilde{\theta} \right\|^2}{2} \left(\sum_{i=1}^n \sum_{q=1}^k \sum_{j=1}^k \left(\mathcal{R}_{k,q,j} \mathcal{Q}_j \mathcal{Q}_q + \mathcal{T}_{k,j} \mathcal{Q}_j \right) \right), \tag{16}$$

where the terms Q_j , Q_q , $\mathcal{T}_{k,j}$, and $\mathcal{R}_{k,q,j}$ are defined in Lemma 3. As a result, defining the polynomial function ρ_0 as

$$\rho_0(\|\sigma\|) \triangleq \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^k \sum_{j=1}^k (\mathcal{R}_{k,q,j} \mathcal{Q}_j \mathcal{Q}_q + \mathcal{T}_{k,j} \mathcal{Q}_j)$$

$$\tag{17}$$

yields $\|R\left(\sigma,\tilde{\theta}\right)\| \leq \rho_0 (\|\sigma\|) \|\tilde{\theta}\|^2$. Because Lemma 3 provides quadratic polynomial bounds on such terms with respect to the input, it follows that ρ_0 is a quadratic function of the form $\rho_0 (\|\sigma\|) = a_2 \|\sigma\|^2 + a_1 \|\sigma\|^1 + a_0$ with constants $a_2, a_1, a_0 \in \mathbb{R}_{>0}$. We note that the explicit values of a_2, a_1, a_0 can be computed by expanding the polynomial formulation in (17).

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