Abstract

The Lipschitz constant of a neural network is a useful metric for provable robustness and generalization. We present a novel analytic result which relates gradient norms to Lipschitz constants for nondifferentiable functions. Next we prove hardness and inapproximability results for computing the local Lipschitz constant of ReLU neural networks. We develop a mixed-integer programming formulation to exactly compute the local Lipschitz constant for scalar and vector-valued networks. Finally, we apply our technique on networks trained on synthetic datasets and MNIST, drawing observations about the tightness of competing Lipschitz estimators and the effects of regularized training on Lipschitz constants.

1. Introduction

We are interested in computing the Lipschitz constant of neural networks with ReLU activations. Formally, for a network $f$ with multiple inputs and outputs, we are interested in the quantity

$$\sup_{x \neq y} \frac{||f(x) - f(y)||_\beta}{||x - y||_\alpha}.$$  

(1)

We allow the norm of the numerator and denominator to be arbitrary and further consider the case where $x, y$ are constrained in a subset of $\mathbb{R}^n$ leading to the more general problem of computing the local Lipschitz constant.

Estimating or bounding the Lipschitz constant of a neural network is an important and well-studied problem. For the Wasserstein GAN formulation (Arjovsky et al., 2017) the discriminator is required to have a bounded Lipschitz constant, and there are several techniques to enforce this (Arjovsky et al., 2017; Cisse et al., 2017; Petzka et al., 2017). For supervised learning Bartlett et al. (2017) have shown that classifiers with lower Lipschitz constants have better generalization properties. It has also been observed that networks with smaller gradient norms are more robust to adversarial attacks. Further, Lipschitz bounds can be used for certifiable robustness against targeted adversarial attacks (Szegedy et al., 2013; Weng et al., 2018a).

The Lipschitz constant of a function is fundamentally related to the maximal norm of its Jacobian matrix. Previous work has demonstrated the relationship between these two quantities for functions that are scalar-valued and continuously differentiable (Latorre et al., 2019; Paulavičius & Žilinskas, 2006). However, neural networks used for multi-class classification with ReLU activations do not meet either of these assumptions. We establish an analytical result that allows us to compute Lipschitz constants of vector-valued ReLU networks by searching only over the subset of inputs where the network is differentiable.

Exactly computing Lipschitz constants of scalar-valued neural networks under the $\ell_2$ norm was shown to be NP-hard (Virmaux & Scaman, 2018). In this paper we establish strong inapproximability results showing that it is hard to even approximate Lipschitz constants of scalar-valued ReLU networks, for $\ell_1$ and $\ell_\infty$ norms.

A variety of algorithms exist that estimate Lipschitz constants for various norms. To the best of our knowledge, none of these techniques are exact: they are either upper bounds, or heuristic estimators with no provable guarantees. In this paper

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we present the first technique to provably exactly compute Lipschitz constants of ReLU networks under certain norms. Our method is called LipMIP and relies on Mixed-Integer Program (MIP) solvers. As expected from our hardness results, our algorithm runs in exponential time in the worst case. At any intermediate time our algorithm may be stopped early to yield valid upper bounds.

We demonstrate an application of LipMIP towards untargeted robustness certificates. Access to a provably correct technique to compute Lipschitz constants of neural networks allows reliable empirical insights about random networks and how various training schemes affect Lipschitz constants of ReLU networks.

Our contributions are as follows:

• We present novel analytic results connecting the Lipschitz constant of an arbitrary function to the supremal norm of the Jacobian, over only the points where the Jacobian is defined.

• We show that that it is provably hard to approximate the Lipschitz constant of a network. Our proof works by developing a strict reduction from maximum independent set, one of the hardest known problems to approximate.

• We present a Mixed-Integer Programming formulation (LipMIP) that is able to exactly compute the Lipschitz constant of a scalar-valued ReLU network over a polyhedral domain.

• We demonstrate how to extend LipMIP to vector-valued networks and apply these results towards the problem of untargeted adversarial robustness.

• We analyze the efficiency and accuracy of LipMIP against other Lipschitz estimators. We provide experimental data demonstrating how Lipschitz constants change under training.

2. Related Work

Lipschitz Estimation Techniques: There are many various settings under which the Lipschitz constant of a neural network may be evaluated. We highlight several techniques to estimate this value in Table 1. The primary settings of interest are: whether the estimator provides an estimate of the local or global Lipschitz constant (Local/Global); whether the returned estimate is guaranteed to be an upper-bound, lower-bound, or a heuristic estimator (Guarantee); which $\ell_p$-norms can be handled in the case that $f$ is scalar-valued ($\ell_p$-norms); and whether differentiable or nondifferentiable activations are supported (Activation). We note that for most applications, the domain of interest is bounded, so local estimators may be used over this entire domain to yield a ‘global’ estimate of the Lipschitz constant.

We will summarize the main idea of each technique listed above. FastLip provides local Lipschitz upper bounds extremely efficiently by using interval-bound propagation (Weng et al., 2018a). LipSDP uses incremental quadratic constraints to yield a global upper bound on the $\ell_2$ Lipschitz constant (Fazlyab et al., 2019). A naive global or local lower bound can be attained by sampling random points and evaluating their gradient norms; CLEVER is a heuristic approach which extends this technique by leveraging extremal value theory (Weng et al., 2018b). SeqLip frames gradient maximization as a combinatorial optimization problem and leverages greedy approaches to provide heuristic estimates (Virmaux & Scaman, 2018). LipOpt provides local and global upper bounds for continuously differentiable networks using polynomial optimization (Latorre et al., 2019).

Adversarial Robustness: As Lipschitz estimation is deeply tied to adversarial robustness, we make the general statement that many techniques estimating certifiable robustness are directly applicable to Lipschitz estimation. FastLip is an example of this, which implicitly applies abstract interpretations to the gradient operator (Weng et al., 2018a). There is a deep body of
work using mixed-integer programming to verify the robustness of a neural network (Lomuscio & Maganti, 2017; Fischetti & Jo, 2018; Tjeng et al., 2017; Dutta et al., 2017; Cheng et al., 2017; Xiao et al., 2018). Our work, then, can be viewed as both an extension of this line of work, where we introduce machinery to compute gradients and their norms as mixed-integer programs. Additionally, our linear programming relaxation can be viewed as an extension of the linear-programming formulation by Wong et al. (Zico Kolter & Wong, 2017).

3. Gradient Norms and Lipschitz Constants

Here we discuss the relation between gradient norms and Lipschitz constants. While the primary focus of this paper is about computing the $\ell_1, \ell_\infty$ local Lipschitz constant of scalar-valued ReLU networks, we present our results for arbitrary norms over vector-valued Lipschitz continuous functions. First we formally define the local Lipschitz constant of a function:

**Definition 1.** We say that a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is locally $(\alpha, \beta)$-Lipschitz continuous over an open domain $\mathcal{X} \subseteq \mathbb{R}^n$ if there exists a constant, $L$, such that

$$
||f(x) - f(y)||_\beta \leq L||x - y||_\alpha \quad \forall x, y \in \mathcal{X}. 
$$

Letting $L$ be the set of constants $L$ for which inequality 2 holds, the **local Lipschitz constant** is defined as

$$
L^{(\alpha, \beta)}(f, \mathcal{X}) := \inf_{L \in L} \sup_{x, y \in \mathcal{X}} \frac{||f(y) - f(x)||_\beta}{||x - y||_\alpha}. 
$$

If $f$ is scalar-valued, then we denote the above quantity $L_\alpha(f, \mathcal{X})$ where $|| \cdot ||_\beta = | \cdot |$ is implicit. For scalar-valued $f$ that are continuously differentiable, this problem has been well studied (Latorre et al., 2019; Paulavičius & Žilinskas, 2006). In particular, if $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and is continuously differentiable over an open set $\mathcal{X}$, then

$$
L_\alpha(f, \mathcal{X}) := \sup_{x \neq y} \frac{|f(x) - f(y)|}{||x - y||_\alpha} = \sup_{x \in \mathcal{X}} ||\nabla f(x)||_\alpha^*, 
$$

where $|| \cdot ||_\alpha$ is an $\ell_p$ norm and $|| \cdot ||_\alpha^*$ is the dual norm of $|| \cdot ||_\alpha$.

However, as far as we know, there are no results that hold for functions that are both Lipschitz continuous, but nondifferentiable, nor for vector-valued functions. To this end, we prove a novel analytic result:

**Theorem 1.** Let $|| \cdot ||_\alpha, || \cdot ||_\beta$ be arbitrary norms over $\mathbb{R}^n, \mathbb{R}^m$, and let $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be locally $(\alpha, \beta)$-Lipschitz continuous over an open set $\mathcal{X}$. Letting $\text{Diff}(\mathcal{X})$ be the subset of $\mathcal{X}$ where the Jacobian of $f$, $\nabla f$, is defined, the following equality holds:

$$
L^{(\alpha, \beta)}(f, \mathcal{X}) = \sup_{x \in \text{Diff}(\mathcal{X})} ||\nabla f(x)||_\alpha^*, 
$$

where the matrix norm $||M||_{\alpha, \beta}$ is defined as $||M||_{\alpha, \beta} := \sup_{||v||_{\alpha} \leq 1} ||Mv||_\beta$.

**Remarks:** In the case where $f$ is scalar-valued, the Jacobian $\nabla f(x)$ is a vector and $||\nabla f(x)||_{\alpha, \beta} = ||\nabla f(x)||_{\alpha^*}$, up to scaling based on $|| \cdot ||_\beta$, thereby recovering the known result from equation 4.

We defer the proof to the appendix, but sketch the main ideas here. The main technical machinery needed is Rademacher’s theorem and the uniform continuity of Lipschitz-continuous functions. We prove a lemma stating that the supremum over directional derivatives is bounded by the right-hand side of equation 5. From here, the proof ideas are a multivariate extension of the scalar-valued continuously differentiable case.

4. Neural Networks and Inapproximability

Now we provide formal definitions for ReLU networks and prove inapproximability results for the optimization problem presented in equation 5.

$^1$The dual norm of $|| \cdot ||_\alpha$ is defined as $||x||_{\alpha^*} := \sup_{||y||_{\alpha} \leq 1} |x^T y|$
We provide an intricate construction, so we will outline a general strategy for developing mixed-integer programming formulations. The key insight in how one develops mixed-integer programming formulations comes from the following simple observation. The inapproximability results of the previous section demonstrate that without structural assumptions, it is hopeless to try to develop polynomial time algorithms that can provably approximate the Lipschitz constant of a ReLU network. Instead we develop polynomial time algorithms that provide provable guarantees but do not run in polynomial time in the worst case. Namely, for a scalar-valued ReLU network \( f \) with only a constant factor increase in encoding size, the size of the max-independent set problem to a ReLU network \( f \), with only a constant factor increase in encoding size. The size of the max-independent set of \( G \) is exactly the maximal \( \ell_1 \) or \( \ell_\infty \) norm attained by \( f \).

### 5. Mixed-Integer Programming

The inapproximability results of the previous section demonstrate that without structural assumptions, it is hopeless to try to develop polynomial time algorithms that can provably approximate the Lipschitz constant of a ReLU network. Instead we can develop algorithms that provide provable guarantees but do not run in polynomial time in the worst case. Namely, for a scalar-valued ReLU networks \( f \), we will demonstrate that we can use mixed-integer programming to solve the optimization problem of Theorem 1:

\[
\max_{x \in \text{Diff}(X)} \| \nabla f(x) \|_*,
\]

where \( \| \cdot \| \) is the \( \ell_1 \) or \( \ell_\infty \) norm. By Theorem 1, this is equivalent to computing \( L^\infty(f, X) \), \( L^1(f, X) \). While mixed-integer programming is intractable in general, the hope is that average-case runtime is significantly better than the worst-case runtime. We provide an intricate construction, so we will outline a general strategy for developing mixed-integer programming formulations. We start by defining the feasible sets we will work with:

**Definition 3.** A **mixed-integer polytope** is a set \( M \subseteq \mathbb{R}^n \times \{0, 1\}^m \) that satisfies a set of linear inequalities:

\[
M := \{ (x, a) \subseteq \mathbb{R}^n \times \{0, 1\}^m \mid Ax + Ba \leq c \}
\]

Mixed-integer programming (MIP) optimizes a linear function over the feasible set of a mixed-integer polytope.

The key insight in how one develops mixed-integer programming formulations comes from the following simple observation. Suppose we wish to solve the optimization problem \( \max_{x \in \mathcal{X}} f(x) \) for some function scalar-valued \( f \). Letting \( \mathcal{Y} \) be the range of \( f \) over \( \mathcal{X}, \mathcal{Y} := \{ f(x) \mid x \in \mathcal{X} \} \), then

\[
\max_{x \in \mathcal{X}} f(x) = \max_{y \in \mathcal{Y}} y.
\]

In particular, if \( \mathcal{X} \) is a mixed-integer polytope and \( f \) has structure such that the range \( \mathcal{Y} \) is also a mixed-integer polytope, then we may rephrase our optimization problem as a linear objective function, where the feasible region is a mixed-integer polytope.
polytope. Further, we note that if instead we wished to optimize \( g(f(x)) \) over \( \mathcal{X} \), if \( \mathcal{Y} \) is defined as above and \( \mathcal{Z} \) is defined \( \mathcal{Z} := \{ g(y) \mid y \in \mathcal{Y} \} \), the optimization becomes
\[
\max_{x \in \mathcal{X}} g(f(x)) = \max_{y \in \mathcal{Y}} g(y) = \max_{z \in \mathcal{Z}} z. \tag{11}
\]
So then the problem of optimizing \( ||\nabla f(x)||_\ast \) for ReLU nets \( f \) becomes one of modeling the range of \( ||\nabla f(x)||_\ast \) over \( \mathcal{X} \) as a mixed-integer polytope. To this end, we define ‘MIP-encodable functions’ as

**Definition 4.** A function \( g : \mathbb{R}^n \times \{0, 1\}^m \rightarrow \mathbb{R}^{n'} \times \{0, 1\}^{m'} \) is **MIP-encodable** if there exists a system of linear inequalities \( \mathcal{L} \), \( \mathcal{G} \), over variables \( (x, x') \) such that \( x' = g(x) \) if and only if \( \mathcal{G}(x, x') \) is satisfied.

Then given a polytope \( M \), and a MIP-encodable function \( g \), one can construct a mixed-integer polytope \( M' := \{ (x, x') \mid x \in M \land \mathcal{G}(x, x') \} \) such that the relation holds
\[
\{ g(x) \mid x \in M \} = \{ x' \mid \exists x \text{ s.t. } (x, x') \in M' \}. \tag{12}
\]
Hence we can model the mapping of mixed-integer polytopes through MIP-encodable functions by lifting dimension and adding constraints. We note that if this procedure is valid for functions \( g, h \), then it is also valid for their composition \( h \circ g \). As our desired function of interest is \( ||\nabla f(\cdot)||_\ast \), a feasible strategy is to write this function as a composition of MIP-encodable functions and iteratively perform this dimension-lifting step.

**MIP-encodable components of ReLU networks:** We aim to show that evaluating \( ||\nabla f(x)||_\ast \) is a composition of three simple MIP-encodable functions: namely, the affine, conditional and switch operators. We define these presently. **Affine operators** \( A : \mathbb{R}^n \rightarrow \mathbb{R}^m \) are defined as
\[
A(x) = Wx + b, \tag{13}
\]
for some fixed matrix \( W \) and vector \( b \).

The **conditional operator** \( C : \mathbb{R} \rightarrow \{0, 1\} \) is defined as
\[
C(x) = \begin{cases} 
1 & \text{if } x \geq 0 \\
0 & \text{if } x < 0. 
\end{cases} \tag{14}
\]

The **switch operator** \( S : \mathbb{R} \times \{0, 1\} \rightarrow \mathbb{R} \) is defined as
\[
S(x, a) = x \cdot a. \tag{15}
\]
Note that \( \text{ReLU}(x) = S(x, C(x)) \). The explicit definition of the conditional operator here is a point of convenience, as we’ll require the output of conditional operators when computing gradients.

We can now claim that \( f(x) \) and \( ||\nabla f(x)||_\ast \) may be written as a composition of these operators.

**Lemma 1.** Let \( f \) be a scalar-valued ReLU network. Then \( f(x) \) may be written as a composition of affine, conditional and switch operators. For all \( x \) such that \( \nabla f(x) \) exists, \( ||\nabla f(x)||_\ast \) may be written as a composition of affine, conditional, and switch operators, for the \( || \cdot ||_1, || \cdot ||_\infty \) norms.

The general idea behind this construction is to notice that both \( f(x) \) and \( \nabla f(x) \) can be constructed recursively, layer-by-layer. Each layer is only an affine and ReLU operator in the forward direction, and each layer is only an affine and a switch operator in the backwards direction. The absolute value operator \( | \cdot | \) can be viewed as an affine operator applied to ReLU operators. Finally, the max operator may also be written using only affine and ReLU operators. Thus we can write the \( || \cdot ||_1, || \cdot ||_\infty \) norms as such a composition. For later convenience, we will generalize the \( || \cdot ||_1, || \cdot ||_\infty \) norms as linear norms:

**Definition 5.** \( || \cdot ||_\alpha \) is a **linear norm** if the unit ball under the dual norm \( || \cdot ||_\alpha \) may be represented as a mixed-integer polytope.

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2Formally we define a linear inequality as a boolean-valued function over \( \mathbb{R}^n \times \{0, 1\}^m \) of the form \( (a_i^T x \leq b_i) \). A system of linear inequalities is a boolean-valued function that is the conjunction of linear inequalities.
Where we note that both the $\ell_\infty$ and $\ell_1$ unit balls are polytopes, and hence $|| \cdot ||_1, || \cdot ||_\infty$ are linear norms.

**MIP-encodability of Affine, Conditional, Switch:** Next we must demonstrate that affine, conditional, and switch operators are indeed MIP-encodable. In general this is not true. However it is true under the assumption that global lower and upper bounds are known. We discuss in detail how to construct these upper and lower bounds in the appendix. In brief, this is done by extending the abstract interpretation work used in certifiable robustness domains (Singh et al., 2019). We encapsulate the MIP-encodability of affine, conditional and switch operators in the following lemma:

**Lemma 2.** Let $g$ be a composition of affine, conditional and switch operators, where global lower and upper bounds are known for each input to the composition. Then $g$ is a MIP-encodable function.

We defer the formal proof of this fact to the appendix. The proof idea for each of the affine, conditional, and switch operators is the same: we define a new variable $x'$ to represent the output of operator $g$. Then we construct a system of linear inequalities, $\Gamma(x, x')$, such that if $x$ lies in between the assumed upper and lower bounds, $(g(x) = x') \iff \Gamma(x, x')$.

**Formulating LipMIP:** With the previous two lemmas at hand, we can now formally define the procedure of how to encode the optimization problem, $\max_{x \in \mathcal{X}} ||\nabla f(x)||$, as a mixed-integer program, where $\mathcal{X}$ is a bounded polytope and the norm is either the $\ell_1$ or $\ell_\infty$ norm.

The first step is to leverage abstract interpretations to generate global lower and upper bounds for each step of the composition of affine, conditional, and switch operators representing $||\nabla f(x)||$. Namely, for each component of the forward and backward pass, we compute bounds $l, u$, such that the inputs to that component lie in the range $l, u$ for all $x \in \mathcal{X}$. As we notice that $\nabla f(x)$ is only a function of the ReLU sign configurations, the next step is to encode these sign configurations. This occurs by encoding the range of the forward pass $f(x)$ as a mixed-integer polytope. Here we leverage the first part of Lemma 1 and make sure to keep track of the variables that represent the output of each conditional operator. As the backward pass is only a composition of affine, conditional and switch operators, defined recursively over only the sign-configuration variables, we iteratively incorporate these into the feasible mixed-integer polytope. Finally, we encode the desired norm by encoding elementwise absolute value operators and, in the case of $|| \cdot ||_\infty$, the $\max$ operator. The objective is set to maximize the variable corresponding to the gradient norm.

### 6. Provable Guarantees of LipMIP

In this section we will address several minor issues so that the mixed-integer programming formulation presented in the previous section is both correct and agrees with the assumptions required by Theorem 1.

**Closed and Open Domains:** The first point of concern arises from the fact that for Theorem 1 to hold, the domain $\mathcal{X}$ needs to be an open set, and this is a necessary assumption for the proofs to go through. On the other hand, mixed-integer programming is optimization over closed mixed-integer polytopes, noting that boundedness is required to compute global lower and upper bounds. As the only sets that are both open and closed are not bounded, we cannot solve the optimization problem in Theorem 1 exactly. Instead, we can say that, given a polyhedral input domain $\mathcal{X}$ over which we use mixed-integer programming to solve $\max_{x \in \mathcal{X}} ||\nabla f(x)||$, we report a solution that optimizes $\max_{x \in N(\mathcal{X})} ||\nabla f(x)||$, where $N(\mathcal{X})$ refers to a neighborhood of $\mathcal{X}$.

**Nondifferentiability of $f$:** The second point of concern arises from the fact that $\nabla f(x)$ is not defined everywhere. Recall the goal is to solve the optimization problem of $\max_{x \in \text{Diff}(\mathcal{X})} ||\nabla f(x)||$, where $\text{Diff}(\mathcal{X})$ is the set of points at which $f$ is differentiable in some set $\mathcal{X}$. We have shown that it suffices to formulate $\mathcal{Y} := \{||\nabla f(x)|| \mid x \in \text{Diff}(\mathcal{X})\}$ and solve $\max_{y \in \mathcal{Y}} y$. From the second part of Lemma 1, $||\nabla f(x)||$, is accurately encoded for $x \in \text{Diff}(\mathcal{X})$. The only problem cases are for the nondifferentiable points. LipMIP will only return an incorrect answer if the MIP-encoded function $||\nabla f(\cdot)||$ attains a value at a nondifferentiable point that is greater than those attained by the differentiable points $x \in \text{Diff}(\mathcal{X})$. As the gradient of $f$ is only defined as a function of the ReLU sign configurations of $f(x)$, certainly it is only the sign-configurations where problems may occur. Indeed, the problematic case occurs when LipMIP assigns a ReLU sign configuration which is not attainable by any differentiable point. Unfortunately, we can demonstrate some networks for which this problem case occurs in LipMIP.

**Counterexample:** To be more concrete, we present as a counterexample, a neural network $f$ for which LipMIP returns a solution based on a ReLU-configuration that is not attainable by any differentiable $x$. Indeed, let $f(x) := \sigma(x) - \sigma(-x)$.
Then LipMIP applied to $f(x) := \sigma(x) - \sigma(-x)$ is a neural network not in general position. For the function $f(x) = x$, The gradient norm at zero is 1 but naively bounding the Lipschitz constant will yield a bound of 2 at zero. In this instance, LipMIP will return an incorrect answer, as both neurons may be considered ‘on’ at $x = 0$.

such that $f(x) = x$ for all $x$ and hence the Lipschitz constant is at most 1. Decomposed into affine, conditional, and switch operators, $\nabla f(x) = C(x) + C(-x)$. And at $x = 0$, by our definition of $C(\cdot)$, LipMIP encodes $\nabla f(x)$ as $C(x) + C(-x)$, where $C(0) + C(-0) = 2$. In particular, we’ve assigned the sign-configuration at $x = 0$ to have both ReLU’s as ‘on’. In this case $\nabla f(0)$ is assigned the value 2, which is certainly greater than the true answer.

**General Position Neural Networks:** To mitigate this, we define a notion of general position for the parameters of ReLU networks. This is a deterministic property of a network. While the formal definition is quite notation-heavy, informally we can say:

**Definition 6. (Informal):** A ReLU network $f$ is said to be in general position if for every ReLU sign-configuration attainable at a nondifferentiable $x$, there exists a differentiable $x'$ that attains the same sign-configuration.

To show this is a reasonable assumption, we present the following theorem, essentially stating that the set of neural networks that are not in general position has measure zero over the parameter space:

**Theorem 3. (Informal):** Let $f$ be a ReLU network and $f'$ be a network where the parameters of $f'$ are those of $f$, but with the biases independently, randomly perturbed. Then $f'$ is in general position almost surely.

Finally we can state our main theorem regarding correctness of LipMIP:

**Theorem 4.** Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a scalar-valued ReLU network in general position, and let $X \subset \mathbb{R}^n$ be a bounded polytope. Then LipMIP applied to $f$ and $X$, returns the value

$$L^\alpha (f, N(X)),$$

where $N(X)$ is a neighborhood of $X$, and $\| \cdot \|$ is understood to be $\| \cdot \|_1$ or $\| \cdot \|_\infty$.

**7. Extensions of LipMIP**

So far, we have only considered exact formulations of computing the $\ell_1$, $\ell_\infty$ norms of the gradient of scalar-valued networks. In this section we will describe how to extend this formulation to vector-valued networks, over linear norms. We will then define a new linear norm which has applications towards robustness and is applicable to other Lipschitz estimation techniques. Finally we will mention natural relaxation techniques to LipMIP.

**Extension to Vector-Valued Networks:** So far, we have only considered real valued networks $f : \mathbb{R}^n \rightarrow \mathbb{R}$. In this section we’ll demonstrate how this can be naturally extended to vector-valued networks $g : \mathbb{R}^n \rightarrow \mathbb{R}^m$. In this case, the Jacobian $\nabla g(x)$, where it exists, is a matrix in $\mathbb{R}^{n \times m}$. From Theorem 1, we wish to optimize

$$||\nabla g(x)^T||_{\alpha, \beta} := \sup_{||y||_{\alpha} \leq 1} ||\nabla g(x)^T y||_{\beta}$$

$$\quad = \sup_{||y||_{\alpha} \leq 1} \sup_{||z||_{\beta} \leq 1} |y^T \nabla g(x) z|.$$  

Unfortunately there is no obvious way to if such a bilinear form is MIP-encodable. Moreover, even if this were possible, a naive formulation would require a significant increase in the size of our mixed-integer polytope, as we have to encode the entire partial Jacobian in each step of backpropagation. We show that we can avoid both of these issues and apply LipMIP when $\| \cdot \|_{\beta}$ is a linear norm. We defer the details to the appendix and instead state the following corollary to Theorem 4:

**Corollary 2.** In the same setting as Theorem 4, if $\| \cdot \|_{\alpha}$ is $\| \cdot \|_1$ or $\| \cdot \|_\infty$ and $\| \cdot \|_{\beta}$ is a linear norm, then LipMIP applied to $f$ and $X$ yields the answer

$$L^{(\alpha, \beta)} (f, N(X)),$$
where the parameters of LipMIP have been adjusted to reflect the norms of interest.

Untargeted Classification Robustness: We can leverage the key insight of Corollary 2 to describe a general application towards untargeted classification robustness certificates. In the binary classification setting, a classifier \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) assigns the label as the sign of the output, \( \text{sign}(f(x)) \), to \( x \). In this case, it is known that for some norm \( ||\cdot||_\alpha \), and some \( x \) such that \( f(x) > 0 \), then for all \( y \in \mathcal{X} \)

\[
||x - y||_\alpha < \frac{f(x)}{L^{\alpha}(f,\mathcal{X})} \implies \text{sign}(f(x)) = \text{sign}(f(y)).
\]

In the multiclassification setting, \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \) assigns the label as the index of the maximum logit, \( \arg\max_i f_i(x) \), to \( x \). We denote this ‘hard classifier’ as \( F(x) \). In this sense, an untargeted robustness certificate in the multiclass setting should look like, for \( x \) such that \( F(x) = i \):

\[
||x - y||_\alpha < \min_j \frac{|f_{ij}(x)|}{L^{\alpha}(f_{ij},\mathcal{X})} \implies F(y) = i.
\]

where \( f_{ij}(x) := (e_i - e_j)^T f(x) \). Naively, computing this requires \( \binom{m}{2} \) estimations of each Lipschitz constant \( L^{\alpha}(f_{ij},\mathcal{X}) \). Alternatively, we can provide a linear norm \( ||\cdot||_\infty \) for which, for every \( x \) with \( F(x) = i \),

\[
\min_j \frac{|f_{ij}(x)|}{L^{\alpha,\infty}(f_{ij},\mathcal{X})} < \min_j \frac{|f_{ij}(x)|}{L^{\alpha}(f_{ij},\mathcal{X})},
\]

Since \( ||\cdot||_\infty \) is defined to be a linear norm, we can apply Corollary 2 to obtain the following theorem:

**Theorem 5.** If \( f \) is defined as above, and if linear norm \( ||\cdot||_\infty \) satisfies 22, then for any \( x \in \mathcal{X} \) such that \( F(x) = i \) and any \( y \in \mathcal{X} \)

\[
||x - y||_\alpha < \min_j \frac{|f_{ij}(x)|}{L^{\alpha,\infty}(f,\mathcal{X})} \implies F(y) = i.
\]

As \( ||\cdot||_\infty \) is defined to be a linear norm, LipMIP can solve the optimization corresponding to \( L^{\alpha,\infty}(f,\mathcal{X}) \) by Corollary 2. We remark that this technique may be applicable to other Lipschitz estimation techniques. We present a construction of \( ||\cdot||_\infty \) and a proof in the appendix.

Natural Relaxation Strategies: Until this point, we have solely considered solving the gradient-norm maximization exactly. While we have shown in Theorem 2 that no efficient approximation algorithms can provide useful bounds in the worst case, every mixed-integer programming formulation we have discussed admits a natural linear programming relaxation. Indeed, by relaxing the constraints on integer variables to instead be continuous variables contained in \([0, 1]\), we attain a linear program. As this is a relaxation, the supremum attained in this setting is at least as great as the mixed-integer programming solution: hence, any optimal LP solution provides an upper bound to the Lipschitz constant. We denote this technique LipLP.

Mixed-integer programming solvers typically use branch-and-bound techniques. This strategy allows for early stopping to be performed using most common MIP optimization frameworks. Provided an early-stopping solution, a valid upper bound can always be attained based on the collection of relaxed versions of the problem solved. A valid lower bound may also be provided by reporting the value for any integral solution. In this sense, an integrality gap is attained. The criteria for when to stop can be defined based on a fixed compute time, or a fixed integrality gap.

8. Experiments

We have described an algorithm to exactly compute the Lipschitz constant of a ReLU network. We now discuss the performance of this tool versus other Lipschitz estimation techniques and then highlight the new empirical insights attainable with LipMIP. Full experimental details and additional data are contained in the Appendix.

**Accuracy vs. Efficiency:** As is typical in approximation techniques, there is frequently a tradeoff between efficiency and accuracy. This is the case for Lipschitz estimation of neural nets. In Tables 2 and 3, we demonstrate where each of the estimation techniques outlined in Table 1 lie on this tradeoff-curve. We evaluate each technique over the unit hypercube across random networks, networks trained on synthetic datasets, and networks trained to distinguish between MNIST 1’s and 7’s.
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| Method      | Time (s)          | Relative Error |
|-------------|-------------------|----------------|
| RandomLB    | 0.334 ± 0.019     | -41.96%        |
| CLEVER      | 20.574 ± 4.320    | -36.97%        |
| LipMIP      | 69.187 ± 70.114   | 0.00%          |
| LipLP       | 0.226 ± 0.023     | +39.39%        |
| FastLip     | 0.002 ± 0.000     | +63.41%        |
| LipSDP      | 20.570 ± 2.753    | +113.92%       |
| SeqLip      | 0.022 ± 0.005     | +119.53%       |
| NaiveUB     | 0.000 ± 0.000     | +212.68%       |

Table 2. Evaluation of Local Lipschitz Estimators on a network trained to distinguish MNIST 1's from 7's. We evaluate the local lipschitz constant where $\mathcal{X}$ is a random $\ell_{\infty}$-ball of radius 0.1.

| Method | Guarantee | Time (s) | Relative Error | Time (s) | Relative Error |
|--------|-----------|----------|----------------|----------|----------------|
| RandomLB | Lower     | 0.238 ± 0.004 | -23.80%     | 0.297 ± 0.004 | -32.68% |
| CLEVER   | Heuristic | 1.420 ± 0.061 | -10.11%     | 1.849 ± 0.054 | +28.45% |
| LipMIP   | Exact     | 325.337 ± 357.716 | 0.00%      | 38.844 ± 34.906 | 0.00%   |
| LipSDP   | Upper     | 2.635 ± 0.025 | +15.16%     | 2.704 ± 0.019 | +39.07% |
| SeqLip   | Heuristic | 0.008 ± 0.001 | +49.55%     | 0.016 ± 0.002 | +98.98% |
| LipLP    | Upper     | 0.019 ± 0.009 | +455.45%    | 0.030 ± 0.002 | +362.43% |
| FastLip  | Upper     | 0.001 ± 0.000 | +485.49%    | 0.001 ± 0.000 | +388.14% |
| NaiveUB  | Upper     | 0.000 ± 0.000 | +1339.31%   | 0.000 ± 0.000 | +996.96% |

Table 3. Lipschitz Estimation techniques applied to random networks with layer sizes [16,16,16,2], and networks of size [10, 20, 30, 20, 2] trained on synthetic datasets, where the evaluation is performed over the unit hypercube. Our method is the slowest, but provides a provably exact answer. This allows us to reliably gauge the accuracy and efficiency of the other techniques.

**Effect of Training On Lipschitz Constant:** We evaluate how the Lipschitz constant of a neural network changes as various regularization schemes are applied during training. These results are plotted in Figure 2. First we remark that for this experiment, the Lipschitz constant grows monotonically with training. Interestingly we also note the strong Lipschitz regularization property that adversarial training with FGSM yields (Szegedy et al., 2013). Counterintuitively, $\ell_2$-weight regularization causes an increase in Lipschitz constants, while $\ell_1$-weight regularization has the opposite effect.

We also consider how training affects the accuracy of the existing Lipschitz estimators. We plot the reported value of a suite of estimators as a network undergoes training on a synthetic dataset in Figure 3. We point out that the absolute error of each estimation technique increases as training proceeds.

**Random networks and Lipschitz Constants:** Studying various properties of random neural networks has been a fruitful area of research, see e.g. (Hanin & Rolnick, 2019; Pennington & Worah, 2017) and references therein. LipMIP can be used as an exact estimation tool for empirical validation of analytical conjectures for random networks. For example, in Figure 4 we show a histogram of Lipschitz constants of random networks for some fixed architecture. The obtained Lipschitz constants seem to have intriguingly regular distribution.

**9. Conclusion and Future Work**

We obtained novel analytical results that relate the Lipschitz constant of a ReLU network to the norm of its Jacobian. Further, we have demonstrated inapproximability results for computing the Lipschitz constant for general networks. We propose a technique to exactly compute this value using mixed integer programming solvers. Our exact method takes exponential time.
Figure 2. Effect of regularization on Lipschitz constants during training. We fix a dataset and network architecture and train with different regularization methods. We compute exact Lipschitz constants with LipMIP. Observe that these values increase as training proceeds. Surprisingly, $\ell_2$ weight regularization increases the Lipschitz constant even compared to the no regularization baseline. Adversarial training (FGSM) is the most effective Lipschitz regularizer we found in this experiment.

Figure 3. Here we plot how the reported bounds from Lipschitz estimators break down as we train a neural network on a synthetic dataset. We notice that as training proceeds, the absolute error of estimation techniques increases relative to the true Lipschitz constant computed with our method (blue dots).

in the worst case but admits natural LP relaxations that trade-off accuracy for efficiency. We also obtained novel results on untargeted robustness certification using our framework.

There are many interesting future directions. We have only started to explore relaxation approaches based on LipMIP and a polynomial time method that scales to large networks may be possible. The reliability of an exact Lipschitz evaluation technique may also prove useful in developing both new empirical insights and mathematical conjectures.

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Figure 4. We plot a histogram of the true Lipschitz constant of \( f \), where \( f \) is a randomly initialized network with layer-sizes [10, 10, 10, 1]. Our method can be used to guide mathematical conjectures about the form of such distributions.

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Appendix

A. Analytical proofs

We first start with formal definitions and known facts. We present our results in general for vector-valued functions, but we will make remarks about the implications for real-valued networks along the way.

A.1. Definitions and Notation

A.1.1. Norms

As we will be frequently referring to arbitrary norms, we recall the formal definition:

Definition 7. A norm \( ||\cdot|| \) over vector space \( V \) is a nonnegative valued function that meets the following three properties:

- **Triangle Inequality:** For all \( x, y \in V \), \( ||x + y|| \leq ||x|| + ||y|| \)

- **Absolute Homogeneity:** For all \( x \in V \), and any field element \( a \), \( ||ax|| = |a| \cdot ||x|| \)

- **Point Separation:** If \( ||x|| = 0 \), then \( x = 0 \), the zero vector of \( V \).

The most common norms are the \( \ell_p \) norms over \( \mathbb{R}^n \), with \( ||x||_p := (\sum_i |x_i|^p)^{1/p} \), though these are certainly not all possible norms over \( \mathbb{R}^n \). We can also describe norms over matrices. One such norm that we frequently discuss is a norm over matrices in \( \mathbb{R}^{m \times n} \) and is induced by norms over \( \mathbb{R}^n \) and \( \mathbb{R}^m \):

Definition 8. Given norm \( ||\cdot||_\alpha \) over \( \mathbb{R}^n \), and norm \( ||\cdot||_\beta \) over \( \mathbb{R}^m \), the matrix norm \( ||\cdot||_{\alpha,\beta} \) over \( \mathbb{R}^{m \times n} \) is defined as

\[
||A||_{\alpha,\beta} := \sup_{||x||_\alpha \leq 1} ||Ax||_\beta = \sup_{x \neq 0} \frac{||Ax||_\beta}{||x||_\alpha}
\]

A convenient way to keep the notation straight is that \( A \), above, can be viewed as a linear operator which maps elements from a space which has norm \( ||\cdot||_\alpha \) to a space which has norm \( ||\cdot||_\beta \), and hence is equipped with the norm \( ||A||_{\alpha,\beta} \). As long as \( ||\cdot||_\alpha, \cdot||_\beta \) are norms, then \( ||\cdot||_{\alpha,\beta} \) is a norm as well in that the three properties listed above are satisfied.

Every norm induces a dual norm, defined as

\[
||x||_* := \sup_{||y|| \leq 1} \langle x, y \rangle
\]

Where the \( \langle \cdot, \cdot \rangle \) is the standard inner product for vectors over \( \mathbb{R}^n \) or matrices \( \mathbb{R}^{m \times n} \). We note that if matrix \( A \) is a row-vector, then \( ||A||_{\alpha,1} = ||A||_{\alpha,*} \) by definition.

We also have versions of Hölder’s inequality for arbitrary norms over \( \mathbb{R}^n \):

Proposition 1. Let \( ||\cdot||_\alpha \) be a norm over \( \mathbb{R}^n \), with dual norm \( ||\cdot||_{\alpha,*} \). Then, for all \( x, y \in \mathbb{R}^n \)

\[
x^T y \leq ||x||_\alpha \cdot ||y||_{\alpha,*}
\]

Proof. Indeed, assuming WLOG that neither \( x \) nor \( y \) are zero, and letting \( u = \frac{x}{||x||_\alpha} \), we have

\[
x^T y = ||x||_\alpha \cdot \frac{u^T y}{||x||_\alpha} \leq ||x||_\alpha \cdot \sup_{||u||_\alpha \leq 1} u^T y = ||x||_\alpha \cdot ||y||_{\alpha,*}
\]

We can make a similar claim about the matrix norms defined above, \( ||\cdot||_{\alpha,\beta} \):
Proposition 2. Letting \( \| \cdot \|_{\alpha,\beta} \) be a matrix norm induced by norms \( \| \cdot \|_{\alpha} \) over \( \mathbb{R}^n \), and \( \| \cdot \|_{\beta} \) over \( \mathbb{R}^m \), for any \( A \in \mathbb{R}^{m \times n} \), \( x \in \mathbb{R}^n \):

\[
\|Ax\|_{\beta} \leq \|A\|_{\alpha,\beta} \|x\|_{\alpha}
\]

(28)

Proof. Indeed, assuming WLOG that neither \( x \) is not zero, letting \( y = x/\|x\|_{\alpha} \) such that \( \|y\|_{\alpha} = 1 \), we have

\[
\|Ax\|_{\beta} = \|x\|_{\alpha} \|Ay\|_{\beta} \leq \sup_{\|y\|_{\alpha} \leq 1} \|x\|_{\alpha} \|Ay\|_{\beta} = \|x\|_{\alpha} \|A\|_{\alpha,\beta}
\]

(29)

A.1.2. Lipschitz Continuity and Differentiability

When \( f : \mathbb{R}^n \to \mathbb{R}^m \) is a vector-valued over some open set \( \mathcal{X} \subseteq \mathbb{R}^n \) we say that it is \((\alpha,\beta)\)-Lipschitz continuous if there exists a constant \( L \) for norms \( \| \cdot \|_{\alpha}, \| \cdot \|_{\beta} \) such that all \( x, y \in \mathcal{X} \),

\[
\|f(x) - f(y)\|_{\beta} \leq L \cdot \|x - y\|_{\alpha}
\]

(30)

Then the Lipschitz constant, \( L^{(\alpha,\beta)}(f, \mathcal{X}) \), is the infimum over all such \( L \). Equivalently, one can define \( L^{(\alpha,\beta)}(f, \mathcal{X}) \) as

\[
L^{(\alpha,\beta)}(f, \mathcal{X}) = \sup_{x,y \in \mathcal{X}, x \neq y} \frac{\|f(x) - f(y)\|_{\beta}}{\|x - y\|_{\alpha}}
\]

(31)

We say that \( f \) is differentiable at \( x \) if there exists some linear operator \( \nabla f(x) \in \mathbb{R}^{n \times m} \) such that

\[
\lim_{h \to 0} \frac{f(x + h) - f(x) - \nabla f(x)^T h}{\|h\|} = 0
\]

(32)

A linear operator such that the above equation holds is defined as the Jacobian

The directional derivative of \( f \) along direction \( v \in \mathbb{R}^n \) is defined as

\[
\delta_v f(x) := \lim_{t \to 0} \frac{f(x + tv) - f(x)}{t}
\]

(33)

Where we note that we are taking limits of a vector-valued function. We now add the following known facts:

- If \( f \) is lipschitz continuous, then it is absolutely continuous.
- If \( f \) is differentiable at \( x \), all directional derivatives exist at \( x \). The converse is not true, however.
- If \( f \) is differentiable at \( x \), then for any vector \( v \), \( \delta_v f(x) = \nabla f(x)^T v \).
- (Rademacher’s Theorem): If \( f \) is Lipschitz continuous, then \( f \) is differentiable everywhere except for a set of measure zero, under the standard Lebesgue measure in \( \mathbb{R}^n \) (Heinonen, 2005).

Finally we introduce some notational shorthand. Letting \( f : \mathbb{R}^n \to \mathbb{R}^m \), be Lipschitz continuous and defined over an open set \( \mathcal{X} \), we denote \( \text{Diff}(\mathcal{X}) \) refer to the differentiable subset of \( \mathcal{X} \). We also let \( \mathcal{D} \) be the set of \((x, v) \in \mathbb{R}^{2n}\) for which \( \delta_v f(x) \) exists and \( x \in \mathcal{X} \). Additionally, let \( D_v \) be the set \( D_v = \{x \mid (x, v) \in \mathcal{D}\} \).

A.2. Relation Between Lipschitz Constants and Gradient Norms

Now we can state our first lemma, which claims that for any norm, the maximal directional derivative is attained at a differentiable point of \( f \):

Lemma 3. For any \((\alpha, \beta)\) Lipschitz continuous function \( f \), norm \( \| \cdot \|_{\beta} \) over \( \mathbb{R}^m \), any \( v \in \mathbb{R}^n \), letting \( D_v := \{x \mid (x, v) \in \mathcal{D}\} \), we have:

\[
\sup_{x \in D_v} \|\delta_v f(x)\|_{\beta} \leq \sup_{x \in \text{Diff}(\mathcal{X})} \|\nabla f(x)^T v\|_{\beta}
\]

(34)
Remark: For real valued functions and norm $\| \cdot \|_\alpha$ over $\mathbb{R}^n$, one can equivalently state that for all vectors $v$ with $\|v\|_\alpha = 1$:

$$ \sup_{x \in \text{Diff}(\mathcal{X})} \|\nabla f(x)\|_{\alpha} \geq \sup_x |\delta_v f(x)| $$

(35)

Proof. Essentially the plan is to say each of the following quantities are within $\epsilon$ of each other: $|\delta_v f(x)|$, the limit definition of $|\delta_v f(x)|$, the limit definition of $|\delta_v f(x')|$, and the norm of the gradient at $x'$ applied to the direction $v$.

We fix an arbitrary $v \in \mathbb{R}^n$. It suffices to show that for every $\epsilon > 0$, there exists some differentiable $x' \in \text{Diff}(\mathcal{X})$ such that $|\nabla f(x')^T \cdot v| \geq \sup_{x \in \mathcal{D}_v} |\delta_v f(x)| - \epsilon$.

By the definition of $\sup$, for every $\epsilon > 0$, there exists an $x \in \mathcal{D}_v$ such that

$$ |\delta_v f(x)|_{\beta} \geq \sup_{y \in \mathcal{D}_v} |\delta f(y)|_{\beta} - \epsilon/4 $$

(36)

Then for all $\epsilon > 0$, by the limit definition of $\delta_v f(x)$ there exists a $\delta > 0$ such that for all $t$ with $|t| < \delta$

$$ \left| |\delta_v f(x) - (f(x + tv) - f(x))|_{\beta} \right| \leq \epsilon/4 $$

(37)

Next we note that, since lipschitz continuity implies absolute continuity of $f$, and $t$ is now a fixed constant, the function $h(x) := f(x)_{||tv||_\alpha}$ is absolutely continuous. Hence there exists some $\delta'$ such that for all $y \in \mathcal{X}$, $z$ with $||z||_\alpha \leq \delta'$

$$ \frac{|f(y + z) - f(y)|_{\beta}}{||tv||_\alpha} = ||h(y + z) - h(y)||_{\beta} \leq \epsilon/4 $$

(38)

Hence, by Rademacher’s theorem, there exists some differentiable $x'$ within a $\delta'$-neighborhood of $x$, such that both $\frac{|f(x') - f(x)|_{\beta}}{||tv||_\alpha} < \epsilon/4$ and $\frac{|f(x' + tv) - f(x + tv)|_{\beta}}{||tv||_\alpha} < \epsilon/4$, hence by the triangle inequality for $| \cdot |_{\beta}$

$$ \left| |h(x + tv) - h(x)|_{\beta} \right| \leq \left| |h(x + tv) - h(x')|_{\beta} \right| + \left| |h(x) - h(x')|_{\beta} \right| + \left| |h(x' + tv) - h(x')|_{\beta} \right| $$

(39)

$$ \leq \epsilon/2 + \left| |h(x' + tv) - h(x')|_{\beta} \right| $$

$$ = \epsilon/2 + \frac{|f(x' + tv) - f(x')|_{\beta}}{||tv||_\alpha} $$

Hence combining equations 37 and 39 we have that

$$ |\delta_v f(x)|_{\beta} \leq 3\epsilon/4 + \frac{|f(x' + tv) - f(x')|_{\beta}}{||tv||_\alpha} $$

(40)

Taking limits over $\delta \to 0$, we get that the final term in equation 40 becomes $3\epsilon/4 + |\delta_v f(x')|_{\beta}$, which is equivalent to $3\epsilon/4 + |\nabla f(x)^T v|_{\beta}$. Hence we have that

$$ |\nabla f(x')^T \cdot v|_{\beta} \geq \sup_{x \in \mathcal{D}_v} |\delta_v f(x)|_{\beta} - \epsilon $$

(41)

as desired, as our choice of $v$ was arbitrary.

Now we can restate and prove our main theorem.

**Theorem 6.** Let $| \cdot |_{\alpha}$, $| \cdot |_{\beta}$ be arbitrary norms over $\mathbb{R}^n, \mathbb{R}^m$, and let $f : \mathbb{R}^n \to \mathbb{R}^m$ be locally $(\alpha, \beta)$-Lipschitz continuous over an open set $\mathcal{X}$. The following inequality holds:

$$ L^{(\alpha, \beta)}(f, \mathcal{X}) = \sup_{x \in \text{Diff}(\mathcal{X})} |\nabla f(x)^T|_{\alpha, \beta} $$

(42)
Remarks: Before we proceed with the proof, we make some remarks. First, note that if \( f \) is scalar-valued and continuously differentiable, then \( \nabla f(x)^T \) is a row-vector, and \( ||\nabla f(x)^T||_{\alpha,\beta} = ||\nabla f(x)||_{\alpha^*} \), recovering the familiar known result. Second, to gain some intuition for this statement, consider the case where \( f(x) = Ax + b \) is an affine function. Then \( \nabla f(x)^T = A \), and by applying the theorem and leveraging the definition of \( L^{(\alpha,\beta)}(f, X) \), we have

\[
L^{(\alpha,\beta)}(f, X) := \sup_{x \neq y \in X} \frac{||A(x-y)||_{\beta}}{||x-y||_{\alpha}} = ||A||_{\alpha,\beta},
\]

where the last equality holds because \( X \) is open.

Proof. We first show that for all \( x, y \in X \) that \( \frac{||f(x) - f(y)||_{\beta}}{||x-y||_{\alpha}} \) is bounded above by \( \sup_{z \in \text{Diff}(X)} ||\nabla f(x)||_{\alpha,\beta} \). Then we will show the opposite inequality.

Fix any \( x, y \in X \), and note that since the dual of a dual norm is the original norm,

\[
||f(x) - f(y)||_{\beta} = \sup_{||c||_{\alpha^*} \leq 1} |c^T(f(x) - f(y))|
\]

(44)

Moving the sup to the outside, we have

\[
||f(x) - f(y)||_{\beta} = \sup_{||c||_{\alpha} \leq 1} ||c||_{\alpha^*} |h_c(0) - h_c(1)|
\]

(45)

for \( h_c : \mathbb{R} \rightarrow \mathbb{R} \) defined as \( h_c(t) := c^T f(x + t(y - x)) \). Then certainly \( h_c \) is lipschitz continous on the interval \([0, 1]\), and the limit \( h'_c(t) \) exists almost everywhere, defined as

\[
h'_c(t) := \lim_{\delta \to 0} \frac{c^T f(x + (t + \delta)(y - x)) - c^T f(x + t(y - x))}{|\delta|} = c^T \delta(y - x) f(x + t(y - x))
\]

(46)

Further, there exists a lebesgue integrable function \( g(t) \) that equals \( h'_c(t) \) almost everywhere and

\[
|h(0) - h(1)| = \int_{0}^{1} g(t) d\mu
\]

(47)

We can assume without loss of generality that

\[
g(t) = \begin{cases} h'_c(t) & \text{if } h'_c(t) \text{ exists} \\ \sup_{s \in [0, 1]} |h'_c(s)| & \text{otherwise} \end{cases}
\]

(48)

where the supremum is defined over all points where \( h'_c(t) \) is defined. Then because \( g \) agrees almost everywhere with \( h'_c \) and is bounded pointwise, we have the following chain of inequalities:

\[
||f(x) - f(y)||_{\beta} = \sup_{||c||_{\alpha^*} \leq 1} |h_c(0) - h_c(1)| = \sup_{||c||_{\alpha} \leq 1} \int_{0}^{1} |g(t)| d\mu
\]

(49)

\[
\leq \sup_{||c||_{\alpha} \leq 1} \int_{0}^{1} |g(t)| d\mu
\]

(50)

\[
\leq \sup_{||c||_{\alpha^*} \leq 1} \sup_{s \in [0, 1]} |h'_c(s)| d\mu
\]

(51)

\[
\leq \sup_{||c||_{\alpha^*} \leq 1} \int_{0}^{1} \sup_{s \in [0, 1]} |c^T \delta(y - x) f(x + s(y - x))| d\mu
\]

(52)

\[
\leq \sup_{||c||_{\alpha^*} \leq 1} \int_{0}^{1} \int_{\mathcal{D}_f(y-x)} |c^T \delta(y - x) f(z)| d\mu
\]

(53)

\[
\leq \sup_{||c||_{\alpha^*} \leq 1} \int_{0}^{1} ||c||_{\alpha^*} \sup_{z \in \mathcal{D}_f(y-x)} ||\delta(y - x) f(z)||_\beta d\mu
\]

(54)

\[
\leq \sup_{z \in \text{Diff}(X)} ||\nabla f(z)(y - x)||_\beta
\]

(55)

\[
\leq \sup_{z \in \text{Diff}(X)} ||\nabla f(z)||_{\alpha,\beta} ||x - y||_\alpha
\]

(56)
Exactly Computing the Local Lipschitz Constant of ReLU Networks

Where Equation 54 holds by Proposition 1, Equation 55 holds by Lemma 3, and the final inequality holds by Proposition 2. Dividing by \( \|x - y\|_\alpha \) yields the desired result.

On the other hand, we wish to show, for every \( \epsilon > 0 \), the existence of an \( x, y \in \mathcal{X} \) such that

\[
\frac{||f(x) - f(y)||_\beta}{\|x - y\|_\alpha} \geq \sup_{x \in \text{Diff}(\mathcal{X})} ||\nabla f(x)||_{\alpha, \beta} - \epsilon
\]  \hspace{1cm} (57)

Fix \( \epsilon > 0 \) and consider any point \( z \in \mathcal{X} \) with \( ||\nabla f(z)||_{\alpha, \beta} \geq \sup_{x \in \mathcal{X}} ||\nabla f(x)||_{\alpha, \beta} - \epsilon/2 \).

Then \( ||\nabla f(z)||_{\alpha, \beta} = \sup_{||v||_\alpha \leq 1} ||\nabla f(z)^Tv||_\beta = \sup_{||v||_\alpha \leq 1} ||\delta_v f(z)||_\beta \). By the definition of the directional derivative, there exists some \( \delta > 0 \) such that for all \( |t| < \delta \),

\[
\frac{||f(z + tv) - f(z)||_\beta}{||tv||_\alpha} \geq ||\delta_v f(z)||_\beta - \epsilon/2 \geq \sup_{x \in \text{Diff}(\mathcal{X})} ||\nabla f(x)||_{\alpha, \beta} - \epsilon
\]  \hspace{1cm} (58)

Hence setting \( x = z + tv \) and \( y = v \), we recover equation \( 57 \). \( \square \)
We are typically interested in combinatorial optimization problems, which we will define informally as follows:

A combinatorial optimization problem is composed of 4 elements: i) A set of valid instances; ii) A set of feasible solutions for each valid instance; iii) A non-negative cost or objective value for each feasible solution; iv) A goal: signifying whether we want to find a feasible solution that either minimizes or maximizes the cost function.

Definition 9. A combinatorial optimization problem is composed of 4 elements: i) A set of valid instances; ii) A set of feasible solutions for each valid instance; iii) A non-negative cost or objective value for each feasible solution; iv) A goal: signifying whether we want to find a feasible solution that either minimizes or maximizes the cost function.

We also note that this definition frames approximation algorithms as a “search problem”.

While many interesting optimization problems are hard to solve exactly, for many of these interesting problems there exist approximation algorithms with approximation ratio \( \alpha \). Optimization problems then typically have 3 formulations, listed in order of decreasing difficulty:

- **Search Problem**: Given an instance \( x \) of optimization problem \( \Pi \), find \( y \) such that \( m(y) = \text{OPT}(x) \).
- **Computational Problem**: Given an instance \( x \) of optimization problem \( \Pi \), find \( \text{OPT}(x) \).
- **Decision Problem**: Given an instance \( x \) of optimization problem \( \Pi \), and a number \( k \), decide whether or not \( \text{OPT}(x) \geq k \).

Certainly an efficient algorithm to do one of these implies an efficient algorithm to do the next one. Also note that by a binary search procedure, the computational problem is polynomially-time reducible to the decision problem. As complexity theory is typically couched in discussion about membership in a language, it is slightly awkward to discuss hardness of combinatorial optimization problems. Since, every computational flavor of an optimization problem has a poly-time equivalent decision problem, we will simply claim that an optimization problem is NP-hard if its decision problem is NP-hard.

While many interesting optimization problems are hard to solve exactly, for many of these interesting problems there exist efficient approximation algorithms that can provide a guarantee about the cost of the optimal solution.

Definition 10. For a maximization problem \( \Pi \), an approximation algorithm with approximation ratio \( \alpha \) is a polynomial-time algorithm that, for every instance \( x \in \Pi \), produces a feasible solution, \( y \), such that \( m(y) \geq \text{OPT}(x)/\alpha \).

Noting that \( \alpha > 1 \) can either be a constant or a function parameterized by \( |x| \), length of the binary encoding of instance \( x \). We also note that this definition frames approximation algorithms as a “search problem”.

A very powerful tool in showing the hardness of approximation problems is the notion of a \( c \)-gap problem. This is a form of promise problem, and proofs of hardness here are slightly stronger than what we actually desire.

Definition 11. Given an instance of an maximization problem \( x \in \Pi \) and a number \( k \), the \( c \)-gap problem aims to distinguish between the following two cases:

- **YES**: \( \text{OPT}(x) \geq k \)
- **NO**: \( \text{OPT}(x) < k/c \)

where there is no requirement on what the output should be, should \( \text{OPT}(x) \) fall somewhere in \([k/c, k]\). For minimization problems, **YES** cases imply \( \text{OPT}(x) \leq k \), and **NO** cases imply \( \text{OPT}(x) > k \cdot c \).

Again we note that \( c \) may be a function that takes the length of \( x \) as an input. We now recall how a \( c \)-approximation algorithm may be used to solve the \( c \)-gap problem, implying the \( c \)-gap problem is at least as hard as the \( c \)-approximation.

**Proposition 3.** If the \( c \)-gap problem is hard for a maximization problem \( \Pi \), then the \( c \)-approximation problem is hard for \( \Pi \).

**Proof.** Suppose we have an efficient \( c \)-approximation algorithm for \( \Pi \), implying that for any instance \( x \in \Pi \), we can output a feasible solution \( y \) such that \( \text{OPT}(x)/c \leq m(y) \leq \text{OPT}(x) \). Then we let \( A_k \) be an algorithm that returns **YES** if...
m(y) \geq k/c, and NO otherwise, where y is the solution returned by the approximation algorithm. Then for the gap-problem, if OPT(x) \geq k, we have that m(y) \geq k/c so the A_k will output YES. On the other hand, if OPT(x) < k/c, then A_k will output NO. Hence, A_k is an efficient algorithm to decide the c-gap problem.

While hardness of approximation results arise from various forms, most notably the PCP theorem, we can black-box the heavy machinery and prove our desired results using only strict reductions, which we define as follows.

**Definition 12.** A strict reduction from problem \( \Pi \) to problem \( \Pi' \), is a function \( f : \Pi \rightarrow \Pi' \) maps problem instances of \( \Pi \) to problem instances of \( \Pi' \). \( f \) must satisfy the following properties for all \( x \in \Pi \):

1. \( |f(x)| \leq \alpha \), where \( \alpha \) is a fixed constant
2. \( \text{OPT}_{\Pi}(x) = \text{OPT}_{\Pi'}(f(x)) \)

For which we can now state and prove the following useful proposition:

**Proposition 4.** If \( f, g \) are a strict reduction from optimization problem \( \Pi \) to optimization problem \( \Pi' \), and the \( c \)-gap problem is hard for \( \Pi \), where \( c \) is polynomial in the size of \( |x| \), then the \( c' \)-gap problem is hard for \( \Pi' \), where \( c' \in \Theta(c) \).

**Proof.** Suppose both \( \Pi \) and \( \Pi' \) are maximization problems, and the \( c \)-gap problem is hard for \( \Pi \). We consider the case where \( c \) is a function that takes as input the encoding size of instances of \( \Pi \). We can define the function \( c'(n) := c(n/\alpha) \) for all \( n \). Hence \( c(|x|) = c'(|f(x)|) \) for all \( x \in \Pi \) by point 1 of the definition of strict reduction. Then for all \( k \) and all \( x \in \Pi \), the following two implications hold

\[
\text{OPT}_{\Pi'}(f(x)) \geq k \implies \text{OPT}_{\Pi}(x) \geq k
\]

\[
\text{OPT}_{\Pi'}(f(x)) < \frac{k}{c(|f(x)|)} \implies \text{OPT}_{\Pi}(x) < \frac{k}{c(|x|)}
\]

Where both implications hold because \( \text{OPT}_{\Pi}(x) = \text{OPT}_{\Pi'}(f(x)) \). If the \( c' \)-gap problem were efficiently decidable for \( \Pi' \), then the \( c' \)-gap problem would be efficiently decidable for \( \Pi \).

If \( \Pi \) is a maximization problem and \( \Pi' \) is a minimization problem, then the following two implications hold:

\[
\text{OPT}_{\Pi'}(f(x)) \leq k' \implies \text{OPT}_{\Pi}(x) \leq k'
\]

\[
\text{OPT}_{\Pi'}(f(x)) > k' \cdot c'(|f(x)|) \implies \text{OPT}_{\Pi}(x) > k' \cdot c(|x|)
\]

Then letting \( k = k' \cdot c(|x|) \) we have that solving the \( c' \)-gap problem for \( \Pi' \) would solve the \( c \)-gap problem for \( \Pi \). The proofs for \( \Pi, \Pi' \) both being minimization problems, or \( \Pi \) being a minimization and \( \Pi' \) being a maximization hold using similar strategies.

**B.2. Hardness and Inapproximability of Lipschitz Constants of Piecewise Linear Neural Networks**

Now we return to ReLU networks and prove novel results about the inapproximability of computing Recall that we have defined ReLU networks as compositions of functions of the form:

\[
f(x) = c^T \sigma(Z_d(x)) \quad Z_i(x) = W_i \sigma(Z_{i-1}(x)) + b_i,
\]

where \( Z_0(x) = x \) and \( \sigma \) is the elementwise ReLU operator. In this section, we only consider scalar-valued networks, \( f : \mathbb{R}^n \rightarrow \mathbb{R} \), in which case, we can define the gradient alternatively as follows:

**Proposition 5.** If \( f \) is differentiable at \( x \), then the \( i^{th} \) coordinate of \( \nabla f(x) \) is given by:

\[
\nabla f(x)_i = \sum_{\Gamma \in \text{Paths}(i)} \left( \prod_{w_j \in \Gamma} w_j \right)
\]

where \( \text{Paths}(i) \) is the set of paths from the \( i^{th} \) input, \( x_i \), to the output in the computation graph, where the ReLU at each vertex is on, and \( w_j \) is the weight of the \( j^{th} \) edge along the path.
We define the following optimization problems:

**Definition 13.** MAX-GRAD is an optimization problem, where the set of valid instances is the set of scalar-valued ReLU networks. The feasible solutions are the set of differentiable points \( x \in X \), which have cost \( ||\nabla f(x)||_1 \). The goal is to maximize this gradient norm.

**Definition 14.** MIN-LIP is an optimization problem where the set of valid instances is the set of piecewise linear neural nets. The feasible solutions are the set of constants \( L \) such that \( L \geq L(f) \). The cost is the identity function, and our goal is to minimize \( L \).

Of course, each of these problems have decision-problem variants, denoted by \( \text{MAX-GRAD}_{dec} \) and \( \text{MIN-LIP}_{dec} \). We also remark that by Theorem 6, and proposition 4, the trivial strict reduction implies that it is at least as hard to approximate \( \text{MIN-LIP} \) as it is to approximate \( \text{MAX-GRAD} \). For the rest of this section, we will only strive to prove hardness and inapproximability results for \( \text{MAX-GRAD} \).

To do this, we recall the definition of the maximum independent set problem:

**Definition 15.** MIS is an optimization problem, where valid instances are undirected graphs \( G = (V,E) \), and feasible solutions are \( U \subseteq V \) such that for any \( v_i, v_j \in U \), \( (v_i, v_j) \notin E \). The cost is the size of \( U \), and the goal is to maximize this cost.

Classically, it has been shown that \( \text{MIS} \) is NP-hard to optimize, but also is one of the hardest problems to approximate and does not admit a deterministic polynomial time algorithm to solve the \( O(n^{1-\epsilon}) \)-gap problem (Zuckerman, 2007).

For ease of exposition, we rephrase instances of \( \text{MIS} \) into instances of an equivalent problem which aims to maximize the size of consistent collections of locally independent sets. Given graph \( G = (V,E) \), for any vertex \( v_i \in V \), we let \( N(v_i) \) refer to the set of vertices adjacent to \( v_i \) in \( G \). We sometimes will abuse notation and refer to variables by their indices, e.g., \( N(i) \). We also refer to the degree of vertex \( i \) as \( d(v_i) \) or \( d(i) \).

**Definition 16.** A locally independent set centered at \( v_i \) is a \( \{-1, +1\} \)-labelling of the vertices \( \{v_i\} \cup N(v_i) \) such that the label of \( v_i \) is \( +1 \) and the label of \( v_j \in N(v_i) \) is \( -1 \). Two locally independent sets are said to be consistent if, for every \( v_j \) appearing in both locally independent sets, the label is the same in both locally independent sets. A consistent collection of locally independent sets is a set of locally independent sets that is pairwise consistent.

Then we can define an optimization problem:

**Definition 17.** LIS is an optimization problem, where valid instances are undirected graphs \( G = (V,E) \), and feasible solutions are consistent collections of locally independent sets. The cost is the size of the collection, and the goal is to maximize this cost.

It is obvious to see that there is a trivial strict reduction between \( \text{MIS} \) and \( \text{LIS} \). Indeed, any independent set defines the centers of a consistent collection of locally independent sets, and vice versa. As we will see, this is a more natural problem to encode with neural networks than \( \text{MIS} \).

Now we can state our first theorem about the inapproximability of \( \text{MAX-GRAD} \).

**Theorem 7.** There is a strict reduction between \( \text{MAX-GRAD} \) and \( \text{LIS} \).

**Proof.** The key idea of the proof is to, given a graph \( G = (V,E) \) with \( |V| = n \), encode a neural network \( h \) with \( n \) inputs, each representing the labeling value. We then build a neuron for each possible locally independent set, where the neuron is ‘on’ if and only if the labelling is close to a locally independent set. And then we also ensure that each locally independent set contributes \( +1 \) to the norm of the gradient of \( f \).

A critical gadget we will use is a function \( \psi(x) : \mathbb{R} \rightarrow \mathbb{R} \) defined as follows:

which is implementable with affine layers and ReLUs as: \( \psi(x) = \sigma(x + 1) - \sigma(x - 1) - 1 \). We are now ready to construct our neural net. For every vertex \( v_i \in V \), we construct an input to the neural net, hence \( f : \mathbb{R}^n \rightarrow \mathbb{R} \). We denote the \( i^{th} \) input to \( f \) as \( x_i \). The first order of business is to map each \( x_i \) through \( \psi(\cdot) \), which can be done by two affine layers and one ReLU layer. e.g., we can define \( \psi(x_i) = A_1(\text{ReLU}(A_0(x_i))) \) where

\[
A_0(x) := \begin{bmatrix} 1 \\ 1 \\ -1 \\ 1 \end{bmatrix} x + \begin{bmatrix} 1 \\ 1 \end{bmatrix}
\]
\[
\psi(x) = \begin{cases} 
-1 & x \in (-\infty, -1] \\
 x & x \in [-1, 1] \\
1 & x \in [1, +\infty)
\end{cases}
\] (60)

Next we define the second layer of ReLU’s, which has width \(n\), and each neuron represents the status of a locally independent set. We define the input to the \(i^{th}\) ReLU in this layer as \(I_i\) with

\[
I_i(x) := \psi(x_i) - \sum_{j \in N(i)} \psi(x_j) - (d + 1 - \epsilon)
\] (61)

for some fixed-value \(\epsilon\) to be chosen later. Finally, we conclude our construction with a final affine layer to our neural net as

\[
h(x) := \sum_{i=1}^{n} \sigma(I_i(x))
\] (62)

Let \(I(x)\) denote the set of indices of ReLU’s that are ‘on’ in the second-hidden layer of \(h\): \(I(x) := \{i \mid I_i(x) > 0\}\). Now we make the following claims about the structure of \(h\).

**Claim B.1.** For every \(i\), if \(i \in I(x)\) then \(x_i > 1 - \epsilon\) and \(x_j < -1 + \epsilon\) for all \(j \in N(i)\). In addition, \(I(x)\) denotes the centers of a consistent collection of locally independent sets.

**Proof.** Indeed, if \(I_i(x) > 0\), then the sum of \((d(i) + 1)\) \(\psi\)-terms is greater than \(1 - \epsilon\). As each \(\psi\)-term is in the range \([-1, 1]\), each \(\psi\)-term must individually be at least \(1 - \epsilon\). And \(\psi(x_j) \geq 1 - \epsilon\) implies \(x_j \geq 1 - \epsilon\). Similarly, \(-\psi(x_j) \geq 1 - \epsilon\) implies that \(x_j \leq -1 + \epsilon\). Now consider any \(i_1, i_2\) in \(I(x)\). Then the pair of locally independent sets centered at \(v_{i_1}\) and \(v_{i_2}\) is certainly consistent. \(\square\)

**Claim B.2.** For any \(x\) such that \(h\) is differentiable at \(x\), \(\nabla h(x)_i \cdot x_i \geq 0\).

---

**Figure 5.** Complete construction of a neural network \(h\) that is the reduction from \(\text{LIS}\), such that the supremal gradient of \(h\) corresponds to the maximum locally independent set. The first step is to map each \(x_i\) to \(\psi(x_i)\), then to construct \(I_i(x)\). Finally, we route each \(\sigma(I_i(x))\) to the output.
Proof. We split into cases based on the value of \( x_i \) and rely on Claim B.1. Suppose \( x_i \in (-1 + \epsilon, 1 - \epsilon) \), then we have \( I_j < 0 \) for any \( j \in \{i\} \cup N(i) \) and hence \( \nabla h(x)_i = 0 \). If \( x_i \geq 1 - \epsilon \), then every \( j \in N(i) \) has \( I_j < 0 \) and hence by Proposition 5, the only contributions to the \( \nabla h(x)_i \) can be from paths that route from \( x_i \) to the output through \( I_i \). Hence

\[
\nabla h(x)_i = \frac{\delta h}{\delta I_i} \cdot \frac{\delta I_i}{\delta x_i} \tag{63}
\]

where both terms are nonnegative and hence so is \( \nabla h(x)_i \). Finally, if \( x_i \leq -1 + \epsilon \), then the only contributions to \( \nabla h(x)_i \) come from paths that route through \( I_j \) for \( j \in N(i) \), hence

\[
\nabla h(x)_i = \sum_{j \in N(i)} \frac{\delta h}{\delta I_j} \cdot \frac{\delta I_j}{\delta x_i} \tag{64}
\]

where the first term is nonnegative and the second term is always nonpositive.

Claim B.3. For any \( x \), let \( \mathcal{I}(x) \) be defined as above, \( \mathcal{I}(x) := \{i \mid I_i(x) > 0\} \). Then \( ||\nabla h(x)||_1 \leq ||\mathcal{I}(x)|| \) and for every \( x \). In addition, for every \( x \), there exists a \( y \) with \( ||\nabla h(y)||_1 \geq ||\mathcal{I}(x)|| \).

Proof. To show the first part, observe that

\[
h(x) = \sum_{i=1}^{n} \sigma(I_i(x)) = \sum_{i \in \mathcal{I}(x)} \frac{I_i(x)}{d(i)+1} \quad \Rightarrow \quad \nabla h(x) = \sum_{i \in \mathcal{I}(x)} \nabla I_i(x) \frac{1}{d(i)+1}
\]

hence

\[
||\nabla h(x)||_1 \leq \sum_{i \in \mathcal{I}(x)} \frac{1}{d(i)+1} ||\nabla I_i(x)||_1 \tag{66}
\]

and

\[
I_i(x) := \psi(x_i) - \sum_{j \in N(i)} \psi(x_j) - (d + 1 - \epsilon) \quad \Rightarrow \quad \nabla I_i(x) = \nabla \psi(x_i) - \sum_{j \in N(i)} \nabla \psi(x_j) \tag{67}
\]

hence

\[
||\nabla I_i(x)||_1 \leq ||\nabla \psi(x_i)||_1 + \sum_{j \in N(i)} ||\nabla \psi(x_j)||_1 \leq d(i) + 1
\]

where the final inequality follows because \( ||\nabla \psi(x_i)||_1 \leq 1 \) everywhere it is defined. Combining equations 66 and 68 yields that \( ||\nabla h(x)||_1 \leq ||\mathcal{I}(x)|| \).

On the other hand, suppose \( \mathcal{I}(x) \) is given. Then we can construct \( y \) such that \( \mathcal{I}(y) = \mathcal{I}(x) \) and \( ||\nabla h(y)||_1 = ||\mathcal{I}(x)|| \). To do this, set \( y_i = 1 - \frac{\epsilon}{2n} \) if \( i \in \mathcal{I}(x) \) and \( y_i = -1 + \frac{\epsilon}{2n} \) otherwise. Then note that \( \mathcal{I}(x) = \mathcal{I}(y) \) and for every \( i \in \mathcal{I}(y) \)

\[
\nabla I_i(y)_k = \begin{cases} +1 & k = i \\ -1 & k \in N(i) \\ 0 & \text{otherwise} \end{cases}
\]

and hence by Claim 2, we can replace the inequalities in equations 66 and 68 we have that

\[
||\nabla h(y)||_1 = \sum_{i \in \mathcal{I}(x)} \frac{1}{d(i)+1} ||\nabla I_i(y)||_1 = ||\mathcal{I}(x)||
\]

as desired.

To demonstrate that this is indeed a strict reduction, we need to define functions \( f \) and \( g \), where \( f \) maps instances of \( \text{LIS} \) to instances of \( \text{MAX-GRAD} \), and \( g \) maps feasible solutions of \( \text{MAX-GRAD} \) back to \( \text{LIS} \). Clearly the construction we have defined above is \( f \). The function \( g \) can be attained by reading off the indices in \( \mathcal{I}(x) \).
To demonstrate that the size of this construction does not blow up by more than a constant factor, observe that by representing weights as sparse matrices, the number of nonzero weights is a constant factor times the number of edges in $G$. Indeed, encoding each $\psi$ in the first layer takes $O(1)$ parameters for each vertex in $G$. Encoding $I_i(x)$ requires only $O(d(i))$ parameters for each $i$, and hence $2|E|$ parameters total. Assuming a RAM model where numbers can be represented by single atomic units, and $\epsilon$ is chosen to be $(n+2)^{-1}$, this is only a constant factor expansion.

The crux of this argument is to demonstrate that $OPT_{\text{MAX-GRAD}}(f(q)) = OPT_{\text{LIS}}(q)$. It suffices to show that for every locally independent set $L$, there exists an $x$ such that $||\nabla h(x)||_1 \geq k$, and for every $y$, there exists a locally independent set $L'$ such that $|L'| \geq ||\nabla h(y)||_1$.

Suppose $L$ is a consistent collection of locally independent sets, with $|L| = k$. Any consistent collection of locally independent sets equivalently defines a labelling of each vertex of $G$, where $l_i$ denotes the label of vertex $v_i$: $l_i := +1$ if the locally independent set centered at $v_i$ is contained in the collection, and $l_i := -1$ otherwise. Then one can construct an $x$ such that $||\nabla h(x)||_1 \geq k$. Indeed, for every $v_i$ with label $l_i$, set $x_i = l_i(1 - \frac{1}{d_i})$. By Claim B.1, under this $x$, $I_i(x) \geq 0$ for every $i$ such that $l_i = +1$, $I_i(x) > 0$. Then $|I(x)| = k$ and by Claim B.3 there exists a $y$ such that $||\nabla h(y)||_1 \geq k$.

On the other hand, suppose the maximum gradient of $h$ is $k$. Then there exists an $x$ that attains this and by Claim B.3, $|I(x)| \geq k$. By Claim B.1, we have that $I(x)$ denotes the centers of a consistent collection of locally independent sets. \(\square\)

The formulation for $\text{MAX-GRAD}$ presented above only considers the $\ell_1$-norm of the gradient. We can define a similar problem $\text{MAX-GRAD}_\infty$ that aims to maximize the $\ell_\infty$ norm of the gradient. We can slightly tweak our construction for the $\text{MAX-GRAD}$ reduction to yield a $\text{MAX-GRAD}_\infty$ reduction.

**Corollary 3.** There is a strict reduction between $\text{MAX-GRAD}_\infty$ and $\text{LIS}$.

**Proof.** We only slightly modify our construction of the reduction for $\text{MAX-GRAD}$. Namely, we add a new input so $h : \mathbb{R}^{n+1} \rightarrow \mathbb{R}$, called $x_{n+1}$. Then we map $x_{n+1}$ through $\psi$ like all the other indices, but instead redefine

$$I_i(x) := \psi(x_i) + (d(i) + 1)\psi(x_{n+1}) - \sum_{j \in N(i)} \psi(x_j) - 2(d(i) + 1 - \epsilon)$$

$$H(x) := \sum_{i=1}^{n} \sigma(I_i(x)) \frac{\sigma(I_i(x))}{2(d(i) + 1)}$$

The rest of the proof is nearly identical with the preceding proof, with the exception being that $||\nabla h(x)||_1$ can be replaced by $\frac{\delta h(x)}{\delta x_{n+1}}$ throughout as an indicator to count the size of $I(x)$. \(\square\)

As an aside, we note that the strict reduction demonstrates that $\text{MAX-GRAD}_{\text{dec}}$ is NP-complete, which implies that $\text{MIN-LIP}_{\text{dec}}$ is CoNP-complete.
C. LipMIP Construction

In this appendix we will describe in detail the necessary steps for LipMIP construction. In particular, we will present how to formulate the gradient norm $||\nabla f||_*$ for scalar-valued $f$ as a composition of affine, conditional and switch operators. Then we will present the proofs of MIP-encodability of each of these operators. Finally, we will describe how the global upper and lower bounds are obtained using abstract interpretation.

C.1. MIP-encodable components of ReLU networks

Our aim in this section is to demonstrate how $||\nabla f||_*$ may be written as a composition of affine, conditional, and switch operators. For completeness, we redefine these operators here:

**Affine operators** $A : \mathbb{R}^n \to \mathbb{R}^m$ are defined as

$$A(x) = Wx + b,$$

for some fixed matrix $W$ and vector $b$.

The **conditional operator** $C : \mathbb{R} \to \{0, 1\}$ is defined as

$$C(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0. \end{cases}$$

The **switch operator** $S : \mathbb{R} \times \{0, 1\} \to \mathbb{R}$ is defined as

$$S(x, a) = x \cdot a.$$  

We will often abuse notation, and let conditional and switch operators apply to vectors, where the operator is applied elementwise. Now we recover Lemma 1 from section 5 of the main paper.

**Lemma 4.** Let $f$ be a scalar-valued ReLU network. Then $f(x)$ may be written as a composition of affine, conditional, and switch operators. For all $x$ such that $\nabla f(x)$ exists, $||\nabla f(x)||$ may be written as a composition of affine, conditional, and switch operators, for the $|| \cdot ||_1, || \cdot ||_\infty$ norms.

**Proof.** We recall that $f$ is defined recursively like:

$$f(x) = c^T \sigma(Z_d(x)) \quad Z_i(x) = W_i \sigma(Z_{i-1}(x)) + b_i \quad Z_0(x) = x$$  

It amounts to demonstrate how $Z_i(x)$ may be computed as a composition of affine, conditional and switch operator. Since $\sigma(x) = S(x, C(x))$, one can write, $Z_1(x) = W_i S(x, C(x)) + b_i$. Letting $A_i(x) := C(Z_i(x))$ and $A_i(x) := W_i(x) + b_i$, one can write $Z_i(x) = A_i \circ S(Z_i(x), A_i(x))$. Since $f(x)$ is an affine operator applied to $Z_d(x)$, $f(x)$ can certainly be encoded using only affine, switch, and conditional operators.

To demonstrate that $\nabla f(x)$ may also be written as such a composition, we require the same definition to compute $Z_i(x)$ as above. Then by the chain rule, we have that

$$\nabla f(x) = W_i^T Y_i(x) = W_i^T \text{Diag}(A_i(x)) Y_{i+1}(x) \quad Y_{d+1}(x) = c$$  

As the $\nabla f(x)$ is an affine operator applied to $Y_1(x)$, and $Y_{d+1}(x)$ is constant, we only need to show that $Y_i(x)$ may be written as a composition of affine, conditional, and switch operators. This follows from the fact that

$$\text{Diag}(A_i(x)) Y_{i+1}(x) = S(Y_{i+1}(x), A_i(x))$$  

Then letting $A_i^T(x) := W_i^T x$ we have that $Y_i(x) = A_i^T \circ (S(Y_{i+1}(x), A_i(x))$. Hence $\nabla f(x)$ may be encoded as a composition of affine, conditional, and switch operators.

All that is left is to show that $|| \cdot ||_1, || \cdot ||_\infty$ may be encoded likewise. For each of these, we require $| \cdot |$ which can equivalently be written $|x| = \sigma(x) + \sigma(-x)$, and hence $|x| = S(x, C(x)) + S(-x, C(-x))$. $|x|_1$ then is encoded as the sum of the elementwise sum over $|x|$. $|| \cdot ||_\infty$ requires the $\max(\ldots)$ operator. To encode this, we see that $\max(x_1, \ldots) = \max(x_1, \max(\ldots))$ and $\max(x, y) = x + \sigma(y - x) = x + S(y - x, C(y - x))$.  

\[\square\]
C.2. MIP-encodability of Affine, Conditional, Switch:

Here we will explain the MIP-encodability each of the affine, conditional, and switch operators. For completeness, we copy the definition of MIP-encodability:

**Definition 18.** A function $g : \mathbb{R}^n \times \{0,1\}^m \rightarrow \mathbb{R}^{n'} \times \{0,1\}^{m'}$ is **MIP-encodable** if there exists a system of linear inequalities, $\Gamma$, over variables $(x, x')$ such that $x' = g(x)$ if and only if $\Gamma(x, x')$ is satisfied.

We now prove Lemma 2 from the main paper:

**Lemma 5.** Let $g$ be a composition of affine, conditional, and switch operators, where global lower and upper bounds are known for each input to each element of the composition. Then $g$ is a MIP-encodable function.

**Proof.** It suffices to show that each of the primitive operators are MIP-encodable. This amounts to, for each operator $f$, to define a system of linear inequalities $\Gamma(x, x')$ which is satisfied if and only if $f(x) = x'$, provided $x \in [l, u]$.

**Affine Operators:** The affine operator is trivially attainable by letting $\Gamma(x, x')$ be the equality constraint

$$x' = Wx + b$$

(75)

**Conditional Operators:** To encode $C(x)$ as a system of linear constraints, we introduce the integer variable $a$ and wish to encode $a = C(x)$, or equivalently, $a = 1 \Leftrightarrow x \geq 0$. We assume that we know values $l, u$ such that $l \leq x \leq u$. Then the implication $a = 1 \Rightarrow x \geq 0$ is encoded by the constraint:

$$x \geq (a - 1) \cdot u$$

(76)

Since if $x < 0$, then $a = 1$ yields a contradiction in that $0 > x \geq (1 - 1) \cdot u = 0$. The implication $x \geq 0 \Rightarrow a = 1$ is encoded by the constraint

$$x \leq a \cdot (1 - l) - 1$$

(77)

Since if $x \geq 0$, then $a = 0$ yields a contradiction in that $0 \leq x \leq (0) \cdot (1 - l) - 1 = -1$. Hence $a = 1 \Leftrightarrow x \geq 0$. We note that if $l > 0$ or $u < 0$, then the value of $a$ is fixed and can be encoded with one equality constraint.

**Switch Operators:** Encoding $S(x, a)$ as a system of linear inequalities requires the introduction of continuous variable $y$. As we assume we know $l, u$ such that $l \leq x \leq u$. Denote $\hat{l} := \min(l, 0)$ and $\hat{u} := \max(u, 0)$. The system of linear inequalities $\Gamma(a, x, y)$ is defined as the conjunction of:

$$y \geq x - u \cdot (1 - a) \quad y \geq l \cdot a$$

$$y \leq x - l \cdot (1 - a) \quad y \leq u \cdot a$$

(78)

We wish to show that $y = S(x, a) \Leftrightarrow \Gamma(a, x, y)$. Suppose that $\Gamma(a, x, y)$ is satisfied. Then if $a = 1$, $x$ must equal $y$, since it is implied by left-column constraints of equation 78. The right-column constraints are satisfied by assumption. Alternatively, if $a = 0$ then $y$ must equal $0$: it is implied by the right-column constraints of equation 78. The left columns are satisfied with $a = 0$ and $y = 1$ since $l \leq x \leq u$ by assumption. On the other hand, suppose $y = S(x, a)$. If $a = 1$, then $y = x$ by definition and we have already shown that $\Gamma(1, x, x)$ satisfied for all $x \in [l, u]$. Similarly, if $a = 0$, then $y = 0$ and we have shown that $\Gamma(0, x, 0)$ is satisfied for all $x \in [l, u]$.

Finally we note that if one can guarantee that $a = 0$ or $a = 1$ always, then only the equality constraint $y = x$ or $y = 0$ is needed.

**More efficient encodings:** Finally we’ll remark that while the above are valid encodings of affine, conditional and switch operators, encodings with fewer constraints for compositions of these primitives do exist. For example, suppose we instead wish to encode a continuous piecewise linear function with one breakpoint over one variable

$$R(x) = \begin{cases} A_1(x) & \text{if } x \geq z \\ A_2(x) & \text{if } x < z \end{cases}$$

(79)
for affine functions $A_1, A_2 : \mathbb{R} \to \mathbb{R}$, with $A_1(z) = A_2(z)$. Certainly we could use affine, conditional and switch operators, as

$$R(x) = A_1(x) + S(A_1(x) - A_2(x), C(z - x)) \quad (80)$$

Where which requires 12 linear inequalities. Instead we can encode this function using only 4 linear inequalities. Supposing we wish to model an abstract domain $A$ we know $l, u$ such that $l \leq x \leq u$, then $R(x)$ can be encoded by introducing an auxiliary integer variable $a$ and four constraints. Letting

$$
\begin{align*}
\zeta^- & = \min_{x \in [l, u]} A_1(x) - A_2(x) \\
\zeta^+ & = \max_{x \in [l, u]} A_1(x) - A_2(x)
\end{align*}
$$

then the constraints $\Gamma(a, x, y)$ are

$$
\begin{align*}
y & \geq A_1(x) - a\zeta^+ & y & \geq A_2(x) + (1 - a)\zeta^- \\
y & \leq A_1(x) - a\zeta^- & y & \leq A_2(x) + (1 - a)\zeta^+
\end{align*}
$$

(83)

This formulation admits a more efficient encoding for functions like $\sigma(\cdot)$, and $| \cdot |$, however it also introduces the issue that both $\Gamma(0, z, A_1(z))$ and $\Gamma(1, z, A_1(z))$ are satisfied, which means that this formulation does not quite meet the definition for being MIP-encodable for functions of the integer variable, $a$, defined above. For our purposes, this will ultimately not cause us problems, as we will assume general position of ReLU networks.

C.3. Abstract Interpretations

Here we discuss techniques to compute the lower and upper bounds needed for the MIP encoding of affine, conditional and switch operators. We will only need to show that for each of our primitive operators, we can map sound input bounds to sound output bounds.

For this, we turn to the notion of abstract interpretation. Classically used in static program analysis and control theory, abstract interpretation develops machinery to generate sound approximations for passing sets through functions. This has been used to great success to develop certifiable robustness techniques for neural networks (Singh et al., 2019). Formally, this requires an abstract domain, abstraction and concretization operators, and a pushforward operator for every function we wish to model. An abstract domain $A^n$ is a family of abstract mathematical objects, each of which represent a set over $\mathbb{R}^n$. An abstraction operator $\alpha^n : \mathcal{P}(\mathbb{R}^n) \to A^n$ maps subsets of $\mathbb{R}^n$ into abstract elements, and a concretization operator $\gamma^n : A^n \to \mathcal{P}(\mathbb{R})^n$ maps abstract elements back into subsets of $\mathbb{R}^n$. A pushforward operator for function $f : \mathcal{R}^n \to \mathcal{R}^m$, is denoted as $f^\# : A^n \to A^m$, and is called sound, if for all $\mathcal{X} \subset \mathbb{R}^n$,

$$\{f(x) \mid x \in \mathcal{X}\} \subseteq \gamma^m(f^\#(\alpha^n(\mathcal{X}))) \quad (84)$$

C.3.1. Hyperboxes and Boolean Hyperboxes

The simplest abstract domains are the hyperbox and boolean hyperbox domains. The hyperbox abstract domain over $\mathbb{R}^n$ is denoted as $H^n$. For each $\mathcal{X} \subset \mathbb{R}^n$ such that $H = \alpha(\mathcal{X})$, $H$ is parameterized by two vectors $l, u$ such that

$$l_i \leq \inf_{x \in \mathcal{X}} x_i \quad u_i \geq \sup_{x \in \mathcal{X}} x_i \quad (85)$$

and $\gamma^n(H) = \{x \mid l \leq x \leq u\}$. An equivalent parameterization is by vectors $c, r$ such that $c = \frac{l + u}{2}$ and $r = \frac{u - l}{2}$. We will sometimes use this parameterization when it is convenient.

Similarly, the boolean hyperbox abstract domain $B^n$ represents sets over $\{0, 1\}^n$. For each $\mathcal{X}_b \subseteq \{0, 1\}^n$ such that $B = \alpha(\mathcal{X}_b)$, $B$ is parameterized by a vector $v \in \{0, 1, ?\}^n$ such that

$$v_i = \begin{cases} 
1 & \text{if } x_i = 1 \ \forall x \in \mathcal{X}_b \\
0 & \text{if } x_i = 0 \ \forall x \in \mathcal{X}_b \\
? & \text{otherwise} 
\end{cases} \quad (86)$$

26
And
\[ \gamma^n(B) = \{ x \mid (x_i = v_i) \lor (v_i = ?) \} \]  
\hfill (87)

Finally, we can compose these two domains to represent subsets of \( \mathbb{R}^n \times \{0, 1\}^m \). For any set \( \mathcal{X} \subseteq \mathbb{R}^n \times \{0, 1\}^m \), we let \( \mathcal{X}_R \) refer to the restriction of \( \mathcal{X} \) to \( \mathbb{R}^n \) and let \( \mathcal{X}_B \) refer to the restriction of \( \mathcal{X} \) to \( \{0, 1\}^m \). Then \( \alpha(\mathcal{X}) := (H, B) \) where \( H = \alpha(\mathcal{X}_R), B = \alpha(\mathcal{X}_B) \). The concretization operator is defined \( \gamma(H, B) := \gamma(H) \times \gamma(B) \).

### C.3.2. Pushforwards for Affine, Conditional, Switch

We will now define pushforward operators for each of our primitives.

#### Affine Pushforward Operators

Provided with bounded set \( \mathcal{X} \subset \mathbb{R}^n \), with \( H = \alpha(\mathcal{X}) \) parameterized by \( c, r \), and affine operator \( A(x) = Wx + b \), the pushforward \( A^\# \) is defined \( A^\#(H) = H' \), where \( H' \) is parameterized by \( c', r' \) with
\[ c' = Wc + b \quad r' = |W|r \]  
\hfill (88)

where \( |W| \) is the elementwise absolute value of \( W \). To see that this is sound, it suffices to show that for every \( x \in \mathcal{X} \), \( c_i' - r_i' \leq A(x_i) \leq c_i' + r_i' \). Fix an \( x \in \mathcal{X} \) and consider \( A(x)_i = w_i^T x + b_i \) where \( w_i \) is the \( i \text{th} \) row of \( W \). Note that \( x = c + e \) for some vector \( e \) with \( |e| \leq r \) elementwise. Then
\[ w_i^T x + b_i = w_i^T c + w_i^T e + b_i \]
\[ \geq w_i^T c - |w_i^T| |e| + b_i \]
\[ \geq w_i^T c - |w_i^T| r + b_i \]
as desired.

#### Conditional Pushforward Operators

Provided with bounded set \( \mathcal{X} \subset \mathbb{R}^n \) with \( H = \alpha^n(\mathcal{X}) \) parameterized by \( l, u \), the elementwise conditional operator is defined \( C^\#(H) = B \) where \( B \) is parameterized by \( v \) with
\[ v_i = \begin{cases} 0 & \text{if } u_i < 0 \\ 1 & \text{if } l_i > 0 \\ \text{?} & \text{otherwise} \end{cases} \]  
\hfill (89)

Soundness follows trivially: for any \( x \in \mathcal{X} \), if \( l_i > 0 \), then \( x_i > 0 \) and \( C(x)_i = 1 \). If \( u_i < 0 \), then \( x_i < 0 \) and \( C(x)_i = 0 \). Otherwise, \( v_i = ? \), which is always a sound approximation as \( C(x)_i \in \{0,1\} \).

#### Switch Pushforward Operators

Provided with \( \mathcal{X} \subset \mathbb{R}^n \times \{0, 1\}^m \), we define \( \mathcal{X}_R := \{ x \mid (x, a) \in \mathcal{X} \} \) and \( \mathcal{X}_B := \{ a \mid (x, a) \in \mathcal{X} \} \). We’ve defined \( \alpha(\mathcal{X}) := (\alpha(\mathcal{X}_R), \alpha(\mathcal{X}_B)) \). Then if \( H := \alpha(\mathcal{X}_R) \) parameterized by \( l, u \), and \( B := \alpha(\mathcal{X}_B) \) parameterized by \( v \), we define the pushforward operator for switch \( S^\#(H, B) = H' \) where \( H' \) is parameterized by \( l', u' \) with
\[ l'_i = \begin{cases} l_i & \text{if } v_i = 1 \\ 0 & \text{if } v_i = 0 \\ \min(l_i, 0) & \text{otherwise} \end{cases} \]  
\hfill (90)
\[ u'_i = \begin{cases} u_i & \text{if } v_i = 1 \\ 0 & \text{if } v_i = 0 \\ \max(u_i, 0) & \text{otherwise} \end{cases} \]  
\hfill (91)

Soundness follows: letting \((x, a) \in \mathcal{X} \), if \( v_i = 0 \), then \( a_i = 0 \), and \( S(x, a)_i = 0 \), hence \( l'_i, u'_i = 0 \) is sound. If \( v_i = 1 \), then \( a_i = 1 \) and \( S(x, a)_i = x_i \) and hence \( l'_i = l_i, u'_i = u_i \) is sound by the soundness of \( H \) over \( \mathcal{X}_R \). Finally, if \( v_i = ? \), then \( a_i = 0 \) or \( a_i = 1 \), and \( S(x, a)_i \in \{0\} \cup [l_i, u_i] \subseteq [\min(l_i, 0), \max(u_i, 0)] \).
C.3.3. **Abstract Interpretation and Optimization**

We make some remarks about the applications of abstract interpretation as a technique for optimization. Recall that, for any set \( \mathcal{X} \) and functions \( g, f \), if \( \mathcal{Y} = \{ f(x) \mid x \in \mathcal{X} \} \) we have that

\[
\max_{x \in \mathcal{X}} g(f(x)) = \max_{y \in \mathcal{Y}} g(y) \quad (92)
\]

Instead if \( \mathcal{Z} \) is such that \( \{ f(x) \mid x \in \mathcal{X} \} \subseteq \mathcal{Z} \), then

\[
\max_{x \in \mathcal{X}} g(f(x)) \leq \max_{z \in \mathcal{Z}} g(z) \quad (93)
\]

In particular, suppose \( f \) is a nasty function, but \( g \) has properties that make it amenable to optimization. Optimization frameworks may not be able to solve \( \max_{x \in \mathcal{X}} g(f(x)) \). On the other hand, it might be the case that the RHS of equation 93 is solvable. In particular, if \( g \) is concave and \( \mathcal{Z} \) is a convex set obtained by \( \mathcal{Z} := \gamma(\mathcal{F}(\alpha(\mathcal{X}))) \), then by soundness we have \( \mathcal{Z} \supset \mathcal{Y} \). In fact, this is the formal definition of a convex relaxation.

Under this lens, one can use the abstract domains and pushforward operators previously defined to recover FastLip (Weng et al., 2018a), though the algorithm was not presented using abstract interpretations. Indeed, using the hyperbox and boolean hyperbox domains, over a set \( \mathcal{X} \), one can recover a hyperbox \( \mathcal{Z} \supseteq \{ \nabla f(x) \mid x \in \mathcal{X} \} \). Then we have that

\[
\max_{x \in \mathcal{X}} \| \nabla f(x) \| \leq \max_{z \in \mathcal{Z}} \| z \| \quad (94)
\]

where it is easy to optimize \( \ell_p \)-norms over hyperboxes. In addition, many convex-relaxation approaches towards certifiable robustness may be recovered by this framework (Zico Kolter & Wong, 2017; Raghunathan et al., 2018; Zhang et al., 2018; Singh et al., 2019).
D. Provable Guarantees of LipMIP

In this section we will present the notions of general position for ReLU networks and present the proofs of Theorems 3 and 4 in the main paper, stating that almost all neural nets are in general position, and that LipMIP operates correctly for general position nets.

D.1. General Position Neural Networks

We start with a formal definition of General Position for ReLU networks.

Let \( f : \mathbb{R}^n \to \mathbb{R} \) be a ReLU network with \( m \) ReLU neurons. We can define a function \( \mathcal{Z}_f : \mathbb{R}^n \to \mathbb{R}^m \) where \( \mathcal{Z}_f(x)_i \) refers to the input to the \( i^{th} \) neuron when applying \( f \) to vector \( x \). Then we can define the sign configuration \( S_f : \mathbb{R}^n \to \{-1, 0, +1\}^m \) as follows:

\[
S_f(x)_i = \begin{cases} 
-1 & \text{if } \mathcal{Z}_f(x)_i < 0 \\
+1 & \text{if } \mathcal{Z}_f(x)_i > 0 \\
0 & \text{if } \mathcal{Z}_f(x)_i = 0
\end{cases}
\]

Now we can define the set of all sign configurations attainable by \( f \) as

\[
\mathcal{A}_f := \{S_f(x) \mid x \in \mathbb{R}^n\}
\]

and we can further partition this set into the sign configurations that contain a 0 and those that don’t.

\[
\mathcal{A}_f^\pm := \mathcal{A}_f \cap \{-1, +1\}^m
\]

\[
\mathcal{A}_f^0 := \mathcal{A}_f \setminus \mathcal{A}_f^\pm
\]

Finally, we define a ‘resolution’ operator \( \mathcal{R}_m : \{-1, 0, +1\}^m \to \mathcal{P}(\{-1, +1\}^m) \) which takes in a sign configuration \( \sigma \), potentially with zeroes in it, and returns a set of sign configurations where each 0 has been replaced by both a -1 and +1. For example

\[
\mathcal{R}_3([+1, 0, 0]) = \left\{ [+1, -1, -1], [+1, -1, +1], [+1, +1, -1], [+1, +1, +1] \right\}
\]

And in general we note that

\[\log_2 (|\mathcal{R}_m(\sigma)|) = |\{i \mid \sigma_i = 0\}|\]

We also define some more notation to describe vector slicing. We use the notation used by the Python programming language to describe prefixes and suffixes. For a vector \( \sigma \), the first \( i \) elements of \( \sigma \) are denoted by \( \sigma[:i] \), and all but the first \( i \) elements are denoted by \( \sigma[i:] \). For a set of vectors \( A \), we let \( A[:i] := \{\sigma[:i] \mid \sigma \in A\} \) and similarly for the suffix operator. We also define the concatenation infix operator \( \land \) which concatenates two vectors together, such that for all \( \sigma, i, \sigma[:i] \land \sigma[i:] = \sigma \).

Now we can define a notion of general position for ReLU networks, which is a deterministic condition, relying on two criteria being met.

**Definition 19.** We say that ReLU Network \( f \) is in general position if the following two criteria are met:

- There are no ‘dead neurons’. That is, for all neurons \( i, \{\mathcal{Z}_f(x)_i \mid x \in \mathbb{R}^n\} \neq \{0\} \).
- All neurons are ‘sufficiently independent’. That is, for all neurons \( i, j \), the intersection of their kernels \( \{x \mid \mathcal{Z}_f(x)_i = 0 \land \mathcal{Z}_f(x)_j = 0\} \) does not contain an \((n-1)\)-dimensional open set.
- All resolved sign configurations are attainable. That is, for all \( x \in \mathbb{R}^n \), \( \mathcal{R}(S_f(x)) \subseteq \mathcal{A}_f \).

Intuitively speaking, a ReLU Network is in general position if there are no neurons that are redundant in a particularly pathological way, and if for every \( x \) for which the input to some ReLU is identically zero, there exists points \( x^+ \) and \( x^- \) for which the input to that ReLU is positive and negative respectively. Next we will show that almost every neural net is in general position. To do this, we introduce the following technical lemma.

**Lemma 6.** Let \( f \) be a ReLU network with no dead neurons, i.e., for every neuron \( i, \{\mathcal{Z}_f(x)_i \mid x \in \mathbb{R}^n\} \neq \{0\} \) and further suppose all neurons are sufficiently independent. Then the following two statements hold:
1. All realizable linear regions are locally realizable. For every \( x \) and every \( \epsilon > 0 \),

\[
(R_m(S_f(x)) \cap A_f) \subseteq \{S_f(y) \mid ||y-x||_2 < \epsilon \}
\]  

which is to say that all attainable resolutions of a sign configuration \( S_f(x) \) are attainable within an \( \epsilon \)-neighborhood of \( x \).

2. All suffix configurations are locally stable. We say that for every \( x \) such that \( S_f(x) \in A_f^0 \), if \( i \) is the largest index such that \( S_f(x)_i = 0 \), then for all \( \zeta \in (R_m(S_f(x)) \cap A_f)\{i\} \) the concatenation of \( \zeta \) with the suffix of \( S_f(x) \) is realizable: \( \zeta \amalg S_f(x)[i:] \in A_f^0 \). This is a direct corollary to the first claim.

Proof. First we state some facts about the geometry of ReLU Network’s. For a more thorough discussion, see also Jordan et al. (2019). Provided that no neuron is dead, we have that for any realizable sign configuration \( \sigma \in A_f^0 \), if \( i \) is the largest index such that \( S_f(x)_i = 0 \), then for all \( \zeta \in (R_m(S_f(x)) \cap A_f)\{i\} \) the concatenation of \( \zeta \) with the suffix of \( S_f(x) \) is realizable: \( \zeta \amalg S_f(x)[i:] \in A_f^0 \). This is a direct corollary to the first claim.

Now we prove part 1. Fix \( x \) and \( \epsilon > 0 \). Assume without loss of generality that \( S_f(x) \in A_f^0 \). Let \( \sigma \) be defined as the sign configuration of \( x \), \( \sigma := S_f(x) \). We refer to the resolution of \( \sigma \) as \( R_m(S_f(x)) \cap A_f \). Unless \( \sigma \) is the zero vector, the set of \( y \) such that \( S_f(y) = \sigma \) is the interior of some lower-dimensional facet of some polytope, and we claim that there exists at least one point \( x_{\sigma'} \) for every sign configuration \( \sigma' \) in the resolution of \( \sigma \), such that \( x_{\sigma'} \) is within \( \epsilon \) distance to some \( y \) such that \( S_f(y) = \sigma \). Indeed, by the continuity of neural networks, for each \( i \) such that \( \sigma_i = 0 \), \( Z_i(x) \) is linear in a neighborhood around \( \{ y \mid S_f(y) = \sigma \} \). Since we have assumed every neuron is sufficiently independent, the kernels of each \( Z_i \) locally form an arrangement of hyperplanes which partitions the space into \( 2^{|\{i \mid \sigma_i = 0\}|} \) regions, thereby attaining every sign configuration in \( R_m(\sigma) \). In other words, for any \( \sigma' \in R_m(S_f(x)) \cap A_f \) we have that there exists a \( y \) arbitrarily close to \( x \) such that \( S_f(y) = \sigma' \) as desired.

Now to prove part 2: fix any \( x \) such that \( S_f(x) \in A_f^0 \) and find the largest index \( i \) such that \( S_f(x)_i = 0 \). For any resolved, realizable sign configuration, consider it’s \( i \)-prefix, letting \( \zeta \in (R_m(S_f(x)) \cap A_f)\{i\} \). Since the input to the \( i \)-th neuron is a ReLU Network itself, namely \( Z_i(\cdot) \), by part 1 there is a point \( y \) that is \( \epsilon \)-close to \( x \) such that \( S_f(y)[i:] = \zeta \), for \( \epsilon \) to be chosen later. Our goal is to show that this \( y \) is such that \( S_f(y)[i:] = S_f(x)[i:] \). Since we have chosen \( i \) such that \( S_f(x)[i:] \in \{\pm 1\}^n \) the input to each of these neurons is bounded away from zero by some value. By the uniform continuity of neural networks, a \( \delta \) can be chosen such that \( S_f(z)[i:] = S_f(x)[i:] \) for all \( z \) such that \( ||z-x|| < \delta \). The result holds by choosing \( y \) based on \( \epsilon = \delta \).

With the lemma in hand, we can now state our general position theorem.

Theorem 8. Let \( f_\theta \) be a ReLU Network that is not in general position, where \( \alpha \) is a vector that parameterizes the biases of the affine layers. Then for any \( \epsilon > 0 \), the probability of \( f_\theta \) being in general position is 1, for \( \theta \sim N(\alpha, \epsilon I) \).

Proof. Note that \( F_\theta \) distribution over neural nets where \( \theta \sim N(\alpha, \epsilon I) \), and induces a measure \( \mu \) over parameter space. The first step is to show that almost surely \( f_\theta \) does not have a dead neuron and that all neurons are sufficiently independent. Recall that a neuron is dead if it’s input is identically zero over all \( x \in \mathbb{R}^n \). Suppose then that neuron \( i \) is dead, where \( Z_i(x) = L(x) + \theta_i \), where \( L(x) \) is a linear combination of the output of ReLU networks. Note that \( Z_i(x) = 0 \) if and only if \( L(x) = \theta_i \) for all \( x \), where \( \theta_i \) is fixed. If \( L \) is nonconstant, then neuron \( i \) is not dead, and if \( L \) is constant, then neuron \( i \) is dead only when \( \theta_i = -L \) where \( \theta_i \sim N(\alpha_i, \epsilon) \) which happens with probability zero. By union bounding over all neurons we can see that the probability that any neuron is dead is zero. Conditioning over the fact that no neurons are dead, we can apply the same argument to demonstrate that the kernel of any \( Z_i(x) \), is a ‘bent hyperplane’ with only finitely many linear regions. Two ‘bent hyperplanes’ only intersect in an \( (n-1) \)-dimensional open set if they are ever locally coplanar, and two hyperplanes are only ever locally coplanar if they are linearly dependent. Because the biases of each \( Z_f(x)_i \), is independently randomly selected, linear independence occurs almost surely for each linear component of every pair of bent hyperplanes. Since there are only finitely many components and pairs, all neurons are sufficiently independent almost surely.

For the rest of the proof, we will condition on the fact that no neuron is dead and that the neurons are sufficiently indepedent. We define the following sets:

\[
B := \{ \theta \mid \exists x \text{ such that } R_m(S_{f_\theta}(x)) \not\subseteq A_{f_\theta} \}
\]  

(97)
Then LipMIP applied to $B$ and $I$, where

$$I_i := \{ \theta \mid \exists x \text{ such that } (S_{f_\theta}(x))_i = 0 \} \land (R_m(\sigma)[: i] \not\subseteq A_{f_\theta}(x)[: i])$$

$$\tilde{I}_i := I_i \setminus \bigcup_{j<i} I_j$$

where $I_i, \tilde{I}_i$ is defined for all neurons $i \in [m]$. Intuitively, $I_i$ represents the set of parameters where the $i^{th}$ neuron makes it bad. $\tilde{I}_i$ is the set of parameters for which the $i^{th}$ neuron is the first one to make the network 'bad'. The rest of the proof proceeds by showing that $B \subseteq \bigcup_i I_i$ and that $\mu(\tilde{I}_i) = 0$, where the measure is over parameters that have no dead neurons. The claim will follow as

$$\mu(B) \leq \mu(\bigcup_i I_i) = \mu(\bigcup_i \tilde{I}_i) \leq \sum_i \mu(\tilde{I}_i) = 0$$

Now we show that $B \subseteq \bigcup_i I_i$. Consider any $\theta \in B$. By definition there exists an $x$ such that $R_m(S_{f_\theta}(x)) \not\subseteq A_{f_\theta}$. Let

$$\sigma := S_{f_\theta}(x)$$

and let $i$ be the largest index such that $\sigma_i = 0$. We would like to claim that

$$R_m(\sigma) \not\subseteq A_{f_\theta} \implies R_m(\sigma)[: i] \not\subseteq A_{f_\theta}[: i]$$

This follows by the contrapositive of Lemma 6: suppose that $R_m(\sigma)[: i] \subseteq A_{f_\theta}[: i]$, which in particular means that any $\zeta \in R_m(\sigma)[: i]$, is such that $\zeta \in A_{f_\theta}[: i]$ and by applying part 2 of Lemma 6, we have that $\zeta \sim \sigma[i :] \in A_{f_\theta}$. By our choice of $i$, $R_m(\sigma) = \{ \zeta \sim \sigma[i :] \mid \zeta \in R_m(\sigma)[: i] \}$, thus completing our claim.

Next we need to prove that $\mu(\tilde{I}_i) = 0$ for all $i$. We prove this by induction. The case for $i = 1$ is trivially true as we have assumed no neuron to be dead. Now assume $\mu(\tilde{I}_j) = 0$ for all $j < k$. Our goal is to show that $\mu(\tilde{I}_k) = 0$. By definition, for any $\theta$ in $\tilde{I}_k$, $\theta \not\in I_j$ for $j < k$, hence the subnetworks $Z_{\theta}(\cdot)_j$ are in general position for all $j < k$ and we only need to consider the case where the bent hyperplane introduced by the $k^{th}$ neuron breaks the general-position-ness. Each sign configuration in $A_{f_\theta}^{+}[: k - 1]$ corresponds to a full dimensional polytope for which $Z_{\theta}(x)_k$ is linear, which in particular implies that within each polytope, the set of $x$ for which $Z_{\theta}(x)_k = 0$ lies in an affine subspace of dimension $n - 1$, which we’ll call $H_{\theta}(\sigma)$. Next that if $H_{\theta}(\sigma)$ does not intersect any vertices of any polytope, then $\theta \not\in \tilde{I}_k$. We can consider the set of biases $\theta_k$ for the $k^{th}$ neuron which intersect a vertex of some polytope. Since there are only finitely many such vertices, there are only finitely many such $\theta_k$ that are in $\tilde{I}_k$, and hence the probability of $\theta_k \sim N(\alpha_k, \epsilon)$ being exactly one of these bad $\theta_k$’s is zero. Thus we can satisfy Equation 100 and complete the proof.

\[ \square \]

D.2. Correctness of LipMIP

Now we restate and prove the main theorem about the correctness of LipMIP:

**Theorem 9.** Let $f : \mathbb{R}^n \to \mathbb{R}$ be a scalar-valued ReLU network in general position, and let $X \subset \mathbb{R}^n$ be a bounded polytope. Then LipMIP applied to $f$ and $X$, returns the value

$$L^\alpha(f, N(X))$$

where $N(X)$ is a neighborhood of $X$ and $|| \cdot ||$ is understood to be $|| \cdot ||_1$ or $|| \cdot ||_\infty$

**Proof.** We put all the pieces together. Theorem 6, states that

$$L^\alpha(f, N(X)) = \sup_{x \in \text{Diff}(N(X))} ||\nabla f(x)||_{\alpha^*}.$$  

(102)

Our goal then is to demonstrate that the mixed-integer program LipMIP yields the answer

$$\sup_{x \in \text{Diff}(N(X))} ||\nabla f(x)||_{\alpha^*}.$$  

(103)
for which it suffices to show that the feasible region of the MIP established by LipMIP $\mathcal{Y}$ is such that $\mathcal{Y} = \{||\nabla f(x)||_{\alpha^*} \mid x \in \text{Diff}(N(\mathcal{X}))\}$.

Then Lemma 4 demonstrates that $||\nabla f(x)||_{\alpha^*}$ may be written as a composition of affine, conditional, and switch operators. Part 2 of Lemma 5 then shows that

$$\mathcal{Y} \supseteq \{||\nabla f(x)||_{\alpha^*} \mid x \in \text{Diff}(\mathcal{X})\}. \quad (104)$$

Now it only amounts to show that the feasible sign configurations of LipMIP are attainable by some point $x \in N(\mathcal{X})$. This fact follows directly from choosing to define the ReLU in the MIP according to the ‘More Efficient Encodings’ subsection. Then, since we have assumed $f$ is in general position, Part 1 of Lemma 6 applies. This allows us to conclude that

$$\mathcal{Y} = \{||\nabla f(x)||_{\alpha^*} \mid x \in \text{Diff}(N(\mathcal{X}))\} \quad (105)$$

as desired.
E. Extensions of LipMIP

This section will provide more details regarding the contents of section 7 of the main paper. First we will describe how to extend LipMIP to handle vector-valued functions, and linear norms over the target space. Then we will present the details for the application towards untargeted classification robustness.

E.1. Extension to Vector-Valued Networks

Letting \( f : \mathbb{R}^n \to \mathbb{R}^m \) be a vector-valued ReLU network, suppose \( \| \cdot \|_\alpha \) is a norm over \( \mathbb{R}^n \) and \( \| \cdot \|_\beta \) is a norm over \( \mathbb{R}^m \). Further, suppose \( \mathcal{X} \) is some open subset of \( \mathbb{R}^n \). Then Theorem 1 states that

\[
L^{(\alpha, \beta)}(f, \mathcal{X}) := \sup_{x \neq y \in \mathcal{X}} \frac{\| f(x) - f(y) \|_\beta}{\| x - y \|_\alpha} = \sup_{x \in \text{Diff}(\mathcal{X})} \| \nabla f(x)^T \|_{\alpha, \beta}.
\]

(106)

And one can rewrite:

\[
\sup_{x \in \text{Diff}(\mathcal{X})} \| \nabla f(x)^T \|_{\alpha, \beta} = \sup_{x \in \text{Diff}(\mathcal{X})} \sup_{\| y \|_\alpha \leq 1} \| \nabla f(x)^Ty \|_\beta = \sup_{x \in \text{Diff}(\mathcal{X})} \sup_{\| y \|_\alpha \leq 1} \sup_{\| \|_\beta \leq 1} \| z \nabla f(x)^T y \|
\]

(107)

The key idea is that we can define function \( g_z : \mathbb{R}^n \to \mathbb{R} \) as

\[
g_z(x) = (z, f(x))
\]

(108)

Where

\[
\nabla g_z(x)^T = z \nabla f(x)^T
\]

(109)

The plan is to make LipMIP optimize over \( x \) and \( z \) simultaneously and maximize the gradient norm of \( g_z(x) \). To be more explicit, we note that the scalar-valued LipMIP solves:

\[
\sup_{x \in \mathcal{X}} \| \nabla f(x)^T \|_{\alpha, \| \cdot \|_\alpha} = \sup_{x \in \mathcal{X}} \| \nabla f(x)^T y \|_\beta
\]

(110)

where we have shown that \( \nabla f(x) \) is MIP-encodable and the supremum over \( y \) can be encoded for \( \| \cdot \|_1, \| \cdot \|_\infty \), because there exist nice closed form representations of \( \| \cdot \|_1, \| \cdot \|_\infty \). The extension, then, only comes from the \( \sup_{\| \|_\alpha \leq 1} \) term. We can explicitly define \( f \) as

\[
f(x) = W_{d+1} \sigma (Z_d(x)) \quad Z_i(x) = W_i \sigma (Z_{i-1}(x)) + b_i \quad Z_0(x) = x
\]

(111)

such that

\[
g_z(x) = z^T W_{d+1} \sigma (Z_d(x)) \quad Z_i(x) = W_i \sigma (Z_{i-1}(x)) + b_i \quad Z_0(x) = x
\]

(112)

And the recursion for \( \nabla g_z(x) \) is defined as

\[
\nabla g_z(x) = W_1^T Y_1(x) \quad Y_i(x) = W_i^T + 1 \text{Diag}(\lambda_i(x)) Y_{i+1}(x) \quad Y_{d+1}(x) = W_{d+1}^T z
\]

(113)

Thus we notice the only change occurs in the definition of \( Y_{d+1}(x) \). In the scalar-valued \( f \) case, \( Y_{d+1}(x) \) is always the constant vector, \( c \). In the vector-valued case, we can let \( Y_{d+1}(x) \) be the output of an affine operator. Thus as long as the dual ball \( \{ z \mid \| z \|_\beta \} \) is representable as a mixed-integer polytope, we may solve the optimization problem of Equation 107.

**Corollary 4.** In the same setting as Theorem 9, if \( \| \cdot \|_\alpha \) is \( \| \cdot \|_1 \) or \( \| \cdot \|_\infty \), and \( \| \cdot \|_\beta \) is a linear norm, then LipMIP applied to \( f \) and \( \mathcal{X} \) yields the answer

\[
L^{(\alpha, \beta)}(f, N(\mathcal{X}))
\]

(114)

where the parameters of LipMIP have been adjusted to reflect the norms of interest.

**Proof.** The proof ideas are identical to that for Theorem 9. The only difference is that the norm \( \| \cdot \|_\beta \) has been replaced from \( \| \cdot \|_1 \) to an arbitrary linear norm. The argument for correctness in this case is presented in the paragraphs preceding the corollary statement.
E.2. Application to Untargeted Classification Robustness

Now we turn our attention towards untargeted classification robustness. In the binary classification setting, we let $f : \mathbb{R}^n \to \mathbb{R}$ be a scalar-valued ReLU network. Then the label that classifier $f$ assigns to point $x$ is $\text{sign}(f(x))$. In this case, it is known that for any open set $\mathcal{X}$, any norm $\| \cdot \|_\alpha$, any $x, y \in \mathcal{X}$,

$$\|x - y\|_\alpha < \frac{|f(x) - f(y)|}{L^\alpha(f, \mathcal{X})} \quad \Rightarrow \quad \text{sign}(f(x)) = \text{sign}(f(y)) \quad (115)$$

Indeed, this follows from the definition of the Lipschitz constant as

$$L^\alpha(f, \mathcal{X}) = \sup_{x \neq y} \frac{|f(x) - f(y)|}{\|x - y\|_\alpha}. \quad (116)$$

Then, by the contrapositive of implication 115, if $\text{sign}(f(x)) \neq \text{sign}(f(y))$ then $|f(x) - f(y)| \geq |f(x)|$ and for all $x, y \in \mathcal{X}$,

$$L^\alpha(f, \mathcal{X}) \geq \frac{|f(x) - f(y)|}{\|x - y\|_\alpha} \quad (117)$$

Rearranging, we have

$$\|x - y\|_\alpha \geq \frac{|f(x) - f(y)|}{L^\alpha(f, \mathcal{X})} \geq \frac{|f(x)|}{L^\alpha(f, \mathcal{X})} \quad (118)$$

arriving at the desired contrapositive implication.

In the multiclass classification setting, we introduce the similar lemma.

**Lemma 7.** $f : \mathbb{R}^n \to \mathbb{R}^m$ assigns the label as the index of the maximum logit. We will define the hard classifier $F : \mathbb{R}^n \to [m]$ as $F(x) = \arg \max_i f(x)_i$. We claim that for any $\mathcal{X}$, and norm $\| \cdot \|_\alpha$, if $F(x) = i$, then for all $y \in \mathcal{X}$,

$$\|x - y\|_\alpha < \min_j \frac{|f_{ij}(x)|}{L^\alpha(f_{ij}, \mathcal{X})} \Rightarrow F(y) = i \quad (119)$$

where we’ve defined $f_{ij}(x) := (e_i - e_j)^T f(x)$.

**Proof.** To see this, suppose $F(y) = j$ for some $j \neq i$. Then $|f_{ij}(x) - f_{ij}(y)| \geq |f_{ij}(x)|$, as by definition $f_{ij}(x) > 0$ and $f_{ij}(y) < 0$. Then by the definition of Lipschitz constant:

$$L^\alpha(f_{ij}, \mathcal{X}) \geq \frac{|f_{ij}(x) - f_{ij}(y)|}{\|x - y\|_\alpha} \geq \frac{|f_{ij}(x)|}{\|x - y\|_\alpha} \quad (120)$$

arriving at the desired contrapositive LHS. We only note that we need to take min over all $j$ so that $f_{ij}(y) \geq 0$ for all $j$. \hfill \square

Now we present our main Theorem regarding multiclassification robustness:

**Theorem 10.** Let $f$ be a vector-valued ReLU network, and let $\| \cdot \|_\infty$ be a norm over $\mathbb{R}^m$, such that for any $x$ in any open set $\mathcal{X}$, with $F(x) = i$,

$$\min_j \frac{|f_{ij}(x)|}{L^{(\alpha, \infty)}(f, \mathcal{X})} \leq \min_j \frac{|f_{ij}(x)|}{L^\alpha(f_{ij}, \mathcal{X})}. \quad (121)$$

Then for $x, y \in \mathcal{X}$ with $F(x) = i$,

$$\|x - y\|_\infty < \min_j \frac{|f_{ij}(x)|}{L^{(\alpha, \infty)}(f, \mathcal{X})} \Rightarrow F(y) = i. \quad (122)$$

In addition, if $\| \cdot \|_\infty$ is a linear norm, then $L^{(\alpha, \infty)}(f, \mathcal{X})$ is computable by LipMIP.

**Proof.** Certainly equation 122 follows directly from Lemma 7 and equation 121. \hfill \square

What remains to be shown is a $\| \cdot \|_\infty$ such that equation 121 holds. To this end, we present a lemma describing convenient formulations for norms:
Lemma 8. Let $C \subseteq \mathbb{R}^n$ be a set that contains an open set. Then
\[
\|x\|_C := \sup_{y \in C} |y^T x|
\] is a norm.

Proof. Nonnegativity and absolute homogeneity are trivial. To see the triangle inequality holds for $\| \cdot \|_C$, we see that, for any $x, y$,
\[
\|x + y\|_C := \sup_{z \in C} |z^T (x + y)| \leq \sup_{z \in C} |z^T x| + \sup_{z' \in C} |z'^T y| \leq \|x\|_C + \|y\|_C
\]
And point separation follows because $C$ contains an open set and if $x \neq 0$, then there exists at least one $y$ in $C$ such that $|y^T x| > 0$. \[\square\]

Now we can define our norm $\| \cdot \|_\times$ that satisfies equation 121:

**Definition 20.** Let $e_{ij} := e_i - e_j$ where each $e_i$ is the elementary basis vector in $\mathbb{R}^m$. Then let $E$ be the convex hull of all such $e_{ij}$ and all $e_i$, $E := \text{Conv}\{e_i \mid i \in [m]\} \cup \{e_{ij} \mid i \neq j \in [m]\}$. We define the cross-norm, $\| \cdot \|_\times$ as
\[
\|x\|_\times := \sup_{y \in E} |y^T x|
\]

We note that by Lemma 8 and since $E$ contains the positive simplex, $E$ contains an open set and hence the cross-norm is certainly a norm. Indeed, because the convex hull of a finite point-set is a polytope, the cross-norm is a linear norm. Further, we note that the polytope $E$ has an efficient H-description.

**Proposition 6.** The set $E \subseteq \mathbb{R}^m$, is equivalent to the polytope $P$ defined as
\[
P = \left\{ x \left| \begin{array}{l} x = x^+ - x^- \\ x^+ \geq 0 : \sum_i x_i^+ \leq 1 \\ x^- \geq 0 : \sum_i x_i^- \leq 1 \\ \sum_i x_i^+ \geq 1 \\ \sum_i x_i^- \leq 1 \end{array} \right. \right\}
\]

Proof. As $E$ is the convex hull of $e_{ij}$ and $e_i$ for all $i \neq j \in [m]$. Certainly each of these points is feasible in $P$, and since $P$ is convex, by the definition of a convex hull, $E \subseteq P$. In the other direction, consider some $x \in P$. Decompose $x$ into $x^+$ and $-x^-$, by only considering the positive and negative components of $x$. The goal is to write $x$ as a convex combination of $(e_{ij}, e_i)$. Further decompose $x^+$ into $y^+, z^+$ such that $x^+ = y^+ + z^+, y^+ \geq 0, z^+ \geq 0, \text{ and } \sum_i y_i^+ = \sum_i x_i^-$. Then we can write $y_i^+ - x_i^- \text{ as a convex combination of } e_{ij}s \text{ and } z_i^+ \text{ is a convex combination of } e_{ij}s \text{ and } 0, \text{ where we note that } 0 \in E \text{ because } e_{ij}, e_{ji} \text{ are in } E. \square$

Now we desire to show equation 121 holds for the cross-norm.

**Proposition 7.** For any open set $X$, the Lipschitz constant with respect to the cross norm, $\| \cdot \|_\times$, and any norm $\| \cdot \|_\alpha$, for $x \in X$ with $F(x) = i$, then
\[
\min_j \frac{|f_{ij}(x)|}{L(\alpha, \times)(f, X)} \leq \min_j \frac{|f_{ij}(x)|}{L(\alpha)(f_{ij}, X)}. \leq \min_j \frac{|f_{ij}(x)|}{L(\alpha)(f, X)}
\]

To see this, notice
\[
\frac{\min_j \frac{|f_{ij}(x)|}{\max_j L(\alpha)(f_{ij}, X)}}{\max_j L(\alpha)(f_{ij}, X)} \leq \min_j \frac{|f_{ij}(x)|}{L(\alpha)(f_{ij}, X)}.
\]
so it amounts to show that $L(\alpha, \times)(f, X) \geq \max_j L(\alpha)(f_{ij}, X)$. By the definition of the Lipschitz constant:
\[
\max_j L(\alpha)(f_{ij}, X) = \max_j \sup_{x \neq y \in X} \frac{|(e_i - e_j, f(x) - f(y))|}{\|x - y\|_\alpha}
\]

By switching the sup and max above, and observing that, for all $z$,
\[
\max_j |(e_i - e_j, z)| \leq \|z\|_\times \leq \|z\|_\alpha \leq \max_j \frac{|f_{ij}(x)|}{\max_j L(\alpha)(f_{ij}, X)}
\]
we can bound
\[ \max_j L^\alpha(f_{ij}, \mathcal{X}) \leq \frac{\|f(x) - f(y)\|_x}{\|x - y\|_\alpha} \leq L^{(\alpha, \times)}(f, \mathcal{X}) \] (131)
as desired.
F. Experiments

In this section we describe details about the experimental section of the main paper and present additional experimental results.

F.1. Experimental Setup

Computing environment: All experiments were run on a desktop with an Intel Core i7-9700K 3.6 GHz 8-Core Processor and 64GB of RAM. All experiments involving mixed-integer or linear programming were optimized using Gurobi, using two threads maximum (Gurobi Optimization, 2020).

Synthetic Datasets: The main synthetic dataset used in our experiments is generated procedurally with the following parameters:

\{dim, num_points, min_separation, num_classes, num_leaders\}

The procedure is as follows: randomly sample $num\_points$ from the unit hypercube in $dim$ dimensions. Points are sampled sequentially, and a sample is replaced if it is within $min\_separation$ of another, previously sampled point. Next, $num\_leaders$ points are selected uniformly randomly from the set of points and uniformly randomly assigned a label from 1 to $num\_classes$. The remaining points are labeled according to the label of their closest ‘leader’. An example dataset and classifier learned to classify it are presented in Figure 6.

![Randomly Generated Data Points](image1)

![Neural Network Decision Boundaries](image2)

Figure 6. (Left): Synthetic dataset used for evaluating effect of training on Lipschitz Estimation. (Right): Decision boundaries of a neural network trained using only CrossEntropy loss for 1000 epochs on the synthetic dataset.

Estimation Techniques: Here we will outline the hyperparameters and computing environment for each estimation technique compared against.

- **RandomLB**: We randomly sample 1000 points in the domain of interest. At each point, we evaluate the appropriate gradient norm that lower-bounds the Lipschitz constant. We report the maximum amongst these sampled gradient norms.

- **CLEVER**: We randomly sample 500 batches of size 1024 each and compute the appropriate gradient norm for each, for a total of 512,000 random gradient norm evaluations. The hyperparameters used to estimate the best-fitting Reverse Weibull distribution are left to their defaults from the CLEVER Github Repository: [https://github.com/IBM/CLEVER-Robustness-Score](https://github.com/IBM/CLEVER-Robustness-Score), (Weng et al., 2018b).



• **LipMIP:** LipMIP is evaluated exactly without any early stopping or timeout parameters, using 2 threads and the Gurobi optimizer.

• **LipSDP:** We use the LipSDP-Network formulation outlined in Fazlyab et al. (2019), which is the slowest but tightest formulation. We note that since this only provides an upper bound of the $\ell_2$-norm of the gradient. We scale by a factor of $\sqrt{n}$ for $\ell_1$, $\ell_\infty$ estimates over domains that are subsets of $\mathbb{R}^n$.

• **SeqLip:** SeqLip bounds are attained by splitting each network into subproblems, with one subproblem per layer. The $\|\cdot\|_2,2$ norm of the Jacobian of each layer is estimated using the Greedy SeqLip heuristic (Virmaux & Scaman, 2018). We scale the resulting output by a factor of $\sqrt{d}$. We remark that a cheap way to make this technique local would be to use interval analysis over a local domain to determine which neurons are fixed to be on or off, and do not include decision variables for these neurons in the optimization step.

• **FastLip:** We use a custom implementation of FastLip that more deeply represents the abstract interpretation view of this technique. As we have noted several times throughout this paper, this is equivalent to the FastLip formulation of Weng et al. (2018a).

• **NaiveUB:** This naive upper bound is generated by multiplying the operator norm of each affine layer’s Jacobian matrix and scaling by $\sqrt{d}$.

F.2. Experimental Details

Here we present more details about each experiment presented in the main paper.

**Accuracy vs. Efficiency Experiments** In the random dataset example, we evaluated 20 randomly generated neural networks with layer sizes $[16, 16, 16, 2]$. Parameters were initialized according to He initialization (He et al., 2015).

In the synthetic dataset example, a random dataset with 2000 points over $\mathbb{R}^10$, 20 leaders 2 classes, were used to train 20 networks, each of layer sizes $[10, 20, 30, 30, 2]$ and was trained for 500 epochs using CrossEntropy loss with the Adam optimizer with learning rate 0.001 and no weight decay (Kingma & Ba, 2014).

In the MNIST example, only MNIST 1’s and 7’s were selected for our dataset. We trained 20 random networks of size $[784, 20, 20, 20, 2]$. We trained for 10 epochs using the Adam optimizer, with a learning rate of 0.001, where the loss was the CrossEntropy loss and an $\ell_1$ weight decay regularization term with value $1 \cdot 10^{-5}$. For each of these networks, 20 randomly centered $\ell_\infty$ balls of radius 0.1 were evaluated.

For each experiment, we presented only the results for compute time and standard deviations, as well as mean relative error with respect to the answer returned by LipMIP.

**Effect of Training on Lipschitz Constant** When demonstrating the effect of different regularization schemes we train a 2-dimensional network with layer sizes $[2, 20, 40, 20, 2]$ over a synthetic dataset generated using 256 points over $\mathbb{R}^2$, 2 classes and 20 leaders. All training losses were optimized for 1000 epochs using the Adam optimizer with a learning rate of 0.001, and no implicit weight decay. Snapshots were taken every 25 epochs and LipMIP was evaluated over the $[0, 1]^2$ domain. All loss functions incorporated the CrossEntropy loss with a scalar value of 1.0. The FGSM training scheme replaced all clean examples with adversarial examples generated via FGSM and a step size of 0.1. The $\ell_1$-weight regularization scheme had a penalization weight of $1 \cdot 10^{-4}$ and the $\ell_2$-weight regularization scheme had a penalization weight of $1 \cdot 10^{-3}$. Weights for $\ell_p$ weight penalties were chosen to not affect training accuracy and were determined by a line search.

The same setup was used to evaluate the accuracy of various estimators during training. The network that was considered in this case was the one trained only using CrossEntropy loss.

**Random Networks and Lipschitz Constants** For the random network experiment, 5000 neural networks with size $[10, 10, 10, 1]$ were initialized using He initialization. LipMIP evaluated the maximal $\ell_1$ norm of the gradient over an origin-centered $\ell_\infty$ ball of radius 1000.
F.3. Additional Experiments

**Effect of Architecture on Lipschitz Estimation** We investigate the effects of changing architecture on Lipschitz estimation techniques. We generate a single synthetic dataset, train networks with varying depth and width, and evaluate each Lipschitz Estimation technique on each network over the \([0, 1]^2\) domain. The synthetic dataset used is over 2 dimensions, with 300 random points, 10 leaders and 2 classes. Training for both the width and depth series is performed using 200 epochs of Adam with learning rate 0.001 over the CrossEntropy loss, with no regularization.

To investigate the effects of changing width, we train networks with size \([2, C, C, C, 2]\) where \(C\) is the x-axis displayed in Figure 7 (left).

To explore the effects under changing depth, we train networks with size \([2] + [20] \times C + [2]\), where \(C\) is the x-axis displayed in Figure 7 (right). Note that the \(y\)-axis is a log-scale: indicating that estimated Lipschitz constants rise exponentially with depth.

**Estimation of \(L^1(f, \mathcal{X})\):** Experiments presented in the main paper evaluate \(L^\infty(f, \mathcal{X})\), which is the maximal \(\ell_1\) norm of the gradient. We can present the same experiments over the \(\ell_\infty\) norm of the gradient. Tables 4 and 5 display results comparing estimation techniques for \(L^1(f, \mathcal{X})\) under the same settings as the “Accuracy vs. Efficiency” experiments in the main paper: that is, we estimate the maximal \(\|\nabla f\|_\infty\) over random networks, networks trained on synthetic datasets, and MNIST networks. Figure 8 demonstrates the effects of training and regularization on Lipschitz estimators on \(L^1(f, \mathcal{X})\). Figure 9 plots a histogram of both \(L^1(f)\) and \(L^\infty(f)\) over random networks.

**Relaxed LipMIP** In section 7 of the main paper, we described two relaxed forms of LipMIP: one that leverages early stopping of mixed-integer programs that can be terminated at a desired integrality gap, and one that is a linear-programming relaxation of LipMIP. Here we present results regarding the accuracy vs. efficiency tradeoff for these techniques. We evaluate LipMIP with integrality gaps of at most \{100\%, 10\%, 1\%, 0\%\} and LipLP over the unit hypercube on the same random networks and synthetic datasets used to generate the data in Table 4. These results are displayed in Table 6.

**Cross-Lipschitz Evaluation** We evaluate the \(\|\cdot\|_\infty\) norm for applications in untargeted robustness verification. We generate a synthetic dataset over 8 dimensions, with 2000 data points, 200 leaders, and 100 classes. We run 10 trials of the following procedure: train a network with layer sizes \([8, 40, 40, 40, 100]\) and pick 20 random data points to evaluate over an \(\ell_\infty\) ball of radius 0.1. We train the network with CrossEntropy loss, \(\ell_1\)-regularization with constant \(5 \cdot 10^{-4}\) and train for 2000 epochs using Adam with a learning rate of 0.001 and no other weight-decay terms. Accuracy is at least 65\% for each trained network. We evaluate the time and reported Lipschitz value for the following metrics, for data points that have label
Exact Computing the Local Lipschitz Constant of ReLU Networks

### Table 4. Accuracy vs. Efficiency tradeoffs for estimating $L^1(f, X)$ over the unit hypercube on random networks of layer sizes $[16, 16, 16, 2]$ and networks with layer sizes $[10, 20, 30, 2]$ trained over a synthetic dataset.

| Method     | Time (s)     | Relative Error | Time (s)     | Relative Error |
|------------|--------------|----------------|--------------|----------------|
| RandomLB   | 0.238 ± 0.004 | -30.43%        | 0.301 ± 0.004 | -29.27%        |
| CLEVER     | 1.442 ± 0.071 | -13.00%        | 55.847 ± 79.212 | 0.00%         |
| LipMIP     | 18.825 ± 19.244 | 0.00%        | 1.873 ± 0.030 | 4.18%         |
| FastLip    | 0.001 ± 0.000 | 167.55%       | 0.028 ± 0.001 | 156.67%       |
| LipLP      | 0.018 ± 0.009 | 167.55%       | 0.001 ± 0.000 | 156.67%       |
| LipSDP     | 2.624 ± 0.026 | 559.97%       | 2.705 ± 0.030 | 432.47%       |
| SeqLip     | 0.007 ± 0.001 | 773.38%       | 0.015 ± 0.002 | 674.84%       |
| NaiveUB    | 0.000 ± 0.000 | 312.15%       | 0.000 ± 0.000 | 11979.62%     |

### Table 5. Accuracy vs. Efficiency for estimating local $L^1(f)$ Lipschitz constants on a network with layer sizes $[784, 20, 20, 20, 2]$ trained to distinguish between MNIST 1’s and 7’s. We evaluate the local lipschitz constant where $X$’s are chosen to be $\ell_1$-balls with specified radius centered at random points in the unit hypercube.

| Method     | Time (s)     | Relative Error | Time (s)     | Relative Error |
|------------|--------------|----------------|--------------|----------------|
| RandomLB   | 0.330 ± 0.006 | -44.25%        | 0.325 ± 0.005 | -35.08%        |
| CLEVER     | 6.855 ± 4.984 | -38.31%        | 23.010 ± 0.612 | -27.24%        |
| LipMIP     | 4.550 ± 2.519 | 0.00%        | 4.292 ± 1.183 | 0.00%         |
| FastLip    | 0.001 ± 0.000 | +43.45%       | 0.233 ± 0.012 | +32.66%       |
| LipLP      | 0.229 ± 0.021 | +43.45%       | 0.002 ± 0.001 | +32.66%       |
| NaiveUB    | 0.000 ± 0.000 | +961.31%      | 0.000 ± 0.000 | +891.10%      |
| LipSDP     | 18.184 ± 1.935 | +16147.15%    | 20.161 ± 2.333 | +14526.92%    |
| SeqLip     | 0.013 ± 0.004 | +16559.65%    | 0.021 ± 0.004 | +14917.94%    |

Figure 8. (Left) Effect of training on various Lipschitz estimators in the $L^1(f, X)$ setting. A network of layer sizes [2, 20, 40, 20, 2] was trained using Adam to minimize CrossEntropy loss over a synthetic dataset. Notice how in this setting, even LipSDP does not provide a tight bound. (Right) Effect of regularization scheme on $L^1(f, X)$. 

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Figure 9. Histograms for $L^1(f)$ and $L^\infty(f)$ over random networks with layer sizes [10, 10, 10, 1]. Notice the much tighter concentration for $L^1(f)$.

| Method      | Random Network | Synthetic Dataset |
|-------------|----------------|-------------------|
|             | Time (s)       | Value | Relative Error | Time (s) | Value | Relative Error |
| LipLP       | 0.017 ± 0.003  | 5.508 | +462.26%       | 0.032 ± 0.003 | 2087.957 | +389.80%       |
| LipMIP(100%)| 132.988 ± 119.857 | 1.937 | +91.98%       | 14.690 ± 12.773 | 742.395 | +69.91%       |
| LipMIP(10%) | 355.974 ± 294.666 | 1.102 | +9.37%       | 50.931 ± 53.403 | 484.550 | +8.75%       |
| LipMIP(1%)  | 357.620 ± 287.511 | 1.015 | +0.72%       | 59.969 ± 63.484 | 448.872 | +0.57%       |
| LipMIP      | 362.533 ± 304.685 | 1.009 | 0.00%       | 60.123 ± 63.721 | 446.327 | 0.00%       |

Table 6. Performance vs. accuracy evaluations of various relaxations of LipMIP. LipLP is the linear programming relaxation, and LipMIP(x%) refers to early stopping of LipMIP once an integrality gap of x% has been attained. It can be significantly more efficient to attain reasonable upper bounds than it is to compute the Lipschitz constant exactly.
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| Method            | Time (s)       | Value       | Relative Error |
|-------------------|----------------|-------------|----------------|
| Naive             | 97.698 ± 104.281 | 72.083      | 0.00%          |
| CrossLip(i)       | 6.156 ± 14.256  | 350.176     | +441.14%       |
| MIPCrossLip(i)    | 6.987 ± 14.704  | 350.176     | +441.14%       |

Table 7. Application to multiclass robustness verification. On networks trained on a synthetic dataset with 100 classes, we evaluate untargeted robustness verification techniques across random datasets. The value column refers to the computed Lipschitz value, and relative error is relative to the Naive value. Notice that a 15x speedup is attainable on average at the cost of providing a 4.5x looser bound on robustness.

\[ \min_j L^\infty(f_{ij}, X), \]  

where we evaluate this naively (Naive), or with the search space of all \( e_{ij} \) encoded directly with mixed-integer-programming (MIPCrossLip(i)). We also evaluate the \( \| \cdot \|_{x(i)} \) norm in lieu of \( \| \cdot \|_\beta \), where \( \| \cdot \|_{x(i)} \) is defined as

\[ \| x \|_{x(i)} := \sup_{y \in P(i)} |y^T x| \]  

where we denote this technique (CrossLip(i)). Times and returned Lipschitz values are displayed in Table 7.