An Efficient Framework for Computing Tight Lipschitz Constants of Neural Networks

Abstract

Lipschitz constants are connected to many properties of neural networks, such as robustness, fairness, and generalization. Existing methods for computing Lipschitz constants either are computationally inefficient or produce loose upper bounds. In this paper, we develop an efficient framework for computing the ℓ_∞ local Lipschitz constant of a neural network by tightly upper bounding the norm of Clarke Jacobian. We view the computation for Clarke Jacobian by chain rule as a higher-order backward computational graph. On this graph, we adopt bound-propagation with linear relaxation to obtain provable bounds, and we derive tight linear relaxations for specific nonlinearities in Clarke Jacobian that previous works could not tightly bound. We further tighten our bounds by Branch-and-Bound (BaB) when time budget allows. Experiments show that on tiny models, our method produces comparable bounds compared to exact methods that cannot scale to slightly larger models; on larger models, our method efficiently produces tighter results than existing relaxed or naive methods, and our method scales to much larger practical models that previous works could not handle. We also demonstrate a potential application of our method for provable monotonicity analysis.

1 Introduction

Lipschitz constants are important for characterizing many properties of neural networks, including robustness [35, 15, 37, 47, 17], fairness [10, 19], generalization [2] and explanation [12]. In order to more precisely characterize the local behavior of a network, we consider local Lipschitz constants which are only required to hold for a small local region. Intuitively they characterize how fast the output of the network changes between any two input within the region.

It is challenging to exactly and efficiently compute local Lipschitz constants. Naive approaches such as computing the product of the induced norm for all layers cannot capture local information and typically produce vacuous bound that are not useful in practice. On the other hand, Jordan & Dimakis [18] used mixed-integer programming (MIP) to compute exact local Lipschitz constants for small ReLU networks (e.g., up to a few hundred neurons), but solving a MIP is often too inefficient and this approach cannot scale to slightly larger networks. Another line of works focus on computing a relaxed upper bound for better scalability compared to MIP. Bound propagation methods [43, 46, 33] which can compute guaranteed lower or upper bounds for neural network verification have been applied to bound the Jacobian [42, 47], which can produce local Lipschitz constant. Bound propagation computes the linear relationship between layers, where nonlinearities in networks are relaxed into linear bounds, e.g., nonlinear activations can be bounded by two lines. However, when bounding the gradient of ReLU activation in the chain rule for computing Jacobian, in nontrivial cases, existing bound propagation methods [42, 47] degenerate to loose interval bounds [16, 28, 14] that only use

bounding lines with zero slopes. Moreover, most of these works only used small toy models and cannot feasibly handle larger practical networks.

In this paper, we aim to efficiently compute relatively tight local Lipschitz constants. We formulate the problem as upper bounding the norm of the Clarke Jacobian by the chain rule; and we view the computation for this norm as a *higher-order backward computational graph* augmented to the original forward graph of the network, which allows us to develop a scalable and flexible framework for practical neural networks.

Our contributions can be summarized as follows: First, we generalize existing bound propagation methods originally used for neural network verification, to a higher-order backward computational graph for bounding Clarke Jacobian. Second, on the backward graph, we propose tight linear relaxations for Clarke gradients in the chain rule, while previous works degenerate to loose interval bounds in nontrivial cases. When time budget allows, we further tighten our bounds via Branch-and-Bound, for a trade-off between tightness and time cost. Lastly, our experiments show that our method efficiently produces tightest local Lipschitz constants compared to other relaxed methods, and is much more efficient than the exact MIP method. Moreover, while previous works commonly used small toy models, our method can scale to much larger models including practical convolutional neural networks (CNN) that previous works could not handle. We also demonstrate an application of our method for provably analyzing the monotonicity of neural networks.

2 Related Work

2.1 Computing Lipschitz Constants

For neural networks, a loose global Lipschitz constant (upper bound) can be computed by the product of layer-wise induced norms [35]. Based on computing this product, Virmaux & Scaman [38] considered the effect of activation and approximated upper bounds which, however, are not guaranteed; Gouk et al. [13] used a power method to handle convolutional layers. LipSDP [11] used semidefinite programming (SDP) to compute tighter bounds. Global Lipschitz constants can be much looser than local Lipschitz constants as they have to hold even for distinct input points, and they cannot characterize the local behavior of neural networks. Thus we focus on local Lipschitz constants in this paper.

To compute local Lipschitz constants, LipMIP [18] used mixed integer programming (MIP) to compute exact results, which is costly and cannot scale to slightly larger models. LipOpt [22] used polynomial optimization, but their method is still inefficient and limited to smooth activations, not including the widely used ReLU. Avant & Morgansen [1] derived layer-wise analytical bounds but only on a simplified definition for Lipschitz constants, which cannot characterize Lipschitzness in the entire local region.

Several other works used methods essentially based on interval bound propagation [16, 28, 14] which computes an interval of lower and upper bounds for each element in the network or the chain rule for Jacobian. Among them, RecurJac [47], improved from FastLip [42], has a recursive procedure to tighten bounds in some special cases but still uses interval bounds in nontrivial cases; and a concurrent work [23] handled non-smooth input perturbations. However, interval bounds are known to be very loose [48]. Bhowmick et al. [3] combined interval bounds with branch-and-bound to compute exact local Lipschitz constants, which is inefficient due to loose interval bounds. In contrast, we propose tight linear relaxation for computing local Lipschitz constants with bound propagation.

2.2 Certified Bounds for Neural Networks

Computing sound local Lipschitz constants is also closely related to neural network verification which computes certified output bounds. Some works computed the exact bounds by satisfiability modulo theory [20] or mixed integer linear programming [36]. For more efficient verification, bound propagation with convex relaxations has been proposed [43, 40, 46, 42, 33, 30]. In addition, Branch-and-Bound can be used to compute tighter certified bounds Katz et al. [20], Bunel et al. [5, 6], Wang et al. [39, 40], Xu et al. [45], Wang et al. [41] by branching activations or input and bounding each smaller subdomain respectively. Although bound propagation has been generalized to support general computational graphs [44], they have not considered high-order computational graphs and did not provide necessary linear relaxation for nonlinearities in Clarke Jacobian.

3 Background

3.1 ReLU Network

Suppose $f(\mathbf{x})$ is a neural network given input $\mathbf{x} \in \mathbb{R}^d$. For the simplicity of presentation, we mainly assume the neural network is feedforward with ReLU activation throughout the paper, but our method can be applied to general network architectures and activations as will be discussed in Section 4. Suppose the network has n layers, it takes input $h_0(\mathbf{x}) = \mathbf{x}$ and then computes

$$\forall i \in [n], \ z_i(\mathbf{x}) = \mathbf{W}_i h_{i-1}(\mathbf{x}) + \mathbf{b}_i, \quad \forall i \in [n-1], \ h_i(\mathbf{x}) = \sigma(z_i(\mathbf{x})), \ h_n(\mathbf{x}) = z_n(\mathbf{x}),$$

where $i \in [n]$ means $1 \leq i \leq n$, $z_i(\mathbf{x})$ is the pre-activation output of the i-th linear layer with weight $\mathbf{W}_i$ and bias $\mathbf{b}_i$, and $h_i(\mathbf{x})$ is the output after activation $\sigma(\cdot)$. This formulation also supports CNNs since convolutional layers are also linear.

3.2 Lipschitz Constant

The (α, β)-Lipschitz constant of a network $f(\mathbf{x})$ over an open set $\mathcal{X} \in \mathbb{R}^d$ is defined as:

$$L^{(\alpha,\beta)}(f, \mathcal{X}) = \sup_{\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{X}, \ \mathbf{x}_1 \neq \mathbf{x}_2} \frac{\|f(\mathbf{x}_1) - f(\mathbf{x}_2)\|_\beta}{\|\mathbf{x}_1 - \mathbf{x}_2\|_\alpha}. \tag{1}$$

If f is smooth and (α, β)-Lipschitz continuous over $\mathcal{X}$, the Lipschitz constant can be computed by upper bounding the norm of Jacobian, i.e., $L^{(\alpha,\beta)}(f, \mathcal{X}) = \sup_{\mathbf{x} \in \mathcal{X}} \|\nabla f(\mathbf{x})\|_{\alpha,\beta}$, where $\|\nabla f(\mathbf{x})\|_{\alpha,\beta}$ is the matrix norm induced by vector norms, i.e., $\|\nabla f(\mathbf{x})\|_{\alpha,\beta} = \sup_{\|\mathbf{z}\|_\alpha = 1} \|\nabla f(\mathbf{x})\mathbf{z}\|_\beta$. Since neural networks with non-smooth ReLU activation are non-smooth functions, we consider Clarke Jacobian (generalized Jacobian) [7] instead, which is defined as the convex hull of $\lim_{i \to \infty} \nabla f(\mathbf{x}_i)$ for any sequence $\{\mathbf{x}_i\}_{i=1}^\infty$ such that every $f(\mathbf{x}_i)$ is differentiable at $\mathbf{x}_i$. We denote the Clarke Jacobian at $\mathbf{x}$ as $\partial f(\mathbf{x})$, and then:

$$L^{(\alpha,\beta)}(f, \mathcal{X}) = \sup_{\mathbf{x} \in \mathcal{X}, \ \mathbf{J}(\mathbf{x}) \in \partial f(\mathbf{x})} \|\mathbf{J}(\mathbf{x})\|_{\alpha,\beta}. \tag{2}$$

Global Lipschitz constant, which considers the supremum over $\mathcal{X} = \mathbb{R}^d$, needs to guarantee Eq. (1) even for distant $\mathbf{x}_1, \mathbf{x}_2$, and thus it can be loose and cannot capture the local behavior of the network. We focus on local Lipschitz constants, where $\mathcal{X}$ is a small local region. Specifically, we consider $\mathcal{X} = B_p(\mathbf{x}_0, \epsilon) := \{\mathbf{x} : \|\mathbf{x} - \mathbf{x}_0\|_p \leq \epsilon\}$ which is a small ℓ_p-ball around $\mathbf{x}_0$, and then the local Lipschitz constant only needs to hold for input near $\mathbf{x}_0$, where $\mathbf{x}_0$ can be data points from clean datasets. When ϵ is large enough to cover any valid input, local Lipschitz constants will become global Lipschitz constants.

3.3 Backward Bound Propagation

To bound the Clarke Jacobian, we will use bound propagation which is originally used to compute the certified output bounds of neural networks. We adopt a backward bound propagation [46, 43, 33, 44] which typically propagates the linear relationship between the output layer to be bounded and all the previous layers it depends on. Suppose we want to compute certified bounds for output layer $h_n(\mathbf{x})$ w.r.t. all $\mathbf{x}$ from a small domain $B_p(\mathbf{x}_0, \epsilon)$. Starting from the output layer, we take $\mathbf{A}_n = \mathbf{I}$, and then $h_n(\mathbf{x}) = \mathbf{A}_n h_n(\mathbf{x})$. For every $i \in [n]$, suppose $h_i(\mathbf{x})$ can be bounded by linear functions w.r.t. $h_{i-1}(\mathbf{x})$ parameterized by $\underline{\mathbf{P}}_i, \overline{\mathbf{P}}_i, \underline{\mathbf{q}}_i, \overline{\mathbf{q}}_i$ (the bounds elementwise hold):

$$\underline{\mathbf{P}}_i h_{i-1}(\mathbf{x}) + \underline{\mathbf{q}}_i \leq h_i(\mathbf{x}) \leq \overline{\mathbf{P}}_i h_{i-1}(\mathbf{x}) + \overline{\mathbf{q}}_i. \tag{3}$$

Then for every $i = n, n-1, \cdots, 1$ in order, $\mathbf{A}_i h_i(\mathbf{x})$ can be recursively bounded by substituting $h_i(\mathbf{x})$ with Eq. (3):

$$\mathbf{A}_i h_i(\mathbf{x}) \leq \mathbf{A}_{i-1} h_{i-1}(\mathbf{x}) + \mathbf{c}_i, \text{where } \mathbf{A}_{i-1} = [\mathbf{A}_i]_+ \overline{\mathbf{P}}_i + [\mathbf{A}_i]_- \underline{\mathbf{P}}_i, \ \ \mathbf{c}_i = [\mathbf{A}_i]_+ \overline{\mathbf{q}}_i + [\mathbf{A}_i]_- \underline{\mathbf{q}}_i, \tag{4}$$

where $[\cdot]_+$ stands for taking positive elements from the matrix or vector, and vice versa for $[\cdot]_-$. $\mathbf{A}_{i-1}$ stands for the coefficients of the linear relationship propagated from layer i to layer $i-1$, and $\mathbf{c}_i$ is a bias term produced at this layer. By this recursive procedure in a backward manner and accumulating

$\mathbf{c}_i (i \in [n])$, eventually bounds are propagated to the input layer as $h_n(\mathbf{x}) \leq \mathbf{A}_0 \mathbf{x} + \sum_{i=1}^{n} \mathbf{c}_i$, which directly represents the linear relationship between the output layer and input. We can eliminate $\mathbf{x}$ from $\mathbf{A}_0 \mathbf{x}$ to obtain final bounds by considering the specific domain of $\mathbf{x}$. In particular, when $\mathbf{x} \in B_p(\mathbf{x}_0, \epsilon)$ $(p \geq 1)$, for every j-th dimension of $h_n(\mathbf{x})$, we can use the fact that $[\mathbf{A}_0]_{j,:}\mathbf{x} \leq [\mathbf{A}_0]_{j,:}\mathbf{x}_0 + \epsilon\|[\mathbf{A}_0]_{j,:}\|_q$, where $[\mathbf{A}_0]_{j,:}$ stands for the j-th row in $\mathbf{A}_0$, $q = 1/(1 - 1/p)$, and q-norm is the dual-norm of p-norm. All the bounds here provably hold for any $\mathbf{x} \in B_p(\mathbf{x}_0, \epsilon)$, and lower bounds can also be obtained by a similar bound propagation.

Parameters in Eq. (3) can be obtained by considering the relation between $h_i(\mathbf{x})$ and $h_{i-1}(\mathbf{x})$. We can first obtain bounds $\mathbf{l}_i \leq z_i(\mathbf{x}) \leq \mathbf{u}_i$ using bound propagation by viewing $z_i(\mathbf{x})$ as the output layer. Then the linear relaxation bounds $h_i(\mathbf{x}) = \sigma(z_i(\mathbf{x}))$ with linear functions of $z_i(\mathbf{x})$:

$$\forall \mathbf{l}_i \leq z_i(\mathbf{x}) \leq \mathbf{u}_i, \quad \underline{\mathbf{s}}_i z_i(\mathbf{x}) + \underline{\mathbf{t}}_i \leq \sigma(z_i(\mathbf{x})) \leq \overline{\mathbf{s}}_i z_i(\mathbf{x}) + \overline{\mathbf{t}}_i. \tag{5}$$

For every neuron j, if $[\mathbf{l}_i]_j \geq 0$ or $[\mathbf{u}_i]_j \leq 0$, $\sigma(z_i(\mathbf{x})) = z_i(\mathbf{x})$ or $\sigma(z_i(\mathbf{x})) = 0$ respectively is already linear, and then we can simply take $[\underline{\mathbf{s}}_i]_j[z_i(\mathbf{x})]_j + [\underline{\mathbf{t}}_i]_j = [\overline{\mathbf{s}}_i]_j[z_i(\mathbf{x})]_j + [\overline{\mathbf{t}}_i]_j = \sigma(z_i(\mathbf{x}))$. Otherwise when $[\mathbf{l}_i]_j < 0 < [\mathbf{u}_i]_j$, as illustrated in Figure 1, the upper bound can be the line passing ReLU activation at $[z_i(\mathbf{x})]_j = [\mathbf{l}_i]_j$ and $[z_i(\mathbf{x})]_j = [\mathbf{u}_i]_j$ respectively, i.e., $[\overline{\mathbf{s}}_i]_j[z_i(\mathbf{x})]_j + [\overline{\mathbf{t}}_i]_j = \left(\frac{\sigma([\mathbf{u}_i]_j) - \sigma([\mathbf{l}_i]_j)}{[\mathbf{u}_i]_j - [\mathbf{l}_i]_j}\right)(z_i(\mathbf{x}) - [\mathbf{l}_i]_j) + \sigma([\mathbf{l}_i]_j)$; the lower bound can be any line with a slope between 0 and 1 and a bias of 0, i.e., $0 \leq [\underline{\mathbf{s}}_i]_j \leq 1$, $[\underline{\mathbf{t}}_i]_j = 0$, where $[\underline{\mathbf{s}}_i]_j$ can be viewed as a parameter optimized with an objective of tightening output bounds [27, 45, 29]. To satisfy Eq. (3), we can take:

$$\underline{\mathbf{P}}_i = \text{diag}(\underline{\mathbf{s}}_i)\mathbf{W}_i, \quad \overline{\mathbf{P}}_i = \text{diag}(\overline{\mathbf{s}}_i)\mathbf{W}_i, \quad \underline{\mathbf{q}}_i = \text{diag}(\underline{\mathbf{s}}_i)\mathbf{b}_i + \underline{\mathbf{t}}_i, \quad \overline{\mathbf{q}}_i = \text{diag}(\overline{\mathbf{s}}_i)\mathbf{b}_i + \overline{\mathbf{t}}_i. \tag{6}$$

Figure 1: Two lines can bound the ReLU activation when the sign of its input is unstable ($-1.5 \leq x \leq 1.5$ in this example) and are used for bound propagation with linear relaxation.

Figure 2: Given the bound on the input to an absolute value function ($-1 \leq x \leq 1.5$ in this example), a line can upper bound the function. We take the blue one with slope $\frac{1}{3}$, while Zhang et al. [47] would take the green one with slope 0, which is a looser upper bound.

4 Methodology

We present our method in this section. We first present a novel view to formulate the local Lipschitz constant computation as a higher-order backward computational graph, and use bound propagation to obtain the bounds of the Clarke Jacobian. We discuss our methods for tightly bounding non-linearities in Clarke Jacobian, including the the norm of Clarke Jacobian and the Clarke gradient of activation. Finally, we use Branch-and-Bound to further tighten the bounds if time budget allows.

4.1 Clarke Jacobian for ReLU Networks

In ReLU networks, the ReLU activation for a single neuron is defined as $\sigma(x) = \max\{x, 0\}$. It is non-smooth at $x = 0$. When computing the Lipschitz constant, we consider Clarke gradient [7]: when $x < 0$, $\partial\sigma(x) = \{0\}$; when $x > 0$, $\partial\sigma(x) = \{1\}$; and when $x = 0$, $\partial\sigma(x) = [0, 1]$. For the i-th layer ($1 \leq i < n$), we use a diagonal matrix $\Delta_i(\mathbf{x})$ to denote the Clarke gradient of ReLU activation for all the neurons in the layer, i.e., $\Delta_i(\mathbf{x}) = \text{diag}\{\partial\sigma([z_i(\mathbf{x})]_j)\}$, where $\partial\sigma([z_i(\mathbf{x})]_j)$ is the Clarke gradient of the j-th neuron. Chain rule can be used to compute the Clarke Jacobian for the whole ReLU network, where Clarke gradient is used for ReLU activations. Denote $\mathbf{J}_i(\mathbf{x}) = \frac{\partial f(\mathbf{x})}{\partial h_{i-1}(\mathbf{x})}$ as the Clarke Jacobian w.r.t. the $(i-1)$-th layer in the chain rule, and we have

$$\mathbf{J}_n(\mathbf{x}) = \mathbf{W}_n, \quad \mathbf{J}_i(\mathbf{x}) = \mathbf{J}_{i+1}(\mathbf{x})\frac{\partial h_i(\mathbf{x})}{\partial h_{i-1}(\mathbf{x})} = \mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})\mathbf{W}_i \quad (i \in [n-1]), \tag{7}$$

Forward graph (original neural network computation)

Backward graph (norm of Clarke Jacobian)

Figure 3: Illustration of our proposed framework where we formulate the computation for local Lipschitz constants by augmenting the original computation graph of the neural network (forward graph) with an additional subgraph for computing the norm of Clarke Jacobian (backward graph). The backward graph relies on the pre-activation values $(\mathbf{z}_1(\mathbf{x}), \cdots, \mathbf{z}_{n-1}(\mathbf{x}))$ in the forward pass to compute the Clarke gradient of activations. Linear relaxation for two categories of nonlinearities in the backward graph (nodes in purple), norm ($\|\mathbf{J}_1(\mathbf{x})\|$) and applying Clarke gradient (σ') are detailed in Figure 2, Figure 4 and Figure 5. We also perform branch-and-bound (BaB) to tighten the bounds, where we branch on pre-activation nodes in the forward graph (nodes in green).

154 and finally $\mathbf{J}_1(\mathbf{x}) \in \partial f(\mathbf{x})$ is the Clarke Jacobian of the network. As we want to compute the Lipschitz
155 constant, by Eq. (2), we upper bound $\|\mathbf{J}_1(\mathbf{x})\|_{\alpha,\beta}$ w.r.t. all $\mathbf{x} \in \mathcal{X}$.

156 Given the forward pass computation of the original network, we can formulate a computational graph
157 for $\|\mathbf{J}_1(\mathbf{x})\|_{\alpha,\beta}$ in a backward pass accordingly as shown in Figure 3. We augment the original
158 forward graph with the backward graph, and the backward graph has a dependency on the output
159 of the forward graph due to $\Delta_1, \Delta_2, \cdots, \Delta_{n-1}$. We build the augmented graph by traversing the
160 forward graph, similar to automatic differentiation for neural network training. The computational
161 graph formulation for Clarke Jacobian allows our method to be easily generalized to different network
162 architectures, with a bound propagation framework for general neural networks [44], as long as the
163 linear relaxation for all the involved nonlinearities is well derived.

164 We use the bound propagation framework described in Section 3.3 to upper bound $\|\mathbf{J}_1(\mathbf{x})\|_{\alpha,\beta}$. On
165 the backward graph, when bounds are propagated to $\mathbf{J}_i(\mathbf{x})$, we use $\widetilde{\mathbf{A}}_i$ to denote the coefficient
166 matrix, and we use $\widetilde{\mathbf{c}}_i$ to denote the bias term (in contrast to $\mathbf{A}_i$ and $\mathbf{c}_i$ in Eq. (4)), and then we
167 have: $\forall i \in [n], \|\mathbf{J}_1(\mathbf{x})\|_{\alpha,\beta} \leq \widetilde{\mathbf{A}}_i \mathbf{J}_i(\mathbf{x}) + \sum_{j=0}^{i-1} \widetilde{\mathbf{c}}_j$. As intermediate bounds for $z_i(\mathbf{x})$ are needed
168 for bounding the forward graph, we also need intermediate bounds $\mathbf{L}_i \leq \mathbf{J}_i(\mathbf{x}) \leq \mathbf{U}_i$ ($\forall \mathbf{x} \in \mathcal{X}$) for
169 the backward graph. And there are particularly two categories of nonlinearities to be tackled on
170 the backward graph: 1) Norm in $\|\mathbf{J}_1(\mathbf{x})\|_{\alpha,\beta}$; 2) $\mathbf{J}_{i+1}(\mathbf{x})\Delta_i$ ($\forall i \in [n-1]$) in the chain rule as Eq.
171 (7), which applies the Clarke gradient of ReLU $\Delta_i(\mathbf{x})$ on the later layer's Clarke Jacobian. We
172 handle them in Section 4.2 and Section 4.3 respectively. Then bounds can be propagated starting
173 at $\|\mathbf{J}_1(\mathbf{x})\|_{\alpha,\beta}$, to $\mathbf{J}_1(\mathbf{x}), \mathbf{J}_2(\mathbf{x}), \cdots, \mathbf{J}_n(\mathbf{x})$ in order. Bounds are eventually propagated to $\mathbf{J}_n(\mathbf{x})$ as
174 $\|\mathbf{J}_1(\mathbf{x})\|_{\alpha,\beta} \leq \widetilde{\mathbf{A}}_n \mathbf{J}_n(\mathbf{x}) + \sum_{j=0}^{i-1} \widetilde{\mathbf{c}}_j$, where $\mathbf{J}_n(\mathbf{x})$ can be substituted by $\mathbf{J}_n(\mathbf{x}) = \mathbf{W}_n$ (Eq. (7)),
175 which yields final bounds on $\|\mathbf{J}_1(\mathbf{x})\|_{\alpha,\beta}$.

4.2 Norm of Clarke Jacobian

177 Norm of Clarke Jacobian is the first nonlinearity we would encounter during backward bound
178 propagation, as it is the last node in the backward graph (see Figure 3). In this paper, we mainly
179 consider ℓ_∞-norm with $\alpha = \beta = \infty$ for simplicity. When $f(\mathbf{x})$ is a K-way classifier and $f(\mathbf{x}) \in \mathbb{R}^k$,
180 we have $\mathbf{J}_1(\mathbf{x}) \in \mathbb{R}^{K \times d}$, and its norm is computed as $\|\mathbf{J}_1(\mathbf{x})\|_\infty = \max_{1 \leq k \leq K} \sum_{j=1}^d |[\mathbf{J}_1(\mathbf{x})]_{kj}|$,
181 where K rows in $\mathbf{J}_1(\mathbf{x})$ can be bounded separately, and after that we can aggregate results on K rows
182 by taking the max. And sometimes we may only care about one particular target class. Thus, for the
183 simplicity of the following analysis, we assume $K = 1$ as we can handle one row in $\mathbf{J}_1(\mathbf{x})$ at each
184 time, but they can still be batched in implementation. Then Clarke Jacobian $\mathbf{J}_i(\mathbf{x})$ ($i \in [n]$) and its
185 bounds $\mathbf{L}_i$, $\mathbf{U}_i$ can be viewed as row vectors, and we will use $[\cdot]_j$ to denote the j-th element. By a
186 tight linear relaxation for $|\cdot|$ as shown in Figure 2 (only the upper bound is needed), we have the
187 following bound for $\|\mathbf{J}_1(\mathbf{x})\|_\infty$:

Proposition 1. *Suppose* $\forall j \in [d]$, $[\mathbf{L}_1]_j \le [\mathbf{J}_1(\mathbf{x})]_j \le [\mathbf{U}_1]_j$ ($\forall \mathbf{x} \in \mathcal{X}$), *the following bound holds:*

$$\|\mathbf{J}_1(\mathbf{x})\|_\infty \le \widetilde{\mathbf{A}}_1 \mathbf{J}_1(\mathbf{x}) + \widetilde{\mathbf{c}}_0, \ \ where \ [\widetilde{\mathbf{A}}_1]_j = \frac{\big|[\mathbf{U}_1]_j\big| - \big|[\mathbf{L}_1]_j\big|}{[\mathbf{U}_1]_j - [\mathbf{L}_1]_j}, \ \ [\widetilde{\mathbf{c}}_0]_j = -[\widetilde{\mathbf{A}}_1]_j[\mathbf{L}_1]_j + \big|[\mathbf{L}_1]_j\big|.$$

We prove it in Appendix C.1, and this propagates bounds from the norm of Clarke Jacobian to $\mathbf{J}_1(\mathbf{x})$.

4.3 Clarke Gradient of the Activation

For each layer $i \in [n-1]$ in the chain rule for computing the Clarke Jacobian as Eq. (7), $\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})$ is involved in addition to fixed weight matrix $\mathbf{W}_i$. $\Delta_i(\mathbf{x})$ is determined by pre-activation value $z_i(\mathbf{x})$ from the forward graph. For the j-th neuron in the layer, $[\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j = [\mathbf{J}_{i+1}(\mathbf{x})]_j[\Delta_i(\mathbf{x})]_{jj}$, when $[\mathbf{u}_i]_j < 0$ or $[\mathbf{l}_i]_j > 0$, we have $[\Delta_i(\mathbf{x})]_{jj} = 0$ and $[\Delta_i(\mathbf{x})]_{jj} = 1$ respectively fixed, and then for these special cases $[\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j$ is linear w.r.t. $[\mathbf{J}_{i+1}(\mathbf{x})]_j$. Otherwise, $[\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j$ is nonlinear since both $[\mathbf{J}_{i+1}(\mathbf{x})]_j$ and $[\Delta(\mathbf{x})]_{jj}$ may vary given different $\mathbf{x} \in \mathcal{X}$. We then focus on relaxing the nonlinearity $[\mathbf{J}_{i+1}(\mathbf{x})]_j[\Delta_i(\mathbf{x})]_{jj}$ given $[\Delta_i(\mathbf{x})]_{jj} = [0, 1]$.

Figure 4: For a neuron j in layer i, when $[\Delta_i(\mathbf{x})]_{jj} = [0, 1]$ is uncertain, we plot $[\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j$ as a group of functions w.r.t. $[\mathbf{J}_{i+1}(\mathbf{x})]_j$ (violet area). In this example, $-1.5 \le [\mathbf{J}_{i+1}(\mathbf{x})]_j \le 1.5$. Our linear relaxation (dashed blue lines) is much tighter than interval bounds (dashed green lines) by Zhang et al. [47].

Figure 5: Computation graph for bounding each Clarke gradient. It is the internal computation for boxes in Figure 3. Two ReLU nodes are inserted as per Proposition 2. In bound propagation, the σ' node takes intermediate bounds from $z_i(\mathbf{x})$ to decide whether bounds are directly propagated from $\mathbf{J}_{i+1}(\mathbf{x})$ (no relaxation needed), or indirectly via $\sigma(\mathbf{J}_{i+1}(\mathbf{x}))$ and $-\sigma(-\mathbf{J}_{i+1}(\mathbf{x}))$ (with relaxation), for each neuron respectively.

As illustrated in Figure 4, the solid blue line and solid red line are the exact upper and lower bound respectively for $[\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j$, which are piecewise linear w.r.t. $[\mathbf{J}_{i+1}(\mathbf{x})]_j$. The most nontrivial case appears when $[\mathbf{L}_{i+1}(\mathbf{x})]_j < 0 < [\mathbf{U}_{i+1}(\mathbf{x})]_j$, where exact bounds for $[\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j$ are nonlinear given the input region. We relax the exact bounds into linear bounds that can be handled by bound propagation with linear relaxation. Previous works such as RecurJac [47] have not tightly bounded this linearity in the nontrivial case and commonly degenerate to interval bounds (dashed green lines with zero slopes in the figure, which are loose bounds).

In contrast, we propose a tight linear relaxation (dashed blue and red lines in Figure 4). We observe that the exact upper bound is essentially a ReLU function of $\mathbf{J}_{i+1}(\mathbf{x})$ (solid blue line in Figure 4), and the exact lower bound can be viewed as a ReLU function flipped both horizontally and vertically (solid red line in Figure 4). Formally, we have:

Proposition 2. *For the j-th neuron in layer $i(i \in [n-1])$, if $[\Delta_i(\mathbf{x})]_{jj} = [0, 1]$, we have:*

$$[\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j \ge \min\{[\mathbf{J}_{i+1}(\mathbf{x})]_j, 0\}, \ \ [\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j \le \max\{[\mathbf{J}_{i+1}(\mathbf{x})]_j, 0\}, \tag{8}$$

which can be rewritten using ReLU activation:

$$\min\{[\mathbf{J}_{i+1}(\mathbf{x})]_j, 0\} = -\sigma(-[\mathbf{J}_{i+1}(\mathbf{x})]_j), \ \ \max\{[\mathbf{J}_{i+1}(\mathbf{x})]_j, 0\} = \sigma([\mathbf{J}_{i+1}(\mathbf{x})]_j). \tag{9}$$

Its correctnesscan be easily verified by considering the sign of $[\mathbf{J}_{i+1}(\mathbf{x})]_j$ as shown in Appendix C.2. We then decompose $[\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j$ into two ReLU activations (Eq. (9)), as illustrated in Figure 5.

ReLU can be further relaxed by Eq. (5), as derived in Appendix C.3, which yields:

Proposition 3. *For the j-th neuron in the i-th layer ($i \in [n-1]$), given $[\Delta_i(\mathbf{x})]_{jj} = [0,1]$ and $[\mathbf{L}_{i+1}]_j \leq [\mathbf{J}_{i+1}(\mathbf{x})]_j \leq [\mathbf{U}_{i+1}]_j$, we have the following relaxation:*

$$[\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j \geq [\widetilde{\underline{\mathbf{s}}}_{i+1}]_j[\mathbf{J}_{i+1}(\mathbf{x})]_j + [\widetilde{\underline{\mathbf{t}}}_{i+1}]_j, \quad [\mathbf{J}_{i+1}(\mathbf{x})\Delta_i(\mathbf{x})]_j \leq [\widetilde{\overline{\mathbf{s}}}_{i+1}]_j[\mathbf{J}_{i+1}(\mathbf{x})]_j + [\widetilde{\overline{\mathbf{t}}}_{i+1}]_j,$$

$$\text{where} \quad [\widetilde{\underline{\mathbf{s}}}_{i+1}]_j = \frac{-\sigma(-[\mathbf{U}_{i+1}]_j) + \sigma(-[\mathbf{L}_{i+1}]_j)}{[\mathbf{U}_{i+1}]_j - [\mathbf{L}_{i+1}]_j}, \quad [\widetilde{\underline{\mathbf{t}}}_{i+1}]_j = -[\widetilde{\underline{\mathbf{s}}}_{i+1}]_j[\mathbf{L}_{i+1}]_j - \sigma(-[\mathbf{L}_{i+1}]_j),$$

$$[\widetilde{\overline{\mathbf{s}}}_{i+1}]_j = \frac{\sigma([\mathbf{U}_{i+1}]_j) - \sigma([\mathbf{L}_{i+1}]_j)}{[\mathbf{U}_{i+1}]_j - [\mathbf{L}_{i+1}]_j}, \quad [\widetilde{\overline{\mathbf{t}}}_{i+1}]_j = -[\widetilde{\overline{\mathbf{s}}}_{i+1}]_j[\mathbf{L}_{i+1}]_j + \sigma([\mathbf{L}_{i+1}]_j).$$

In the following theorem, we show that relaxation in Proposition 3 is the tightest linear relaxation:

Theorem 4. *For the j-th neuron in the i-th layer ($i \in [n-1]$), and any $\underline{s}, \underline{t}, \overline{s}, \overline{t}$ satisfying*

$$\forall J \in \left[[\mathbf{L}_{i+1}]_j, [\mathbf{U}_{i+1}]_j\right], \forall [\Delta_i(\mathbf{x})]_{jj} \in [0,1], \quad \underline{s}J + \underline{t} \leq J \cdot [\Delta_i(\mathbf{x})]_{jj} \leq \overline{s}J + \overline{t}, \quad (10)$$

we have

$$(\underline{s}, \underline{t}) \neq ([\widetilde{\underline{\mathbf{s}}}_{i+1}]_j, [\widetilde{\underline{\mathbf{t}}}_{i+1}]_j) \implies \forall [\mathbf{L}_{i+1}]_j < J < [\mathbf{U}_{i+1}]_j, \quad \underline{s}J + \underline{t} < [\widetilde{\underline{\mathbf{s}}}_{i+1}]_j J + [\widetilde{\underline{\mathbf{t}}}_{i+1}]_j,$$

$$(\overline{s}, \overline{t}) \neq ([\widetilde{\overline{\mathbf{s}}}_{i+1}]_j, [\widetilde{\overline{\mathbf{t}}}_{i+1}]_j) \implies \forall [\mathbf{L}_{i+1}]_j < J < [\mathbf{U}_{i+1}]_j, \quad \overline{s}J + \overline{t} > [\widetilde{\overline{\mathbf{s}}}_{i+1}]_j J + [\widetilde{\overline{\mathbf{t}}}_{i+1}]_j,$$

where $[\widetilde{\underline{\mathbf{s}}}_{i+1}]_j, [\widetilde{\underline{\mathbf{t}}}_{i+1}]_j, [\widetilde{\overline{\mathbf{s}}}_{i+1}]_j, [\widetilde{\overline{\mathbf{t}}}_{i+1}]_j$ are by Proposition 3.

This theorem states that our proposed linear relaxation is provably tighter than any other valid linear relaxation. We prove this theorem in Appendix C.4.

4.4 Branch and Bound

Formulating the backward computational graph also enables the use of Branch-and-Bound (BaB) to further tighten the bounds if time budget allows. We denote $\mathcal{C}_0 = \{(\mathbf{l}_1, \mathbf{u}_1), (\mathbf{l}_2, \mathbf{u}_2), \cdots (\mathbf{l}_{n-1}, \mathbf{u}_{n-1})\}$ as the domain of all pre-activation bounds of ReLU neurons before BaB, not including ReLU from Eq. (9). We use $\mathcal{C}$ to denote a pool of domains that we currently have, and initially $\mathcal{C} = \{\mathcal{C}_0\}$. BaB aims to recursively split domains in $\mathcal{C}$ into smaller subdomains $\mathcal{C}_1, \mathcal{C}_2, \cdots$, where $\mathcal{C}_0 = \mathcal{C}_1 \bigcup \mathcal{C}_2 \bigcup \cdots$), and bounds for each domain can be computed respectively using bound propagation, since linear relaxation can generally be tighter with smaller domains.

At each iteration, we take B domains in $\mathcal{C}$ with loosest bounds, where B is the batch size for BaB (we take all if there are fewer domains). For each domains, we choose one layer $\hat{i}$ and one ReLU neuron $\hat{j}$ in layer $\hat{i}$ on the forward graph, such that the neuron has uncertain Clarke gradient for this domain, i.e., $[\mathbf{l}_{\hat{i}}]_{\hat{j}} \leq 0 \leq [\mathbf{u}_{\hat{i}}]_{\hat{j}}$. We branch this domain into two subdomains with intermediate bounds $([\mathbf{l}_{\hat{i}}]_{\hat{j}}, -\tilde{\epsilon})$ and $(\tilde{\epsilon}, [\mathbf{l}_{\hat{i}}]_{\hat{j}})$ respectively, where $\tilde{\epsilon}$ is a sufficiently small value (e.g., 10^{-9}). Thereby, the Clarke gradient for ReLU becomes certain in each subdomain (0 and 1 respectively) with other neurons unchanged. We compute the bounds for the new subdomains, and we repeat this process until reaching a time limit or there is no domain with uncertain Clarke gradient to branch.

We use a heuristic score to decide which neuron to branch for a given domain, by estimating the potential improvement to the bounds after the branching [5]. Here for branching a ReLU neuron on the forward graph, we estimate the potential improvement on the bounds of the backward graph. In particular, suppose neuron $\hat{j}$ in layer $\hat{i}$ is branched, the gap between the upper and lower bound in the liner relaxation is eliminated, which can tighten the final bound. We estimate the area of the gap before branching (the gap between the blue dashed line and the red dashed line in Figure 4) as $\frac{1}{2}([\mathbf{U}_{\hat{i}+1}]_{\hat{j}} - [\mathbf{L}_{\hat{i}+1}]_{\hat{j}})^2$, multiplied by the coefficient $[\widetilde{\mathbf{A}}_{\hat{i}}]_{\hat{j}}$ from the bound propagation as the heuristic score. We thereby branch neurons with highest scores.

5 Experiments

In our experiments, we focus on evaluating the tightness of local Lipschitz bounds and the efficiency of computation. There are three parts: 1) We compare the tightness and efficiency on relatively small models and synthetic data, to accommodate slow baselines; 2) We also use practical image datasets with larger models. 3) Finally, we demonstrate an application of our method on analyzing the monotonicity of neural networks. Additional experimental details are provided in Appendix B.

256 **Baselines** We compare our methods to the following baselines: **NaiveUB** upper bounds Lipschitz
257 constants simply by multiplying the induced norm of each layer, which can scale to arbitrarily large
258 models but the bound is often vacuous; **LipMIP** [18] computes exact local Lipschitz constants using
259 MIP, which compute the exact (tightest) bound but can only work for very small models. **LipSDP** [11]
260 computes upper bounds of ℓ_2 local Lipschitz constants using SDP, and we convert their ℓ_2 results
261 into upper bounds for the ℓ_∞-case by a $\sqrt{d}$ factor. **LipBaB** [3] uses loose interval bounds with
262 branch-and-bound. **RecurJac** [47] uses bound propagation with interval bounds in nontrivial cases
263 but has tightened bounds for some special cases. All the baselines do not support CNN in their
implementation, and we need to convert CNN models to equivalent MLP models for baselines.

Table 1: Local Lipschitz constant values and runtime (seconds) on MLP and CNN models with
growing width for a synthetic input data point with 16 dimensions. Smaller values indicate tighter
results. Width for MLP stands for number of neurons in each hidden layer, and width for CNN stands
for number of filters in each convolutional layer. "C" and "F" in the model name for CNN denote
number of convolutional layers and fully-connected layers respectively. We set a timeout of 1000s for
LipMIP and LipSDP, and 60s for BaB. "*" denotes that we report the upper bound LipMIP returns at
timeout, and "-" means LipSDP cannot return an upper bound at timeout.

| Method | 4-Layer MLP | | | | | | CNN-2C1F | | | | | |
| | Width=32 | | Width=64 | | Width=128 | | Width=4 | | Width=8 | | Width=16 | |
	Value	Runtime	Value	Runtime	Value	Runtime	Value	Runtime	Value	Runtime	Value	Runtime
NaiveUB	24.31	0.05	33.02	0.01	49.39	0.00	24.38	0.00	39.99	0.01	51.68	0.03
LipMIP	12.13	16.25	102.64	1,000.05*	456.89	1,000.12*	9.54	1,000.08*	57.88	1,000.17*	628.91	1,000.40*
LipSDP	21.49	11.01	27.27	103.04	-	-	11.03	729.92	-	-	-	-
LipBaB	12.13	2.92	30.59	63.16	73.71	60.98	5.39	61.62	15.34	61.43	36.40	81.82
RecurJac	12.38	17.40	20.25	17.07	47.23	16.66	5.02	16.21	9.02	16.73	38.19	16.38
Ours (w/o BaB)	12.28	6.95	17.45	6.42	35.66	6.67	4.69	7.29	8.41	7.40	30.28	7.29
Ours (w/ BaB)	12.13	8.13	16.30	13.57	28.69	60.10	4.69	7.59	8.19	52.29	28.6	60.1

5.1 Comparison on a Synthetic Dataset

266 We follow Jordan & Dimakis [18] and train several small models on a synthetic dataset. We compare
267 different methods on models with varying width as shown in Table 1, and we also show results with
268 varying depth and ϵ in Appendix A.1. Since some of these models are already large for LipMIP, we
269 set a time limit of 1000 seconds, and we report the upper bound it returns at timeout. For our BaB,
270 we set a timeout of 60 seconds and stop further branching at timeout.

271 Without BaB, our method is very efficient while it already outperforms baselines on tightness except
272 for LipMIP on the smallest MLP. Compared to LipMIP, for the smallest MLP on which LipMIP does
273 not timeout, our result without BaB is very close to their exact result; and for other relatively larger
274 models, LipMIP cannot produce exact results within the timeout and our result is much tighter than
275 the upper bounds by LipMIP. And LipSDP fails to yield results within the timeout on many models.
276 Although LipBaB has BaB to tighten bounds, their results are still loose within the time budget,
277 since their BaB is based on loose interval bounds and is thus inefficient. RecurJac is a relatively
278 efficient baseline but still returns looser bounds compared to our method. Our BaB further improves
279 the tightness of our bounds, and our method with BaB consistently produces tightest results within a
280 reasonable time budget, compared to all the baselines.

5.2 Comparison on Image Datasets

Table 2: Average local Lipschitz constant values and runtime (seconds) on MNIST. Clean accuracy is
evaluated on the entire test set, and Lipschitz constants are evaluated on the first 100 examples in the
test set. We set a timeout value of 120s for LipMIP and 60s for BaB. "-" means LipMIP and LipBaB
cannot return any valid upper bound at timeout on the CNN model.

| Model | Clean acc. | NaiveUB | | LipMIP | | LipBaB | | RecurJac | | Ours (w/o BaB) | | Ours (w/ BaB) | |
		Value	Runtime	Value	Runtime	Value	Runtime	Value	Runtime	Value	Runtime	Value	Runtime
3-layer MLP	94.90%	3,257.16	0.00	14,218.99*	120.51	947.69	62.77	1,091.31	0.22	667.35	4.95	397.25	52.23
CNN-2C2F	98.83%	80,239.62	0.00	-	-	-	-	12,514.55	115.43	5,473.03	8.21	5,458.84	60.04

282 To further evaluate the scalability of different methods to relatively large models, we then conduct
283 experiments on image datasets including MNIST [25], CIFAR-10 [21], and TinyImagenet [24]. We
284 use a 3-layer MLP and a 4-layer CNN on MNIST, and we use 4-layer and 6-layer CNN models on
285 CIFAR-10 and TinyImageNet. All the models here are too large for LipSDP; LipMIP and LipBaB
286 can only handle the MLP model on MNIST, and they cannot return any valid upper bound for the

Table 3: Average local Lipschitz constant values and runtime (seconds) on CIFAR-10 and TinyImageNet. Clean accuracy is evaluated on the entire test set, and Lipschitz constants are evaluated on the first 100 examples in the test set. Baselines except NaiveUB cannot handle these models.

| Dataset | CIFAR-10 | | TinyImageNet | |
Model	CNN-2C2F	CNN-4C2F	CNN-2C2F	CNN-4C2F
Clean accuracy	76.53%	78.91%	29.97%	29.1%
NaiveUB	1707252.88	365293440.00	1512185.25	87148664.00
Value (ours)	18638.14	1049447.88	4556.61	25096.26
Runtime (ours)	11.17	29.79	95.42	137.04

Table 4: Percentage of examples on which the predicted confidence for high income level is monotonically increasing ($\uparrow$) or decreasing ($\downarrow$) w.r.t. each feature.

Feature	$\uparrow$	$\downarrow$
Age	40%	0%
Education num	58%	0%
Capital gain	5%	0%
Capital loss	7%	0%
Hours-per-week	98%	0%

CNN models within a reasonable time budget; RecurJac can handle the CNN model on MNIST, but other CNN models on CIFAR-10 and TinyImageNet are still too large for RecurJac after converted to equivalent MLP models. In contrast, our formulation for the backward computational graph allows us to utilize the efficient bound propagation for convolutional layers from Xu et al. [44]. We do not enable BaB to save time cost on these large datasets. We show results in Table 2 and Table 3. Our results are much tighter compared to the baselines even if we do not enable BaB, and BaB can further tighten results. More importantly, our method can scale to larger CNN models on CIFAR-10 and TinyImageNet that previous works could not handle. We present additional results in Appendix.

5.3 An Application on Monotonicity Analysis

We further use an application to demonstrate that our proposed method can be used to check the monotonicity of neural networks. Given a network, we aim to check whether the network's output is a monotonic function w.r.t. each input feature. Monotonicity can be preferred properties in some real-world scenarios [32, 8, 26, 34]. In this experiment, we adopt the Adult dataset [4], with a binary classification task about predicting income level. There are only several continuous features, and we aim to check the monotonicity of income level w.r.t. age, education number, capital gain, capital loss, and hours per week. We train an MLP model on this dataset and verify its monotonicity on the first 100 test examples. Signs of Clarke Jacobian can be used to check monotonicity [31], and we achieve this by checking the bounds of Clarke Jacobian. For each continuous feature j we concern, we set an input domain $\mathcal{X}_j$ where only this particular feature can be varied between the minimum and maximum possible values of this feature in the dataset, while we keep other features fixed. And then we obtain bounds on the Clarke Jacobian of the output class for high income level, as $\mathbf{L}_1 \leq \mathbf{J}_1(\mathbf{x}) \leq \mathbf{U}_1$ ($\forall \mathbf{x} \in \mathcal{X}_j$). Then if $[\mathbf{L}_1]_j > 0$, the predicted confidence on high income level is monotonically increasing w.r.t. feature j, and vice versa. We count the percentage of examples that satisfy each type of monotonicity respectively. We show results in Table 4. It suggests that the predicted confidence on high income level tends to be monotonically increasing w.r.t. age, education number, and hours per week, which is reasonable. Results also suggest that the models learn little monotonicity on capital gain or loss features.

6 Conclusion

In this paper, we propose an efficient framework to compute tight local Lipschitz constants for neural networks by upper bounding the norm of Clarke Jacobian. We model the computation for the Clarke Jacobian as a backward computational graph. On the backward graph, we conduct bound propagation and propose tight linear relaxation for nonlinearities in Clarke Jacobian. We further tighten bounds with branch-and-bound when time budget allows. Experiments show that our method efficiently produces much tighter results compared to existing relaxed methods and can scale to larger convolutional networks on which previous works cannot handle. However, it remains challenging to handle even more large-scale models such as those for ImageNet [9], and it will be interesting for future work to further extend the scalability. Lastly, we also use our method to analyze the monotonicity of neural networks as a potential application.

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