Hierarchical Verification for Adversarial Robustness

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Abstract

We introduce a new framework for the exact pointwise $\ell_p$ robustness verification problem that exploits the layer-wise geometric structure of deep feed-forward networks with rectified linear activations (ReLUs). The activation regions of the network partition the input space, and one can verify the $\ell_p$ robustness around a point by checking all the activation regions within the desired radius. The GeoCert algorithm (Jordan et al., 2019) treats this partition as a generic polyhedral complex in order to detect which region to check next. In contrast, our LayerCert framework considers the nested hyperplane arrangement structure induced by the layers of the ReLU network and explores regions in a hierarchical manner. We show that, under certain conditions on the algorithm parameters, LayerCert provably reduces the number and size of the convex programs that one needs to solve compared to GeoCert. Furthermore, our LayerCert framework allows the incorporation of lower bounding routines based on convex relaxations to further improve performance. Experimental results demonstrate that LayerCert can significantly reduce both the number of convex programs solved and the running time over the state-of-the-art.

1. Introduction

Deep neural networks have been demonstrated to be susceptible to adversarial perturbations of the inputs (e.g., Szegedy et al. (2013); Biggio et al. (2013); Goodfellow et al. (2014)). Hence, it is important to be able to measure how vulnerable a neural network may be to such noise, especially for safety-critical applications. We study the problem of pointwise exact verification for $\ell_p$-norm adversarial robustness for trained deep feed-forward networks with ReLU activation functions. The point-wise $\ell_p$ robustness with respect to an input $x \in \mathbb{R}^n$ and a classifier $c : \mathbb{R}^n \to |C| := \{1, 2, 3, \ldots, C\}$ is defined as

$$e^*(x; c) := \min_{\|v\|_p \leq \epsilon} \epsilon \text{ s.t. } c(x + v) \neq c(x). \quad (1)$$

The goal of exact or complete robustness verification is to check if $\epsilon > r$ for some desired radius $r$. The choices of $p$ studied in the literature are typically 1, 2, and $\infty$; our work applies to all $p \geq 1$. Solving Problem (1) exactly (or within a factor of $1 - o(1) \ln n$) is known to be NP-hard (Weng et al., 2018). Developing methods that perform well in practice would require a better understanding of the mathematical structure of neural networks.

In this work, we approach the problem from the angle of how to directly exploit the geometry induced in input space by the neural network. Each activation pattern (i.e., whether each neuron is on or off) corresponds to a polyhedral region in the input space, and the decision boundary within each region is linear. A natural geometric approach to the verification problem is then to check regions in order of their distance. We illustrate this in Figure 1. We can terminate this process either when we have reached the desired verification radius or when we have exceeded the distance to the closest decision boundary found. In the latter case the distance to that boundary is the solution to Problem (1).

Jordan et al. (2019) proposed the first algorithm for this distance-based exploration of the regions. Their GeoCert algorithm navigates the regions in order of distance by maintaining a priority queue containing all the polyhedral faces that make up the frontier of all regions that have been visited. The priority associated with each face is computed via an optimization problem that can be solved by a generic convex programming solver. Under a limited time budget, GeoCert finds a stronger computational lower bound for $e^*(x; c)$ compared to a complete method that directly uses mixed-integer programming (Tjeng et al., 2019).

In this paper we introduce the LayerCert framework that makes use of the layer-wise structure of neural networks. The first layer of ReLUs induce a hyperplane arrangement structure, and each subsequent layer induces one within each region of the hyperplane arrangement from the previous layer. This forms a nested hyperplane pattern and a
We demonstrate the first advantage by studying a simplified version of LayerCert (LayerCert-Basic), which introduces a hierarchy of regions/subregions that our algorithm will use to navigate the input space. This hierarchical approach has two main advantages over GeoCert:

1. **Provable** reduction in the number and size of convex programs solved when using a convex distance-based priority function.

2. The ability to incorporate convex-relaxation-based lower bounding/incomplete methods for Problem (1) to reduce the number of regions that are processed.

We use subscripts for vectors and matrices to refer to entries and superscripts are used to index distinct objects, with the exception of $\mathbb{R}^n$ and $\mathbb{R}^+$ to denote the $n$-dimensional Euclidean space and the nonnegative real numbers respectively. We use subscripts for vectors and matrices to refer to entries in the objects and subscripts for sets to refer to distinct sets. We use typewriter fonts to denote subroutines.

**2. Related work**

Besides GeoCert (Jordan et al., 2019), the majority of exact or complete verification methods are based on branch-and-bound (e.g. Katz et al. (2017); Wang et al. (2018); Tjeng et al. (2019); Anderson et al. (2019a); Lu & Kumar (2020)), and Bunel et al. (2018; 2019) provide a detailed overview. These methods construct a search tree over the possible individual ReLU activations and use upper and lower bounds to prune the tree. The upper bounds come from adversarial examples, while the lower bounds are obtained by solving a relaxation of the original problem, which we briefly discuss in the next paragraph. Since our focus in this work is on methods that directly leverage the geometry of the neural network function in the input space, we leave a detailed comparison against these methods to future work.

Instead of exactly measuring or verifying, we can instead overapproximate or relax the set reachable by an $\epsilon$-ball around the input point (e.g. Dvijotham et al. (2018); Xiang et al. (2018); Singh et al. (2018); Weng et al. (2018); Wong et al. (2018); Wong et al. (2019)).
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& Kolter (2018); Zhang et al. (2018); Singh et al. (2019b)). These incomplete approaches give us a lower bound for Problem (1). These can only certify that there is no perturbation that changes the class within some radius \( r \) for some \( r \) that can be much smaller than \( \epsilon(\mathbf{x}; \mathbf{c}) \). The majority of the works focus on different convex relaxations of the ReLU activations (see Salman et al. (2019) for a discussion of the tightness of the different approaches), though recent works have started going beyond single ReLU relaxations (Singh et al., 2019a; Anderson et al., 2019b). Another line of work studies how to efficiently bound the Lipschitz constant of the neural network function (Szegedy et al., 2013; Bartlett et al., 2017; Weng et al., 2018; Combettes & Pesquet, 2019; Fazlyab et al., 2019; Zou et al., 2019).

The complexity of geometric methods (and many other exact methods) for robustness verification can be upper bounded by a constant \( \times \) (number of activation regions) \( \times \) (complexity of solving a convex program). There have been several works in recent years that study the number of these activation regions (patterns and regions in hyperplane arrangements) Given a hyperplane arrangement \( \mathcal{A} \) is a finite intersection of halfspaces.

### 3. Hierarchical Structure of ReLU Networks

In this section, we describe the structure induced by the ReLU neurons in the input space and how this leads naturally to a hierarchy of regions that we use in our approach.

#### 3.1. Hyperplane Arrangements

**Definition 3.1.** (Hyperplanes and hyperplane arrangements) A hyperplane \( H \subset \mathbb{R}^n \) is an \((n-1)\)-dimensional affine space that can be written as \( \{ \mathbf{x} \mid \alpha^\top \mathbf{x} = b \} \) for some \( \alpha \in \mathbb{R}^n \) and \( b \in \mathbb{R} \). A hyperplane arrangement \( \mathcal{A} \) is a finite set of hyperplanes.

**Definition 3.2.** (Halfspaces) Given a hyperplane \( H \coloneqq \{ \mathbf{x} \mid \alpha^\top \mathbf{x} = b \} \), the halfspaces \( H^\leq \) and \( H^\geq \) correspond to the sets \( \{ \mathbf{x} \mid \alpha^\top \mathbf{x} \leq b \} \) and \( \{ \mathbf{x} \mid \alpha^\top \mathbf{x} \geq b \} \), respectively. A polyhedron is a finite intersection of halfspaces.

**Definition 3.3.** (Patterns and regions in hyperplane arrangements) Given a hyperplane arrangement \( \mathcal{A} \) and a pattern \( P : \mathcal{A} \to \{-1, 1\} \), the corresponding region is

\[
R_+ := \bigcap_{P(H) = 1} H^\leq \cap \bigcap_{P(H) = -1} H^\geq.
\]

We say that another pattern \( Q : \mathcal{A} \to \{-1, 1\} \) (or region \( R_Q \)) is a neighbor of \( P \) (\( R_P \) resp.) if \( P \) and \( Q \) differ only on a single hyperplane.

#### 3.2. Geometric Structure of Deep ReLU Networks

A ReLU network with \( L \) hidden layers for classification with \( C \) classes and \( n_i \) neurons in the \( i \)-th layer for \( i \in [L] \) can be represented as follows:

\[
x^0 := \mathbf{x} \quad \text{input},
\]

\[
z^i+1 := W^i x^i + b^i \quad \text{for } i \in \{0, 1, \ldots, L - 1\}, \tag{2}
\]

\[
x^i := \text{relu}(z^i) \quad \text{for } i \in \{1, \ldots, L\},
\]

\[
f(\mathbf{x}) := W^L x^L + b^L \quad \text{output},
\]

where \( W^i, b^i \) describe the weight matrix and bias in the \( i \)-th layer and the ReLU function is defined as \( \text{relu}(v)_i := \max(0, v_i) \). The length of \( b^i \) is \( n_i+1 \) for \( i \in [L - 1] \) and \( b^0 \in \mathbb{R}^n \) and \( b^L \in \mathbb{R}^C \). The classification decision is given by \( \arg\max_i (f(\mathbf{x})){i} \), and the decision boundary between classes \( i \) and \( j \) is the set \( \{ x \mid f_i(x) - f_j(x) = 0 \} \).

Note that layers like batch normalization layers, convolutional layers, and average pooling layers can be included in this framework by using the appropriate weights and biases. We can also have a final softmax layer since it does not affect the decision boundaries as it is a symmetric monotonically increasing function.

**Definition 3.4.** (Full activation patterns) Let \( n_i \) denote the number of neurons in the \( i \)-th layer: A (full) activation pattern \( A = (A_1, \ldots, A_L) \) is a collection of functions \( A_i : [n_i] \to (-1, +1) \). Two activation patterns are neighbors if they differ on exactly one layer for exactly one neuron.

We can define a neighborhood graph over the set of activation patterns where each node presents a pattern and we add an edge between neighboring patterns.

**Definition 3.5.** (Activation patterns and the input space) For an input \( \mathbf{x} \), the (full) activation pattern of \( \mathbf{x} \) is \( A^x \) where

\[
A^x_i(j) := \begin{cases} +1 & \text{if } z^i_j \geq 0, \\ -1 & \text{if } z^i_j < 0, \end{cases} \tag{3}
\]

where the \( z^i_j \) terms are defined according to (2). Conversely, given an activation pattern \( A \), the corresponding activation region is \( R_A := \{ x \mid A^x = A \} \).

Given an activation pattern \( A \) and some \( x \in R_A \), the corresponding \( z \) terms are given by

\[
z^{i+1} = W^i I^{A_i} z^i + b^i \tag{4}
\]

where \( I^{A_i} \) is the diagonal 0-1 matrix such that

\[
I^{A_i}_{j,k} := \begin{cases} 1 & \text{if } j = k \text{ and } A_i(j) = 1, \\ 0 & \text{otherwise.} \end{cases}
\]

By letting

\[
e_i := \sum_{j=0}^{i} \left( \prod_{k=j+1}^{i} W^k I^{A_k} \right) b^i
\]
we can expand Eq. (4) as
\[ z^{l+1} = \left( \prod_{j=0}^{i} W^j I^{A_j} \right) x + c^i. \] (5)

Hence, each \( z^i \) term and \( f(x) \) can be expressed as a linear expression over \( x \) involving \( W^i, I^{A^i} \), and \( b^i \) terms. This also allows us to write \( R_A \) in the form of linear inequalities over \( x \) as a polyhedron
\[ \{ x \mid A_i(j)z_j^i \geq 0 \text{ for } i \in [L], \ j \in [n_i] \} \] (6)

Since the neural network function \( f \) is linear within each activation region, each decision boundary is also linear within each activation region. This allows us to efficiently compute the classification decision boundaries.

The set of activation regions for a network with one hidden layer corresponds to the regions of a hyperplane arrangement (where each row of \( W^0 \) and the corresponding entry in \( b^0 \) defines a hyperplane). With each additional layer, we take the regions corresponding to the previous layer and add a hyperplane arrangement to each region. Thus, this leads to a nested hyperplane arrangement. Figure 2 illustrates this structure and the corresponding neighborhood graph.

In addition to full activation patterns, it is useful to consider the patterns for all neurons up to a particular layer.

**Definition 3.6.** (Partial activation patterns and regions) Given some \( l < L \), an \( l \)-layer partial activation pattern \( A = (A_1, \ldots, A_l) \) is a collection of functions \( A_i : [n_i] \rightarrow \{-1, +1\} \). The corresponding partial activation region \( R_A \) is \( \{ x \mid A_i(j)z_j^i \geq 0 \text{ for } i \in [L], \ j \in [n_i] \} \).

The partial activation regions naturally induce a hierarchy of regions. We can describe the relationship between the regions in the different levels in the following terms:

**Definition 3.7.** For a \( l \)-layer activation pattern \( A = (A_1, \ldots, A_l) \), let parent(\( A \)) := (\( A_1, \ldots, A_{l-1} \)). The terms child and descendant are defined analogously.

We can use Definition 3.7 and 3.8 to define a hierarchical search graph with \( L + 1 \) levels. The nodes in the \( l \)-th level represent the \( l \)-th layer activation patterns. We connect two activation patterns in the same level if they are neighboring siblings.

Figure 3 illustrates this hierarchy of activation regions and the corresponding hierarchical search graph. In Sections 4 and 5, we describe how to leverage this hierarchical structure to design efficient algorithms for verification.

### 4. Exploring Activation Regions Geometrically

In this section, we first describe the GeoCert algorithm (Jordan et al., 2019) that provides a method for navigating the activation regions in order of increasing distance from the input. We subsequently consider the hierarchy of partial regions and describe LayerCert-Basic that leverages the geometric structure to provably reduce the number and size of convex programs compared to GeoCert. We then introduce the full LayerCert framework in Section 5.

#### 4.1. Prior Work: GeoCert

GeoCert performs a process akin to breadth-first search over the neighbourhood graph (see Figure 2). In each iteration, GeoCert selects the activation region corresponding to the
We provide a formal description of GeoCert in Algorithm 1 and demonstrate an iteration of the algorithm in Figure 4. Setting the input \( U \) term to a radius \( r \) solves the robustness verification problem for that radius, while setting it sufficiently high measures the robustness (i.e., Problem (1)).

We describe the subroutines in detail below.

**Measuring the distance to a distance boundary restricted to a region.** The subroutine `decision_bound` with inputs \( A, x, y \) solves the problem

\[
\min_v \| x - v \|_p \quad \text{s.t.} \quad v \in R_A, f_y(v) - f_j(v) = 0
\]

for all classes \( j \neq y \) and returns the minimum (or \( \infty \) if all the problems are infeasible). This is equivalent to computing the \( \ell_p \) projection of \( x \) onto the respective set. We can use algorithms specifically designed for projection onto sets such as Dykstra’s method (Boyle & Dykstra, 1986). We can also use generic convex optimization solvers to handle a wider range of priority functions.

**Computing the priority function.** From (6), we can write each activation region \( R_A \) as a polyhedron 
\[
\{ x \mid A_i(j) z_j^i \geq 0 \text{ for } i \in [L], j \in [n_i] \}
\]

A neighbouring region \( R_A' \) that differs only on the \( a \)-th neuron on the \( b \)-th layer will intersect with \( R_A \) within the hyperplane 
\[
H = \{ x \mid b^b_z \geq 0 \}.
\]

We name the set \( R_A \cap H = R_A' \cap H \) as `Face\( (A, A') \)` since this set is a face of both \( A \) and \( A' \). As with \( R_A \) and (6), we can write `Face\( (A, A') \)` as
\[
\{ x \mid A_i(j) z_j^i \geq 0 \text{ for } i \in [L], j \in [n_i], z_0^a = 0 \}
\]

where \( z_j^i \) can be expressed in terms of the \( x \) variables using the expression in (5). Given some function \( q : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^n \), the subroutine `priority` with inputs \( x, \text{Face}(A, A') \)` solves the following optimization problem:

\[
\min_v q(x, v) \quad \text{s.t.} \quad v \in \text{Face}(A, A').
\]

For \( \ell_p \)-robustness, a natural choice of \( q \) is the \( \ell_p \) distance function. Jordan et al. (2019) also propose an alternative variant of GeoCert where they incorporate an additional term \( \min_{y \neq j} \frac{f_y(v) - f_j(v)}{L} \) priority function, where \( L \) denotes an upper bound on the Lipschitz constant. This makes the priority function nonconvex. We will refer to the \( \ell_p \) priority variant of GeoCert as just GeoCert and specifically use the term GeoCert-Lip for the Lipschitz variant.

**4.2. Our Approach – LayerCert**

Instead of exploring the neighborhood graph of full activation regions, we develop an algorithm that makes use of the nested hyperplane arrangement and the graph induced by it. See Definition 3.7 and Figure 3 for a description of this graph. We first give a description of a basic form of LayerCert in Algorithm 2, followed by theoretical results about this method.

In each iteration, LayerCert processes the next nearest partial activation pattern by computing the distances to all sibling patterns to the queue. This is in contrast to GeoCert which computes the distance to all neighbouring patterns of the next nearest full activation pattern.

The new subroutine in LayerCert-Basic is `next_layer`, which takes an \( l \)-layer activation pattern \( A \) and an input vector \( v \) and returns the \( l + 1 \) layer activation pattern that is a child of \( A \) and contains \( v \):

\[
\text{next}\_\text{layer}(A,v) := (A_1, \ldots, A_l, A_l^{v+1})
\]

where \( A^v \) is the full activation pattern of \( v \) (Definition 3.5).
Algorithm 2 LayerCert-Basic

1: **Input:** $x, y$ (label of $x$), $U$ (upper bound)
2: $A^x \leftarrow$ activation pattern of $x$ at first layer
3: $Q \leftarrow$ empty priority queue
4: $Q$.push((0, $A^x$, $x$))
5: $S \leftarrow \emptyset$
6: **while** $Q \neq \emptyset$ **do**
7: $(d, A, v) \leftarrow Q$.pop()
8: **if** $U \leq d$ **then**
9: \hspace{1em} **return** $U$
10: **else**
11: \hspace{2em} **if** $A$ is a full activation pattern **then**
12: \hspace{3em} $U \leftarrow \min(\text{decision bound}(A, x, y), U)$
13: \hspace{2em} **else**
14: \hspace{3em} **for** $A' \in N_{\text{current layer}}(A) \setminus S$ **do**
15: \hspace{4em} **if** Face($A, A'$) is nonempty **then**
16: \hspace{5em} $v', d' \leftarrow \text{priority}(x, \text{Face}(A, A'))$
17: \hspace{6em} $Q$.push($((d', A', v')), S \leftarrow S \cup \{A'\}$

We prove in the appendix that when the priority function is a convex distance function, LayerCert-Basic visits full activation patterns in ascending order of distance, which implies that it returns the correct solution.

**Theorem 4.1.** *(Correctness of LayerCert-Basic)* If the priority function used is a convex distance function, LayerCert processes full activation patterns in ascending order of distance and returns the distance of the closest point with a different class from $x$.

As a corollary of Theorem 4.1, LayerCert-Basic and GeoCert equipped with the same priority function visit the activation patterns in the same order (allowing for permutations of patterns with the exact same priority).

The primary difference in computational difficulty between the two methods is the number and complexity of priority computations is reduced in LayerCert. There are three main reasons for this. First, LayerCert-Basic updates the set of seen patterns $S$ with $A$ once we have processed any neighbour of $A$. Hence, we only do a single priority computation for each $A$. This is not necessarily the case in GeoCert. Secondly, the convex programs corresponding to nodes further up the hierarchy have less constraints since they only need to consider all neurons to the respective layer. Finally, in LayerCert-Basic we do not need to compute priority between two $l$-layer partial activation patterns that differ on exactly a single neuron that is not in layer $l$ (i.e., these patterns are not siblings). GeoCert in contrast computes the priority between any two neighbours as long as the corresponding Face is non-empty. This allows us to amortize the number of convex programs to compute for a single full activation region in GeoCert over multiple levels in LayerCert — Consider a full activation pattern $A = (A_1, \ldots, A_L)$ and the set of all ancestor patterns $B_1, \ldots, B_{L-1}$ where $B_i := (A_1, \ldots, A_i)$. We have $\sum_i n_i$ neighbours for GeoCert when processing pattern $A$. For LayerCert-Basic, we have up to $n_i$ siblings when processing each $B_i$, for a total of $\sum_i n_i$ patterns when processing $B_1, \ldots, B_{L-1}, A$.

These facts can be used to prove our main theoretical result about the complexity of LayerCert-Basic. The proof of these and the main theorem are in the supplementary material.

**Theorem 4.2.** *(Complexity of LayerCert-Basic)* Given an input $x$, suppose the distance to the nearest adversary returned by LayerCert/GeoCert is not equal to the distance of any activation region from $x$. Suppose we formulate the convex problems associated with decision bound and next layer using Formulations (6) and (8). We can construct an injective mapping from the set of convex programs solved by LayerCert to the corresponding set in GeoCert such that the constraints in the LayerCert program is a subset of those in the corresponding GeoCert program.

5. The LayerCert Framework

We now describe how our hierarchical approach is amenable to the use of convex relaxation-based lower bounds to prune the search space. For simplicity, in this section we will assume that we are performing verification with respect to a targeted class $y'$. The general LayerCert framework is presented in Algorithm 3. The two new subroutines in the algorithm are contains_db and restriction.
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Let $B_{p,r}(x)$ denote the $\ell_p$-ball of radius $r$ around $x$. The subroutine `contains<>(A,x,r)` returns `false` when $R_A \cap B_{p,r}(x)$ is guaranteed not to intersect with a decision boundary. This means that we can remove $A$ and all its descendants from consideration. Otherwise, it returns `maybe` and we proceed on to the next level.

The routine `restriction(x,r)` explicitly computes a convex set $M$ that is a superset of the part of the decision boundary contained in $B_{p,r}(x)$. This both restricts the search directions we need to consider and also allows us to warm start the algorithm by projecting the initial point onto this set. In the following we describe some possible choices for these subroutines. In the appendix we discuss a version of LayerCert that recursively applies a modified version of `restriction` to aggressively prune the search space.

### Pruning partial activation regions.

We can use incomplete verifiers (see Section 2 for references) to check if the region $B_{p,U}$ might contain a decision boundary. These methods work by implicitly or explicitly computing some overapproximation of the set

$$\{ f_{\theta}(v) - f_{\theta'}(v) \mid v \in B_{p,U} \}. \quad (10)$$

If all values in (10) are strictly positive, then we know that the decision boundary cannot be in $R_A \cap B_{p,U}$.

Many incomplete verifiers work by constructing convex relaxations of each nonlinear ReLU function. If a neuron is guaranteed to be always on or always off over all points in the region of interest, we can use this to tighten the convex relaxation. This allows us to incorporate information from the current partial activation region into incomplete verifiers.

For our experiments, we choose to use the efficient interval arithmetic approach (first applied in the context of neural network verification by Xiang et al. (2018)). Below we describe a version of the method that incorporates information about partial regions:

$$X^0 := B_{p,U}(x),$$
$$Y^i := \text{Interval}_A(X^{i-1}) \quad \text{for } i \in [L + 1],$$
$$Z^i := W^{i-1} Y^{i-1} + b^{i-1} \quad \text{for } i \in [L],$$
$$X^i := \text{relu}(Z^i) \quad \text{for } i \in [L],$$

where `Interval_A(X)` is given by the following set:

$$\left\{ v \mid \min_{w \in X} w_j \leq v_j \leq \min_{w \in X} (p_j, \max_{w \in X} w_j) \right\}$$

where $p_j$ is 0 if $A(i,j) = -1$ and infinite otherwise. We can use the fact that $f(B_{p,U}(x) \cap R_A) \subseteq W^L Y^{L+1} + b^L$ to check if we need to explore the descendants of $A$.

### Warm starts via restricting search area.

Certain incomplete verifiers implicitly generate enough information to allow us to efficiently compute a convex set $M$ that contains the decision boundary. We will describe how to do this for verifiers based on simple linear underestimates of $f_{\theta} - f_{\theta'}$ in the ball $B_{p,U}(x)$ such as Fast-Lin (Weng et al., 2018) and CROWN (Zhang et al., 2018). These methods construct a linear function $g \leq f_{\theta} - f_{\theta'}$ by propagating linear and upper bounds of the ReLUs through the layers. The resulting set $\{ v \mid g(v) \leq 0 \}$ is a halfspace that we can efficiently project onto. Figure 5 illustrates this concept. For the purposes of this paper we use the lower bound from the CROWN verifier (Zhang et al., 2018) to compute a halfspace $M$.

Once we have computed $M$, we can use it throughout our algorithm. In particular, if a face does not overlap with $M$, we can remove it from consideration in our algorithm. We discuss this in more detail in the supplementary.

Instead of just using linear approximations, we can also use tighter approximations such as the linear programming relaxation that models single ReLUs tightly (see for example Salman et al. (2019)) These result in a smaller convex set $M$ that is still guaranteed to contain the decision boundary but overlaps with less regions, resulting in a reduction in the search space. The drawback of using such methods is that the representation of $M$ can get significantly more complicated, which in turn increases the cost of solving Problems (9) and (7).

### 6. Experimental Evaluation

We use an experimental setup similar to the one used in Jordan et al. (2019). The two experiments presented here are taken directly from them, except for an additional neural network in the first and a larger neural network in the second. Additional results are presented in the appendix.

We consider a superset of the networks used in GeoCert. The fully connected ReLU networks we use in the paper have two to five hidden layers, with between 10 to 50 neurons.
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Table 1. Average number of convex programs and running time over 100 inputs for 12 different networks for $\ell_\infty$-distance. The green shaded entries indicate the best performing method for each neural network under each metric. The gray shaded entries indicates the algorithm timed out before an exact solution to Problem (1) could be found for at least one input. Whenever a timeout occurs, we use a time of 1800 seconds in its place, which leads to an underestimate of the true time.

|                  | [10, 50, 10] | 2 x [20] | 3 x [20] | 4 x [20] | 5 x [20] | 2 x [30] |
|------------------|-------------|---------|---------|---------|---------|---------|
|                  | #LPs | Time(s) | #LPs | Time(s) | #LPs | Time(s) | #LPs | Time(s) | #LPs | Time(s) | #LPs | Time(s) |
| GeoCert          | 48.8 | 3.68    | 488.0 | 22.85   | 3297.7| 212.32  | 275.2 | 26.46   | 82.0 | 9.50    | 92.0 | 6.51    |
| GeoCert-Lip      | 39.4 | 4.19    | 183.4 | 11.11   | 1055.0| 90.23   | 154.7 | 18.36   | 61.3 | 8.79    | 55.1 | 4.91    |
| LayerCert        | 28.4 | 1.56    | 227.7 | 8.60    | 1617.8| 62.53   | 111.8 | 5.62    | 44.0 | 3.36    | 45.9 | 2.28    |
| LayerCert-IA     | 26.4 | 1.34    | 208.1 | 7.72    | 1258.0| 44.17   | 90.7  | 3.52    | 38.6 | 2.66    | 45.6 | 2.23    |
| LayerCert-CROWN  | 26.8 | 1.46    | 116.7 | 5.80    | 648.1 | 24.34   | 73.7  | 3.43    | 31.1 | 2.36    | 39.1 | 1.93    |
| LayerCert-Both   | 25.4 | 1.38    | 116.7 | 5.82    | 613.0 | 22.63   | 67.2  | 2.83    | 29.9 | 2.08    | 39.1 | 1.91    |

6.1. Exact measurement experiments.

We randomly picked 100 ‘1’s and ‘7’s from MNIST and collected the wall-clock time and number of linear programs solved. Since some instances can take a very long time to solve fully, we set a time limit of 1800s for each instance.

Averaged metrics. We measure (1) the average of the wall-clock time taken to measure the distances and (2) the average of number of linear programs solved. The first geometric-certificates and modifies it to make use of open-source convex programming solvers to enable further research to a wider community, as the original code uses Gurobi (Gurobi Optimization, 2019), which is a commercial software. We use CVXPY (Diamond & Boyd, 2016) to model the convex programs and the open-source ECOS solver (Domahidi et al., 2013) as the main solver. Since ECOS can occasionally fail, we also use OSQP (Stellato et al., 2017) and SCS (Odonoghue et al., 2016) as backup solvers. In our tests, ECOS and OSQP are significantly faster than SCS which we use only as a last resort.

We implemented LayerCert in Python using the packages numpy, PyTorch, numba (for the lower bounding methods), and the aforementioned packages for solving convex programs. Our experiments were performed on an Ubuntu 18.04 server on an Intel Xeon Gold 6136 CPU with 12 cores. We restricted the algorithms to use only a single core and do not allow the use of the GPU. All settings, external packages, and compute are identical for all the methods compared.

Methods evaluated. We test the following variants of GeoCert and LayerCert. All variants of LayerCert use an $\ell_p$ distance priority function.

- GeoCert with $\ell_p$ distance priority function.
- GeoCert-Lip: GeoCert with $\|x - v\|_p + \min_{y \neq j} \frac{f_y(v) - f_j(v)}{L}$ priority function, where $L$ denotes an upper bound on the Lipschitz constant found by the Fast-Lip method (Weng et al., 2018).
- LayerCert-Basic.
- LayerCert with interval arithmetic pruning.
- LayerCert with warmstart in the initial iteration using CROWN (Zhang et al., 2018) to underestimate $f_y - f_j$.
- LayerCert-Both: with both interval arithmetic pruning and CROWN-based warm start.

We initialize each algorithm with a target verification radius of 0.3. Each method terminates when we have exactly computed the answer to (1) or when it has determined that the lower bound is at least the radius.

Implementation details. Our implementation of GeoCert (Jordan et al., 2019) starts with the original code provided by the authors at https://github.com/revbucket/geometric-certificates and modifies it to make use of open-source convex programming solvers to enable further research to a wider community, as the original code uses Gurobi (Gurobi Optimization, 2019), which is a commercial software. We use CVXPY (Diamond & Boyd, 2016) to model the convex programs and the open-source ECOS solver (Domahidi et al., 2013) as the main solver. Since ECOS can occasionally fail, we also use OSQP (Stellato et al., 2017) and SCS (Odonoghue et al., 2016) as backup solvers. In our tests, ECOS and OSQP are significantly faster than SCS which we use only as a last resort.

We implemented LayerCert in Python using the packages numpy, PyTorch, numba (for the lower bounding methods), and the aforementioned packages for solving convex programs. Our experiments were performed on an Ubuntu 18.04 server on an Intel Xeon Gold 6136 CPU with 12 cores. We restricted the algorithms to use only a single core and do not allow the use of the GPU. All settings, external packages, and compute are identical for all the methods compared.

We randomly picked 100 ‘1’s and ‘7’s from MNIST and collected the wall-clock time and number of linear programs solved. Since some instances can take a very long time to solve fully, we set a time limit of 1800s for each instance.

Averaged metrics. We measure (1) the average of the wall-clock time taken to measure the distances and (2) the average of number of linear programs solved. The first
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Figure 6. Performance profiles comparing LayerCert-Both (orange, ‘x’ markers) with GeoCert-Lip (blue, dotted, circle markers) over 12 different networks using $\ell_{\infty}$ norm. Marks are placed for every 10 input points.

Performance profiles. Performance profiles (Dolan & Mor, 2002) are a commonly-used technique to benchmark the performance of different optimization methods over sets of instances. A performance profile is a plot of a cumulative distribution, where the $x$-axis denotes the amount of time each method is allowed to run for, and the $y$-axis the number of problems that can be solved within that time period. If the performance profile of a method is consistently above the performance profile of another method, it indicates that the former method is always able to solve more problems regardless of the time limit. We illustrate the performance profiles for GeoCert-Lip and LayerCert-Both in Figure 6. LayerCert-Both consistently dominates GeoCert-Lip.

7. Conclusion

We have developed a novel hierarchical framework LayerCert for exact robustness verification that leverages the nested hyperplane arrangement structure of ReLU networks. We prove that a basic version of LayerCert is able to reduce the number and size of the convex programs over GeoCert using the equivalent priority functions. We showed that LayerCert is amenable to the use of lower bounding methods that use convex relaxations to both prune and warm start the algorithm. Our experiments showed that LayerCert can significantly outperform variants of GeoCert.

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Hierarchical Verification for Adversarial Robustness

References

Anderson, G., Pailoor, S., Dillig, I., and Chaudhuri, S. Optimization and abstraction: a synergistic approach for analyzing neural network robustness. In Proceedings of the 40th ACM SIGPLAN Conference on Programming Language Design and Implementation, PLDI 2019, pp. 731–744, Phoenix, AZ, USA, June 2019a. Association for Computing Machinery. ISBN 978-1-4503-6712-7.

Anderson, R., Huchette, J., Tjandraatmadja, C., and Vielma, J. P. Strong Mixed-Integer Programming Formulations for Trained Neural Networks. In Lodi, A. and Nagaraajan, V. (eds.), Integer Programming and Combinatorial Optimization, Lecture Notes in Computer Science, pp. 27–42. Springer International Publishing, 2019b. ISBN 978-3-030-17953-3.

Balan, R., Singh, M., and Zou, D. Lipschitz properties for deep convolutional networks. arXiv preprint arXiv:1701.05217, 2017.

Bartlett, P. L., Foster, D. J., and Telgarsky, M. J. Spectrally-normalized margin bounds for neural networks. In Advances in Neural Information Processing Systems, pp. 6240–6249, 2017.

Biggio, B., Corona, I., Maiorca, D., Nelson, B., Šrndić, N., Laskov, P., Giacinto, G., and Roli, F. Evasion attacks against machine learning at test time. In Joint European conference on machine learning and knowledge discovery in databases, pp. 387–402. Springer, 2013.

Boyle, J. P. and Dykstra, R. L. A Method for Finding Projections onto the Intersection of Convex Sets in Hilbert Spaces. In Dykstra, R., Robertson, T., and Wright, F. T. (eds.), Advances in Order Restricted Statistical Inference, Lecture Notes in Statistics, pp. 28–47, New York, NY, 1986. Springer. ISBN 978-1-4613-9940-7.

Bunel, R., Turkaslan, I., Torr, P. H., Kohli, P., and Kumar, M. P. A Unified View of Piecewise Linear Neural Network Verification. In Proceedings of the 32Nd International Conference on Neural Information Processing Systems, NIPS’18, pp. 4795–4804, USA, 2018. Curran Associates Inc. event-place: Montral, Canada.

Bunel, R., Lu, J., Turkaslan, I., Torr, P. H. S., Kohli, P., and Kumar, M. P. Branch and Bound for Piecewise Linear Neural Network Verification. arXiv:1909.06588 [cs, stat], November 2019. arXiv: 1909.06588.

Combettes, P. L. and Pesquet, J.-C. Lipschitz certificates for neural network structures driven by averaged activation operators. arXiv preprint arXiv:1903.01014, 2019.

Diamond, S. and Boyd, S. CVXPY: A Python-embedded modeling language for convex optimization. Journal of Machine Learning Research, 17(83):1–5, 2016.

Dolan, E. D. and Mor, J. J. Benchmarking optimization software with performance profiles. Mathematical Programming, 91(2):201–213, January 2002. ISSN 1436-4646.

Domahidi, A., Chu, E., and Boyd, S. ECOS: An SOCP solver for embedded systems. In European Control Conference (ECC), pp. 3071–3076, 2013.

Dvijotham, K., Stanforth, R., Gowal, S., Mann, T., and Kohli, P. A dual approach to scalable verification of deep networks. In Proceedings of the Thirty-Fourth Conference Annual Conference on Uncertainty in Artificial Intelligence (UAI-18), pp. 162–171, Corvallis, Oregon, 2018. AUAI Press.

Fazlyab, M., Robey, A., Hassani, H., Morari, M., and Pappas, G. J. Efficient and Accurate Estimation of Lipschitz Constants for Deep Neural Networks. arXiv:1906.04893 [cs, math, stat], June 2019. arXiv: 1906.04893.

Gondzio, J. Presolve Analysis of Linear Programs Prior to Applying an Interior Point Method. INFORMS Journal on Computing, 9(1):73–91, February 1997. ISSN 1091-9856. doi: 10.1287/ijoc.9.1.73.

Goodfellow, I. J., Shlens, J., and Szegedy, C. Explaining and harnessing adversarial examples. arXiv preprint arXiv:1412.6572, 2014.

Gurobi Optimization, L. Gurobi optimizer reference manual, 2019. URL http://www.gurobi.com.

Hanin, B. and Rolnick, D. Deep relu networks have surprisingly few activation patterns. In Wallach, H., Larochelle, H., Beygelzimer, A., d’Alché Buc, F., Fox, E., and Garnett, R. (eds.), Advances in Neural Information Processing Systems 32, pp. 359–368. Curran Associates, Inc., 2019.

Jordan, M., Lewis, J., and Dimakis, A. G. Provable Certificates for Adversarial Examples: Fitting a Ball in the Union of Polytopes. In Wallach, H., Larochelle, H., Beygelzimer, A., d’Alché Buc, F., Fox, E., and Garnett, R. (eds.), Advances in Neural Information Processing Systems 32, pp. 14059–14069. Curran Associates, Inc., 2019.

Katz, G., Barrett, C., Dill, D. L., Julian, K., and Kohcenderfer, M. J. Reluplex: An Efficient SMT Solver for Verifying Deep Neural Networks. In Majumdar, R. and Kunak, V. (eds.), Computer Aided Verification, Lecture Notes in Computer Science, pp. 97–117, Cham, 2017. Springer International Publishing. ISBN 978-3-319-63387-9.

Lu, J. and Kumar, M. P. Neural Network Branching for Neural Network Verification. In International Conference on Learning Representations, 2020.
Hierarchical Verification for Adversarial Robustness

Odonoghue, B., Chu, E., Parikh, N., and Boyd, S. Conic optimization via operator splitting and homogeneous self-dual embedding. *Journal of Optimization Theory and Applications*, 169(3):1042–1068, 2016.

Salman, H., Yang, G., Zhang, H., Hsieh, C.-J., and Zhang, P. A Convex Relaxation Barrier to Tight Robustness Verification of Neural Networks. In Wallach, H., Larochelle, H., Beygelzimer, A., Alch-Buc, F. d., Fox, E., and Garnett, R. (eds.), *Advances in Neural Information Processing Systems 32*, pp. 9832–9842. Curran Associates, Inc., 2019.

Serra, T., Tjandraatmadja, C., and Ramalingam, S. Bounding and Counting Linear Regions of Deep Neural Networks. In Dy, J. and Krause, A. (eds.), *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pp. 4558–4566, Stockholmsmssan, Stockholm Sweden, July 2018. PMLR.

Singh, G., Gehr, T., Mirman, M., Pschel, M., and Vechev, M. Fast and Effective Robustness Certification. In Bengio, S., Wallach, H., Larochelle, H., Grauman, K., Cesa-Bianchi, N., and Garnett, R. (eds.), *Advances in Neural Information Processing Systems 31*, pp. 10802–10813. Curran Associates, Inc., 2018.

Singh, G., Ganvir, R., Pschel, M., and Vechev, M. Beyond the Single Neuron Convex Barrier for Neural Network Certification. In Wallach, H., Larochelle, H., Beygelzimer, A., Alch-Buc, F. d., Fox, E., and Garnett, R. (eds.), *Advances in Neural Information Processing Systems 32*, pp. 15072–15083. Curran Associates, Inc., 2019a.

Singh, G., Gehr, T., Pschel, M., and Vechev, M. An Abstract Domain for Certifying Neural Networks. *Proc. ACM Program. Lang.*, 3(POPL):41:1–41:30, January 2019b. ISSN 2475-1421.

Stellato, B., Banjac, G., Goulart, P., Bemporad, A., and Boyd, S. OSQP: An operator splitting solver for quadratic programs. *ArXiv e-prints*, November 2017.

Szegedy, C., Zaremba, W., Sutskever, I., Bruna, J., Erhan, D., Goodfellow, I., and Fergus, R. Intriguing properties of neural networks. *arXiv preprint arXiv:1312.6199*, 2013.

Tjeng, V., Xiao, K. Y., and Tedrake, R. Evaluating Robustness of Neural Networks with Mixed Integer Programming. In *International Conference on Learning Representations*, 2019.

Wang, S., Pei, K., Whitehouse, J., Yang, J., and Jana, S. Formal Security Analysis of Neural Networks using Symbolic Intervals. In *27th USENIX Security Symposium (USENIX Security 18)*, pp. 1599–1614, Baltimore, MD, August 2018. USENIX Association. ISBN 978-1-939133-04-5.

Weng, L., Zhang, H., Chen, H., Song, Z., Hsieh, C.-J., Daniel, L., Boning, D., and Dhillon, I. Towards Fast Computation of Certified Robustness for ReLU Networks. In *International Conference on Machine Learning*, pp. 5276–5285, July 2018.

Wong, E. and Kolter, Z. Provable Defenses against Adversarial Examples via the Convex Outer Adversarial Polytope. In *International Conference on Machine Learning*, pp. 5286–5295, July 2018.

Xiang, W., Tran, H.-D., and Johnson, T. T. Output Reachable Set Estimation and Verification for Multilayer Neural Networks. *IEEE Transactions on Neural Networks and Learning Systems*, 29(11):5777–5783, November 2018. ISSN 2162-2388.

Zhang, H., Weng, T.-W., Chen, P.-Y., Hsieh, C.-J., and Daniel, L. Efficient Neural Network Robustness Certification with General Activation Functions. In Bengio, S., Wallach, H., Larochelle, H., Grauman, K., Cesa-Bianchi, N., and Garnett, R. (eds.), *Advances in Neural Information Processing Systems 31*, pp. 4939–4948. Curran Associates, Inc., 2018.

Zou, D., Balan, R., and Singh, M. On lipschitz bounds of general convolutional neural networks. *IEEE Transactions on Information Theory*, 2019.
A. An Example Comparing GeoCert and LayerCert-Basic

The following simple example of a network with two hidden layers over a 2D input demonstrates the advantage of LayerCert-Basic over GeoCert. Recall the definition of the neural network from (2). We pick the following values for weights and biases of the network:

\[
W_0 := \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad b_0 := \begin{bmatrix} 0 \\ 0 \end{bmatrix},
\]

\[
W_1 := \begin{bmatrix} 1 & 1 \end{bmatrix}, \quad b_1 := -1,
\]

\[
W_2 := \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad b_2 := \begin{bmatrix} 0 \\ 10 \end{bmatrix}.
\]

Let the input point be \( x := [-1, -1.25]^T \). The input space and the corresponding graphs for LayerCert and GeoCert are illustrated in Figure 7. We leave the decision boundary off the figure.

![Figure 7. Input space with hierarchical graph for LayerCert and neighborhood graph for GeoCert.](image)

The next figure shows the order in which GeoCert processes the nodes and the edges (distance computations). At each node, we check if there is a decision boundary contained within the region. As for each each, we compute the distance from the input \( x \) to the boundary of the two regions that is connected by the edge.

![Figure 8. GeoCert Node and Edge Processing Order.](image)

For LayerCert, we visit more nodes. Note that we still visit all nodes in the last layer in the same relative order. We only need to check for decision boundaries for the nodes in the last layer. In addition, within the first layer, we do not have to compute the distance to the top-right green node more than once.

![Figure 9. LayerCert Node and Edge Processing Order.](image)
B. Proofs for LayerCert-Basic

B.1. Lemmas on Hyperplane Arrangements

Before we prove the result for the full hierarchical structure, we focus on the simpler case of just hyperplane arrangements. We show that for each pattern \( A \), \( \text{dist}(R_A, x) \) can be obtained by considering any neighboring pattern \( A' \) such that \( R_A \) is closer to \( x \) than \( R_{A'} \). This fact is allows us to skip the computation of some of the distances compared to GeoCert.

**Proposition B.1.** Let \( \text{dist} \) be a convex distance function. Given a nonempty region \( R_A \) and a nonempty neighboring region \( R_{A'} \) such that \( \text{dist}(R_A, x) \geq \text{dist}(R_{A'}, x) \), we have \( \text{dist}(R_A, x) = \text{dist}(\text{Face}(A, A'), x) \).

Proposition B.1 is a special case of the following lemma:

**Lemma B.2.** Let \( C \) be a closed convex set and \( f, g : \mathbb{R}^n \to \mathbb{R} \) be convex functions. Suppose the sets \( D := C \cap \{ v \mid g(v) \leq 0 \} \) and \( C \setminus D \) are nonempty and suppose \( \min_{x \in C \setminus D} f(x) \leq \min_{x \in D} f(x) \). Then there exists \( x^* \in \arg\min_{x \in D} f(x) \) satisfying \( g(x^*) = 0 \).

**Proof.** Pick some \( z \in \arg\min_{x \in C \setminus D} f(x) \) and \( y \in \arg\min_{x \in D} f(x) \). If \( g(z) = 0 \) or \( g(y) = 0 \), we are done. Suppose then that \( g(z) > 0 \) and \( g(y) < 0 \). Let \( w = z - y \) and pick \( \lambda \in (0, 1) \) such that \( g(y + \lambda w) = 0 \). It follows that \( y + \lambda w \) is in \( D \) and by the convexity of \( f \) we have \( f(y + \lambda w) \leq f(y) \). Hence \( y + \lambda w \) satisfies the claim. \( \square \)

The next thing we show about hyperplane arrangements will be useful when we consider nested hyperplane structures.

**Proposition B.3.** Let \( C \) be a convex set in \( \mathbb{R}^n \) and consider a hyperplane arrangement. Let \( \text{dist} \) be a convex distance function. Let \( A \) be a pattern that contains a point in \( \arg\min_{v \in C} \text{dist}(v, x) \) and consider another pattern \( A' \) such that \( R_A \cap C \) is nonempty. Then there is a sequence of patterns \( A = A_1, A_2, \ldots, A_k, A_{k+1} = A' \) such that we have

- \( A_i \) and \( A_{i+1} \) are neighboring patterns for \( i \in [k] \),
- \( \text{dist}(R_{A_i} \cap C, x) \leq \text{dist}(R_{A_{i+1}} \cap C, x) \) for \( i \in [k] \), and
- \( R_{A_i} \cap C \) is nonempty for \( i \in [k + 1] \).

Before we prove Proposition B.3, we will prove the following result about the hyperplane arrangements. We use the terms ‘regions’ and ‘neighbors’ here similar to their use in Definitions 3.4 and 3.5.

**Lemma B.4.** Consider a hyperplane arrangement, a convex set \( C \), and a line with endpoints contained entirely within \( C \). Consider the undirected graph \( G \) where the nodes correspond the regions of the arrangement and edges are formed between neighboring regions. For all regions in the arrangement that have a nonempty intersection with the line, there is a path in \( G \) between two regions that only passes through regions that touch the line.

**Proof.** We will first show that any two regions that share a common point can be connected through regions that share that same point \( v \). Suppose this is true if there are \( k \) hyperplanes going through the point \( v \). Let \( A \) and \( A' \) be neighboring regions that contain \( v \). After introducing another hyperplane through \( v \), suppose \( A \) gets split into two neighboring regions \( A_1, A_2 \). The addition of the hyperplane either splits \( A' \) into two regions or keeps it as one. Let \( A_3 \) be one of the nonempty regions. It must be the case that \( A_1 \) is on the same side of the hyperplane as one of \( A_1, A_2 \), so \( A_3 \) is a neighbor to one of them. Hence, all the regions around the point remain connected to each other through each other.

We will now show we can move from one end of the line to the other. The hyperplane arrangement partitions the line into line segments \( \{ s_1, s_2, \ldots, s_k \} \). There is a region that covers each line segment, so we can connect any two such line segment covering regions through a path. Furthermore, any region touching the line must touch one of the endpoints of the line segment, and hence there is a path between that point and the corresponding line segment covering region. \( \square \)

**Proof of Proposition B.3.** Let \( v, v' \) be the minimizers of \( \text{dist}(\cdot, x) \) when restricted to \( R_A \cap C \) and \( R_{A'} \cap C \) respectively. If \( \text{dist}(R_A \cap C, x) = \text{dist}(R_{A'} \cap C) \), then the straight line segment connecting \( v \) and \( v' \) only passes through patterns with the same distance by convexity of the distance function and the fact that \( A \) contains a minimizer of \( \text{dist}(\cdot, x) \) in \( C \).

Suppose the set \( C \) and corresponding pattern \( A \) are fixed. We now prove this for all valid \( A' \) patterns by performing induction on the distance \( \text{dist}(R_{A'} \cap C, x) \) since there are only finitely many. Suppose this is true for all patterns of distance less than...
We return to considering partial activation patterns and Theorem 4.1, which claims that LayerCert-Basic returns the distance of the closest point with a different label from the input. Recall the \textit{hierarchical search graph} described in Section 3.2:

- Root node (level 0): an empty ‘activation pattern’ corresponding to the ‘activation region’ $\mathbb{R}^n$.
- Nodes at level $l$: the nonempty layer-$l$ partial activation region.
- Edges at level $l$: between $A$ and $A'$ if they are $l$-layer neighbors (i.e. $A$ and $A'$ differ on a single $l$th layer neuron).
- Edges between levels $l$ and $l + 1$: between $\text{parent}(A)$ and $A$ if $A$ is obtained by $\text{next\_layer}(A, v)$ during the GeoCert algorithm.

In each iteration of the outer loop of LayerCert-Basic, the algorithm considers all nodes adjacent to those that have been processed. It picks a closest unprocessed node and computes the distance to all the neighboring nodes.

\textbf{Lemma B.5.} Let $H$ denote the hierarchical search graph of LayerCert-Basic for some network and input point $x$. There is a path in $H$ from the initial layer-1 activation pattern $A^x$ to every pattern $A$ such that the distances of the patterns on the path are monotonically increasing.

\textit{Proof.} Suppose the main claim holds for all patterns up to layer $l - 1$. We will now show this for layer $l$. The claim holds for any pattern obtained through the $\text{next\_layer}$ operation since the distance of this pattern is equal to that of its parent. Given an arbitrary $l$-layer region $R_A$ of distance $d$ from $x$, as a consequence of Proposition B.3 there is a path in $H$ of monotonically increasing distances from the pattern $B$ obtained by applying $\text{next\_layer}$ to $\text{parent}(A)$.

The proof of correctness follows from Lemma B.5.

\textit{Proof of Theorem 4.1.} Since the distance to the distance boundary contained within a full region is further or equal to the distance of the region, if we process all the regions in order of distance we will terminate only when we have computed all regions closer than the closest decision boundary.

The first region processed is the region associated the empty activation pattern which has distance 0 from $x$. Again consider the straight line segment connecting $v$ and $v'$. All regions touching $v'$ have distance at most $d'$. Furthermore, since the number of regions is finite, by the convexity of the line segment there must be some pattern $B$ where $d' \in R_B$ and $R_B$ also contains other points on the line segment closer to $v$. The convexity of the distance function implies that $\text{dist}(R_B \cap C, x) < d'$. By Lemma B.4 there must be a series of neighboring regions connecting $B$ to $A'$, and as a result $A'$ is connected to a region of at most distance $d$ through regions of at most distance $d'$.

\textbf{B.2. Correctness Proof}

We refer to considering partial activation patterns and Theorem 4.1, which claims that LayerCert-Basic returns the distance of the closest point with a different label from the input. Recall the \textit{hierarchical search graph} described in Section 3.2:

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The proof of correctness follows from Lemma B.5.

\textit{Proof of Theorem 4.1.} Since the distance to the distance boundary contained within a full region is further or equal to the distance of the region, if we process all the regions in order of distance we will terminate only when we have computed all regions closer than the closest decision boundary.

The first region processed is the region associated the empty activation pattern which has distance 0 from the input point. Again consider the straight line segment connecting $v$ and $v'$. All regions touching $v'$ have distance at most $d'$. Furthermore, since the number of regions is finite, by the convexity of the line segment there must be some pattern $B$ where $d' \in R_B$ and $R_B$ also contains other points on the line segment closer to $v$. The convexity of the distance function implies that $\text{dist}(R_B \cap C, x) < d'$. By Lemma B.4 there must be a series of neighboring regions connecting $B$ to $A'$, and as a result $A'$ is connected to a region of at most distance $d$ through regions of at most distance $d'$.

Let $H$ denote the hierarchical search graph of LayerCert-Basic for some network and input point $x$. There is a path in $H$ from the initial layer-1 activation pattern $A^x$ to every pattern $A$ such that the distances of the patterns on the path are monotonically increasing.

\textit{Proof.} Suppose the main claim holds for all patterns up to layer $l - 1$. We will now show this for layer $l$. The claim holds for any pattern obtained through the $\text{next\_layer}$ operation since the distance of this pattern is equal to that of its parent. Given an arbitrary $l$-layer region $R_A$ of distance $d$ from $x$, as a consequence of Proposition B.3 there is a path in $H$ of monotonically increasing distances from the pattern $B$ obtained by applying $\text{next\_layer}$ to $\text{parent}(A)$.

The proof of correctness follows from Lemma B.5.
B.3. Main Proof

Proof of Theorem 4.2. From Theorem 4.1, we know that LayerCert-Basic processes the full activation patterns in order of increasing distance. GeoCert does the same, and therefore both methods will process the same full activation patterns.

We will first show that the only nodes LayerCert processes are those that are full activation patterns or ancestors of the full activation patterns processed. Suppose for contradiction that this is not the case. Then, there is some processed pattern \( A \) that is not a full activation pattern where we process no child. However, LayerCert will apply \textit{next-layer} to \( A \), adding the child node \( B \) with the same priority as \( A \) to the priority queue. By assumption we have \( U \) larger than the distance of \( B \), so we will process \( B \) eventually, contradicting our earlier claim.

For any full activation pattern \( A \), there is a one-to-one mapping between the convex programs processed by GeoCert and the convex programs processed LayerCert for \( A \) and all ancestors of \( A \). This is because we form one program for each neuron in the ReLU network. Consider the \( j \)-th neuron in the \( l \)-th layer. The constraints in the convex program formed by GeoCert for \( A \) and a neighboring full pattern \( A' \) are

\[
A_i(j)z_j^i \geq 0 \text{ for } i \in [L], j \in [n_i], \text{ and } z_j^i = 0
\]

where \( z_j^i \) is defined as in (2). In contrast, LayerCert uses

\[
A_i(j)z_j^i \geq 0 \text{ for } i \in [L], j \in [n_i], \text{ and } z_j^i = 0
\]

which only has a subset of the constraints. Since the only nodes we have to consider for LayerCert are ancestors of full activation patterns, this concludes the proof of the theorem.

C. Simplifying Projection Problems via Upper Bounds

To reduce the number of constraints in Problems (7) and Problems (9), Jordan et al. (2019) note that we can quickly decide if a constraint of the form \( a^T x \leq b \) is necessary by checking if the hyperplane \( \{ x \mid a^T x = b \} \) overlaps with the ball \( B_{p,U}(x) \). This can be done via performing an \( \ell_p \) projection of \( x \) onto the hyperplane given by \( a^T x = b \), which can be done in a linear number of elementary operations. This technique of using upper and lower bounds on variables (corresponding to the case where \( p = \infty \) to prune constraints is standard in the linear programming literature (see for example Gondzio (1997)). Each time a tighter upper bound \( U \) is obtained, the ball \( B_{p,U}(x) \) shrinks, allowing us to remove more constraints.

We can apply this technique to GeoCert and any variant of the LayerCert method. Under the additional assumption that GeoCert and LayerCert-Basic process full activation patterns in the same order, LayerCert-Basic maintains its advantage in number and size of convex programs solved.

**Theorem C.1.** (Complexity of LayerCert-Basic with Domain-based Constraint Pruning) Suppose LayerCert-Basic and GeoCert process full activation patterns in the same order. Suppose we formulate the convex problems associated with decision bound and next-layer using Formulations (6) and (8). We can construct an injective mapping from the set of convex programs solved by LayerCert to the corresponding set in GeoCert such that the constraints in the LayerCert program is a subset of those in the corresponding GeoCert program.

The proof of this is similar to the proof of Theorem 4.2. The addition of domain-based pruning does not affect the result since the same constraints are pruned for both methods.

D. LayerCert Framework and Convex Restrictions

We expand on the discussion on the use in Section 5 on how to use incomplete verifiers such as those presented in Weng et al. (2018); Zhang et al. (2018) or the full linear programming relaxation of single ReLUs to improve LayerCert. Once we compute a convex set \( M \) that contains the closest decision boundary, we can subsequently restrict our attention to just the intersection of activation regions with \( M \). The correctness of this follows from the fact that Proposition B.3 accommodates the use of such a set \( M \) and from modifying the hierarchical search graph in Lemma B.5.

Instead of just applying \textit{restriction} at the initiation iteration, one can apply it at every iteration. This version of \textit{restriction} also takes in an activation pattern and forms the restriction based on this. We describe the full algorithm in Algorithm 4. The use of \textit{restriction} in every iteration can add significant overhead to the algorithm, so there is
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there are trade-offs between (1) the choice of restriction used and (2) the frequency in which restriction is applied, and these choices can depend heavily on the width and depth of the neural networks that we are verifying. We leave a computational study of this to future work.

Algorithm 4 LayerCert with Recursive Convex Restrictions

1: Input: $x, y$ (label of $x$), $U$ (upper bound)
2: $d, A, M \leftarrow \text{restriction}(\emptyset, x, ub)$
3: $Q \leftarrow \text{empty priority queue}$
4: $Q.\text{push}((d, A, M))$
5: $S \leftarrow \emptyset$
6: while $Q \neq \emptyset$ do
7:   $(d, A, M) \leftarrow Q.\text{pop}()$
8:   if $ub \leq d$ then
9:     return $U$
10:   if $A$ is a full activation pattern then
11:     $ub \leftarrow \min(\text{decision bound}(A, x, ub))$
12:   else
13:     if contains$_{\text{db}}(A, x, ub) = \text{maybe}$ then
14:       $(d', A', M') \leftarrow \text{restriction}(A, x, ub)$
15:       $Q.\text{push}((d', A', M'))$
16:     for $A' \in N_{\text{current layer}}(A) \setminus S$ do
17:       if Face$(A, A') \cap M$ is nonempty then
18:         $d' \leftarrow \text{priority}(x, \text{Face}(A, A') \cap M)$
19:         $Q.\text{push}((d', A', M))$
20:     $S \leftarrow S \cup \{A'\}$

E. Additional Experiments and Details
E.1. Parameter Choices

Convex programming software. We used the following package versions and settings for handling convex programs. All the solvers are accessed through CVXPY’s interface:

- Modeling language: CVXPY v1.0.25 (Diamond & Boyd, 2016).
- Primary solver: ECOS v2.0.7 (Domahidi et al., 2013) – ‘abstol’:$1 \times 10^{-5}$, ‘reltol’:$1 \times 10^{-4}$, ‘feastol’:$1 \times 10^{-5}$, ‘abstol_inacc’:$5 \times 10^{-3}$, ‘reltol_inacc’:$5 \times 10^{-2}$, ‘feastol_inacc’:$5 \times 10^{-3}$.
- Secondary solver: OSQP v0.6.0 (Stellato et al., 2017) – ‘eps_abs’:$0.001$, ‘eps_rel’:$0.001$.
- Backup solver: SCS v2.1.1 (Odonoghue et al., 2016) – default settings.

Use of constraint-reducing techniques. We used the same domain-based techniques mentioned in Section C for all the methods. Before adding a constraint to a convex program to solve, we check if the constraint overlaps with $B_{p, U}(x)$.

E.2. Additional Results

$\ell_2$-norm experiments. In Table 2 we present the averaged results for $\ell_2$-norm. We used an upper bound radius of 3.0. As with the $\ell_\infty$ results presented in Table 1, the LayerCert methods consistently outperform the GeoCert methods in terms of the timing. We note that some of the difference in running times is partially due to the solvers – ECOS and OSQP failed frequently, and whenever SCS is invoked the running time is significantly increased. This issue persisted over a range of hyperparameter settings for ECOS and OSQP. We note that this is rare for the $\ell_\infty$-norm experiments.

As for the number of quadratic programs, LayerCert-CROWN and LayerCert-Both consistently outperform both GeoCert methods, while LayerCert and LayerCert-IA mostly but not always outperforms GeoCert-Lip. GeoCert is consistently the worst performing method in terms of number of QPs and running time.
Table 2. Average number of convex programs and running time over 100 inputs for 12 different networks for $\ell_2$-norm distance. The green shaded entries indicate the best performing method for each neural network under each metric. The gray shaded entries indicates the algorithm timed out before an exact solution to Problem (1) could be found or before a radius of 3 is reached for at least one input. Whenever a timeout occurs, we use a time of 1800 seconds in its place, which leads to an underestimate of the true time.

|                | [10, 50, 10] | 2 x [20] | 3 x [20] | 4 x [20] | 5 x [20] | 2 x [30] |
|----------------|-------------|----------|----------|----------|----------|----------|
|                | #QPs | Time (s) | #QPs | Time (s) | #QPs | Time (s) | #QPs | Time (s) | #QPs | Time (s) | #QPs | Time (s) |
| GeoCert        | 22.0  | 1.80     | 56.3  | 10.47    | 96.0  | 6.21     | 49.3  | 25.30    | 64.9  | 304.80   | 24.6  | 1.77     |
| GeoCert-Lip    | 19.0  | 1.70     | 34.9  | 9.77     | 51.0  | 3.58     | 41.8  | 22.00    | 62.7  | 242.47   | 22.6  | 1.77     |
| LayerCert      | 15.3  | 0.76     | 36.4  | 1.34     | 53.7  | 2.03     | 27.9  | 1.43     | 29.0  | 49.45    | 16.0  | 0.86     |
| LayerCert-IA   | 15.3  | 0.79     | 36.4  | 1.38     | 53.7  | 2.07     | 24.0  | 1.12     | 29.0  | 49.35    | 16.0  | 0.89     |
| LayerCert-CROWN| 15.3  | 0.79     | 28.9  | 1.20     | 41.3  | 1.58     | 25.4  | 1.95     | 27.8  | 52.12    | 14.6  | 0.75     |
| LayerCert-Both | 15.3  | 0.82     | 28.9  | 1.24     | 41.3  | 1.61     | 22.7  | 1.74     | 27.8  | 51.87    | 14.6  | 0.79     |

Ablation Study for LayerCert-Basic. In Section 4.2, one of the reasons provided for the reduction in the number of priority computations for LayerCert-Basic over GeoCert was that was LayerCert marked a pattern $A$ as ‘seen’ after the first priority computation involving $A$, whereas GeoCert only did so after it selected $A$ at the start of an iteration. To test the effect of this particular change, we created a new variant of LayerCert where we only marked a pattern as seen after it is chosen at the start of a main iteration, akin to GeoCert.

The results are presented in Table 3. We see that this leads to a slight overhead over LayerCert, but overall this accounts only for a small fraction of the improvement in performance over GeoCert. This indicates that the majority of the improvement comes from hierarchical structure and the way that it allows us to avoid a large number of priority computations while reducing the complexity of each computation.

Experiments for Larger Networks To compare the performance of LayerCert and GeoCert for large networks, we chose the following fully-connected networks and used $\ell_\infty$-distance.

- $8 \times [20]$,
- $6 \times [30]$,
- $5 \times [50]$,
- $5 \times [60]$.

We chose the 10 instances where none of the methods were able to converge within 1800 seconds and compared the performance of GeoCert with Lipschitz term and LayerCert with both heuristics. Figures 10, 11, 12, 13 contain these results. The orange solid line in each represent LayerCert while the blue dotted line represents GeoCert.
Table 3. Ablation Study: Average number of convex programs and running time over 100 inputs for 12 different networks for $\ell_\infty$-norm distance, focusing on GeoCert, LayerCert-Basic, and a variant of LayerCert that allows repeated priority computations by shifting when we mark a pattern as ‘seen’. The gray shaded entries indicates the algorithm timed out before an exact solution to Problem (1) could be found or before a radius of 0.3 is reached for at least one input. Whenever a timeout occurs, we use a time of 1800 seconds in its place, which leads to an underestimate of the true time.

|                  | 3 x [30] | 4 x [30] | 5 x [30] | 2 x [50] | 3 x [50] | 4 x [50] |
|------------------|----------|----------|----------|----------|----------|----------|
|                  | #LPs Time (s) | #LPs Time (s) | #LPs Time (s) | #LPs Time (s) | #LPs Time (s) | #LPs Time (s) |
| GeoCert          | 867.4 88.92 | 18.0 1.48 | 392.7 96.08 | 1739.7 252.82 | 1567.1 410.47 | 814.8 336.03 |
| LayerCert + Repeat | 568.3 29.95 | 12.4 0.69 | 203.5 22.88 | 1870.2 120.88 | 3500.9 248.85 | 1001.3 108.04 |
| LayerCert        | 440.4 25.52 | 12.1 0.68 | 176.7 22.00 | 1620.0 111.61 | 3131.7 239.81 | 826.3 99.61 |

Figure 10. Timing for 10 Instances, $8 \times [20]$ network.

Figure 11. Timing for 10 Instances, $6 \times [30]$ network.
Figure 12. Timing for 10 Instances, $5 \times [50]$ network.

Figure 13. Timing for 10 Instances, $5 \times [60]$ network.