Bounding the Complexity of Formally Verifying Neural Networks: A Geometric Approach

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ABSTRACT
In this paper, we consider the computational complexity of formally verifying the input/output behavior of Rectified Linear Unit (ReLU) Neural Networks (NNs): that is, we consider the complexity of determining whether the output of a NN lies in a specific convex polytopic region (in its range) whenever its input lies in a specific polytopic region (in its domain). Specifically, we show that for two different NN architectures—shallow NNs and Two-Level Lattice (TLL) NNs—the verification problem with (convex) polytopic constraints is polynomial in the number of neurons in the NN to be verified, when all other aspects of the verification problem held fixed (e.g., input dimension). We achieve these complexity results by exhibiting an explicit verification algorithm for each type of architecture. Nevertheless, both algorithms share a commonality in structure. First, they directly (or almost directly) translate the NN parameters into a partitioning of the NN’s input space by means of hyperplanes; this has the effect of partitioning the original verification problem into sub-verification problems derived from the geometry of the NN itself. Indeed, these partitionings have two further important properties. First, the number of these hyperplanes is polynomially related to the number of neurons, and hence so is the number of sub-verification problems. Second, each of the subproblems is solvable (in polynomial time) by means of a Linear Program (LP). Thus, to attain an overall polynomial time algorithm for the original verification problem, it is only necessary to enumerate these subproblems in polynomial time. To achieve this final step, we also contribute a novel algorithm to enumerate the regions in a hyperplane arrangement in polynomial time; our algorithm is based on a poset ordering of the regions for which poset successors are polynomially easy to compute. Taken together, the runtime of either verification algorithm has the following form: polynomially many subproblems times polynomial time to enumerate all of the subproblems times polynomial time to solve each subproblem.

KEYWORDS
Neural Networks, Neural Network Verification, Rectified Linear Units

1 INTRODUCTION
Neural Networks (NNs) are increasingly used in modern cyber-physical systems, where they are often employed as feedback controllers. Typically, however, these NNs are not designed analytically or explicitly, but rather trained from data in an end-to-end learning paradigm. Such data-trained controllers are popular in this context because they often perform quite well, but because they are obtained by an implicit design methodology, they do not come with crucial safety guarantees per se. Thus, algorithms that can independently verify the safety of a NN (controller) are a very active area research, even though progress in this area not kept pace with the momentum of NN controller adoption in safety-critical applications.

Despite the importance—and abundance—of such NN verification algorithms, relatively little attention has been paid to a theoretical analysis of their computational complexity. While it is known that the satisfiability of any 3-SAT formula, \( \varphi \), can be encoded as a NN verification problem, this result requires the variables in \( \varphi \) to be in correspondence with the input dimensions to the network [15]. On the one hand, this makes it clear that the complexity of verifying a NN depends unfavorably on the dimension of its input space. On the other hand, this result doesn’t speak directly to the relative difficulty of verifying a NN with a fixed input dimension but an increasing number of neurons. The only results that hint at this second consideration are those that exhibit networks for which the number of affine regions grows exponentially in the number of neurons in the network—see e.g. [18]. However, these kinds of results merely suggest that the verification problem is still “hard” in the number of neurons in the network (input and output dimensions are fixed). There are not, to our knowledge, any concrete complexity results that address this second question.

In this paper, we prove two such concrete complexity results that explicitly describe the computational complexity of verifying a NN as a function of its size. In particular, we consider two specific NN architectures—shallow NNs and Two-Level Lattice NNs [9]—and prove that the complexity of verifying either type of NN grows only polynomially in the number of neurons in the network to be verified, all other aspects of the verification problem held fixed. These results appear in Section 3 as Theorem 2 and Theorem 3 for shallow NNs and TLL NNs, respectively. Our proofs for both of these complexity results are existential: that is we propose two concrete verification algorithms, one for shallow NNs and one for TLL NNs. However, we note that although our proposed algorithms do have polynomial time complexities, the constants and exponents prevent them from being amenable to real-world problems; they are merely proof devices to establish categories of NNs for which polynomial verification is possible (if not practical).

Despite some network specific differences, the algorithms we propose for shallow NNs and TLL NNs depend on the following common observations.

- The parameters of both architectures readily expose an arrangement of hyperplanes that partitions the input space into affine regions of the NN to be verified. Consequently, the regions of this arrangement constitute a partitioning
of the original verification problem into a number of sub-verification problems, each of which can be solved in polynomial time directly with Linear Programs (LPs). Moreover, the number of hyperplanes in these arrangements can be chosen to depend polynomially on the size of the NN to be verified; thus, since the number of regions in such an arrangement further depends polynomially on the number of hyperplanes, this partitioning results in polynomially many sub-verification problems. Thus, for both shallow NNs and TLL NNs, it is possible to replace the original verification problem with polynomially many verification problems over affine regions of the original NN, each of which may in turn be verified in polynomial time.

- Given the prequel, a polynomial verification algorithm is to exhaustively verify the (polynomially many) sub-problems — that is provided the regions in the associated hyperplane arrangement can be enumerated in polynomial time. Thus, we also introduce a novel algorithm that does exactly that. Our algorithm is based on a long-known poset for the regions in a hyperplane arrangement [6], but we show that successors in this arrangement can be obtained in polynomial time. Thus, traversing the (poset of) regions in such an arrangement is itself a polynomial operation.

Finally, we note that our results should be viewed in the context of three observations. First, by their mere existence, the complexity results we prove herein demonstrate that the NN verification problem is not per se a “hard” problem as a function of the size of the NN to be verified. Second, although our results show that complexity of verifying a shallow or a TLL NN scales polynomially with its size, all other aspects of the problem held constant, our complexity claim do scale exponentially in the dimension of the input to the NN. Thus, our results do not contradict the known “hardness” of the verification problem as a function of the NN’s input dimension — i.e. the results in [15]. Finally, while our results do speak directly to the complexity of the verification problem as a function of the number of neurons, they do not speak as directly to the complexity of the verification problem as a function of the input dimension of the problem held constant, our complexity results, although many have noticed empirically that there is a significant complexity associated with the input dimension; [15] is a notable exception, since it also included an NP-completeness result based on the 3-SAT encoding mentioned above. Other examples of pragmatic NN verification approaches include: (i) SMT-based methods [7, 15, 16]; (ii) MILP-based solvers [1–4, 11, 17, 22]; (iii) Reachability based methods [8, 13, 14, 23, 26, 29, 30]; and (iv) convex relaxations methods [5, 25, 28]. By contrast, a number of works have focused on the computational complexity of various other verification-related questions for NNs ([15] is the exception in that it expressly considers the verification problem itself). Some NN-related complexity results include: the minimum adversarial disturbance to a NN is NP hard [27]; computing the Lipschitz constant of a NN is NP hard [24]; reachability analysis is NP hard [20].

2 PRELIMINARIES

2.1 Notation

Throughout this paper, ℝ will refer to the real numbers. For an (n × m) matrix (or vector), A, we will use the notation A[i, j] to denote the element in the i-th row and j-th column of A. Analogously, the notation A[i, :], will denote the i-th row of A, and [A](:, j) will denote the j-th column of A; when A is a vector instead of a matrix, both notations will return a scalar corresponding to the corresponding element in the vector. Let \(a_{m,n}\) be an (n × m) matrix of zeros. We will special bold parenthesis \((\cdot)\) to delineate the arguments to a function that returns a function. For example, given an (m × n) matrix, \(W\), (possibly with \(m = 1\)) and an (m × 1) dimensional vector, \(b\), we define the linear function:

\[
\mathcal{L}(W, b) : x \mapsto \|Wx + b\|_i.
\]

(1)

(that is \(\mathcal{L}(W, b)\) is itself a function). We also use the functions \(\text{First}\) and \(\text{Last}\) to return the first and last elements of an ordered list (or by overloading, a vector in \(\mathbb{R}^n\)). The function \(\text{Concat}\) concatenates two ordered lists, or by overloading, concatenates two vectors in \(\mathbb{R}^n\) and \(\mathbb{R}^m\) along their (common) nontrivial dimension to get a third vector in \(\mathbb{R}^{n+m}\). We will use an overbar to indicate (topological) closure of a set: i.e. \(\bar{A}\) is the closure of \(A\). Finally, \(B(x, \delta)\) will denote an open Euclidean ball centered at \(x\) with radius \(\delta\).

2.2 Neural Networks

In this paper, we will exclusively consider Rectified Linear Unit Neural Networks (ReLU NNs). A K-layer ReLU NN is specified by composing \(K\) layer functions (or just layers). We allow two kinds of layers: linear layers and nonlinear layers. A nonlinear layer with \(l\) inputs and \(o\) outputs is specified by a \((o \times l)\) real-valued matrix of weights, \(W\), and a \((o \times 1)\) real-valued matrix of biases, \(b\), as follows:

\[
L_\theta : \mathbb{R}^l \rightarrow \mathbb{R}^o, \quad L_\theta : z \mapsto \max\{Wz + b, 0\}
\]

(2)

where the max function is taken element-wise, and \(\theta = (W, b)\) for brevity. A linear layer is the same as a nonlinear layer, except for the omission of the nonlinearity \(\max\{\cdot, 0\}\) in the layer function; a linear layer will be indicated with a superscript “\(\text{lin}\)” as in \(L_\theta^{\text{lin}}\).

Thus, a K-layer ReLU NN function as above is specified by \(K\) layer functions \(L_{\theta^{(i)}} : i = 1, \ldots, K\) whose input and output dimensions are composable: that is they satisfy \(i_1 = i_{0,1} : i = 2, \ldots, K\). We further adopt the convention that the final layer is always a linear layer; however, other layers are allowed to be linear as desired. Specifically:

\[
\mathcal{N}(x) = (L_{\theta^{(K)}} \circ L_{\theta^{(K-1)}} \circ \cdots \circ L_{\theta^{(2)}})(x).
\]

(3)

When we wish to make the dependence on parameters explicit, we will index a ReLU function \(\mathcal{N}\) by a list of matrices \(\Theta \doteq (\theta^{(1)}, \ldots, \theta^{(K)})\) in this respect, we will often abuse notation slightly, and use \(\mathcal{N}_{\Theta}\) and \(\Theta\) interchangeably when no confusion will result.

Note that specifying the number of layers and the dimensions of the associated matrices \(\theta^{(i)} = (W^{(i)} b^{(i)})\) specifies the architecture of the ReLU NN. Therefore, we will use:

\[
\text{Arch}(\Theta) \doteq ((n, o_1), (i_1, o_2), \ldots, (i_{K-1}, o_{K-1}), (i_K, m))
\]

(4)

\(^1\)That is \(\Theta\) is not the concatenation of the \(\theta^{(i)}\) into a single large matrix, so it preserves information about the sizes of the constituent \(\theta^{(i)}\).
to denote the architecture of the ReLU NN \(\mathcal{M}_\Theta\). Note that our definition is quite general since it allows the layers to be of different sizes, as long as \(\theta_{i-1} = 1\) for \(i = 2, \ldots, K\).

**Definition 1 (Shallow NN).** A shallow NN is a NN with two layers, the first of which is nonlinear and the second of which is linear.

### 2.3 Special NN Operations

**Definition 2 (Sequential (Functional) Composition).** Let \(\mathcal{M}_\Theta_1\) and \(\mathcal{M}_\Theta_2\) be two NNs where \(\text{Last}(\text{Arch}(\Theta_1)) = (i, c)\) and \(\text{First}(\text{Arch}(\Theta_2)) = (c, 0)\) for some nonnegative integers \(i\) and \(c\). Then the **sequential (or functional) composition** of \(\mathcal{M}_\Theta_1\) and \(\mathcal{M}_\Theta_2\), i.e. \(\mathcal{M}_\Theta_1 \circ \mathcal{M}_\Theta_2\), is a well defined NN, and can be represented by the parameter list \(\Theta_1 \circ \Theta_2 \triangleq \text{Concat}(\Theta_1, \Theta_2)\).

**Definition 3.** Let \(\mathcal{M}_\Theta_1\) and \(\mathcal{M}_\Theta_2\) be two \(K\)-layer NNs with parameter lists:

\[
\Theta_1 = ((W_1^{i_1}, b_1^i), \ldots, (W_K^{i_K}, b_K^i)), \quad i = 1, 2.
\]

Then the **parallel composition** of \(\mathcal{M}_\Theta_1\) and \(\mathcal{M}_\Theta_2\) is a NN given by the parameter list

\[
\Theta_1 \parallel \Theta_2 \triangleq \left( \begin{pmatrix} W_1^{i_1} & W_2^{j_1} & \cdots & W_K^{j_K} \\ b_1^i & b_2^j & \cdots & b_K^j \end{pmatrix} \right).
\]

2.4 Two-Level-Lattice (TLL) Neural Networks

In this paper, we will be especially concerned with ReLU NNs that have a particular architecture: the Two-Level Lattice (TLL) architecture introduced as part of the AREN algorithm in [9]. We describe the TLL architecture in two separate subsections, one for scalar output TLL NNs, and one for multi-output TLL NNs.

#### 2.4.1 Scalar TLL NNs

A scalar-output TLL NN can be characterized entirely by integers \(N\) and \(M\) as follows.

\[
\mathcal{M}_{N, M} \triangleq \Theta_{\text{max}} \circ \left( (\Theta_{\text{min}_1} \circ \Theta_{S_1}) \parallel \cdots \parallel (\Theta_{\text{min}_N} \circ \Theta_{S_N}) \right) \circ \Theta_T.
\]

In the above,

\[
\Theta_T \triangleq ((W_t, b_t)),
\]

and each \(\Theta_{S_j}, j = 1, \ldots, M\) has the form

\[
\Theta_{S_j} = (S_j, \Theta_{M, 1})
\]

where

\[
S_j = [I_N^T, \ldots, I_N^T]^T\text{ for some sequence } i_k \in \{1, \ldots, N\}\text{ (recall that } I_N \text{ is the } (N \times N) \text{ identity matrix).}
\]

The linear functions implemented by the mapping \(x \mapsto \left[ W_1^i, \ldots, W_i^j \right]^T + [b_1^i, \ldots, b_i^j]^T\) for \(i = 1, \ldots, N\) will be referred to as the **local linear functions** of \(\mathcal{M}_{N, M}\); we assume for simplicity that these linear functions are unique. The matrices \(S_j|j = 1, \ldots, M\) will be referred to as the **selector matrices** of \(\mathcal{M}_{N, M}\). Each set \(S_j \triangleq \{k \in \{1, \ldots, N\}| \exists x \in \{1, \ldots, N\} \parallel S_j \|_k = 1\}\) will be called the selector set of \(S_j\).

#### 2.4.2 Multi-output TLL NNs

For the purposes of this paper, we will define a multi-output TLL NN with range space \(\mathbb{R}^m\) using \(m\) equally sized scalar TLL NNs. This is for two reasons. First, it will make the eventual computational complexity expressions for our algorithms more compact. Second, it will make straightforward the connection to assured architecture designs, such as the one in [9]: if \(N\) local linear functions are needed in a NN with \(m\) real-valued outputs, then an architecture with \(m\) component TLL NNs, each with its own \(N\) local linear functions, will have enough local linear functions to meet the assurance (a consequence of [9, Theorem 3]). We will likewise assume that all of the component TLLs have a common number of selector matrices.

**Definition 6 (Multi-output TLL NN).** A ReLU NN that maps \(\mathbb{R}^n \rightarrow \mathbb{R}^m\) is said to be an **m-output TLL NN of size** \((N, M)\) if its parameters \(\Sigma_{N, M}^{(m)}\) are the parallel composition of \(m\) scalar-output TLL NNs, each of size \((N, M)\). That is:

\[
\Sigma_{N, M}^{(m)} \triangleq \left( \Sigma_{N, M}^1 \parallel \cdots \parallel \Sigma_{N, M}^m \right).
\]

The subnetworks \(\Sigma_{N, M}^i, i = 1, \ldots, m\) will be referred to as the **component (TLL) networks** of \(\Sigma_{N, M}^{(m)}\).

### 2.5 Hyperplanes and Hyperplane Arrangements

In this section, we review mostly notation for hyperplanes and hyperplane arrangements; [21] is the primary reference for this section, although we don’t need any of the sophisticated theorems therein.

**Definition 7 (Hyperplanes and Half-spaces).** Let \(t : \mathbb{R}^n \rightarrow \mathbb{R}\) be an affine map. Then define:

\[
H^t_\ell \triangleq \left\{ \left. x \in \mathbb{R}^n \right| t(x) < 0 \right\} = -1, \quad H^t_{\ell^+} \triangleq \left\{ \left. x \in \mathbb{R}^n \right| t(x) > 0 \right\} = +1
\]

We say that \(H^t_\ell\) is the **hyperplane defined by** \(t\) **in dimension** \(n\), and \(H^{-1}_\ell\) and \(H^{+1}_\ell\) are the **negative and positive half-spaces defined by** \(t\), respectively.

**Definition 8 (Normal Vector to a Hyperplane).** Let \(H^t_\ell\) be a hyperplane. Then let \(\perp(H^t_\ell)\) be the unit normal vector to \(H^t_\ell\) such that for any \(x \in H^t_\ell\), \((x + \perp(H^t_\ell)) \in H_\ell^{+1}\).

**Definition 9 (Rank of a Set of Hyperplanes).** Let \(S = \{H^t_1, \ldots, H^t_N\}\) be a set of hyperplanes with associated affine functions \(t_1, \ldots, t_N\). Then we define:

\[
\text{rank}(S) \triangleq \text{rank}(\{\perp(H^t_1), \ldots, \perp(H^t_N)\} \subseteq \mathbb{R}^n).
\]

**Definition 10 (Hyperplane Arrangement).** Let \(\mathcal{L}\) be a set of affine functions for which each \(\ell \in \mathcal{L}\) is a function \(\ell : \mathbb{R}^n \rightarrow \mathbb{R}^m\).
Then \( \{ H^f_\ell : \ell \in \mathcal{L} \} \) is said to be an arrangement of hyperplanes in dimension \( n \).

**Definition 11 (Region of a Hyperplane Arrangement).** Let \( \mathcal{H} \) be an arrangement of \( N \) hyperplanes in dimension \( n \) defined by corresponding set of affine functions, \( \mathcal{L} \). Then a non-empty open subset \( R \subseteq \mathbb{R}^n \) is said to be an \( m \)-dimensional region of \( \mathcal{H} \) if there is an indexing function \( s : \mathcal{L} \rightarrow \{-1, 0, +1\} \) such that rank(\( \{ H^f_\ell : \ell \in \mathcal{L}, s(\ell) = 0 \} \)) = \( n - m \) and

\[
R = \bigcap_{\ell \in \mathcal{L}} H^f_\ell(s(\ell)).
\]

(14)

When the dimension of a region is omitted, it will be assume to be the same as the dimension of the arrangement. The set of all regions of an arrangement \( \mathcal{H} \) will be denoted by \( \mathcal{R} \).

**Definition 12 (Face).** Let \( \mathcal{H} \) be an arrangement of \( N \) hyperplanes in dimension \( n \) defined by affine functions \( \mathcal{L} \), and let \( R \) be an \( m \)-dimensional region of \( \mathcal{H} \) that is specified by the indexing function \( s : \mathcal{L} \rightarrow \{-1, 0, +1\} \). Then a closed set \( F \subseteq \mathbb{R}^n \) is an \( m' \) \( \leq m \) dimensional face of \( R \) if \( F \) is the closure of an \( m' \)-dimensional region contained in \( R \). That is there exists an indexing function \( s' : \mathcal{L} \rightarrow \{-1, 0, +1\} \) such that

\[
F = \bigcap_{\ell \in \mathcal{L}} H^f_\ell(s'(\ell)),
\]

(15)

where

- \( s(\ell) = s'(\ell) \) for all \( \ell \in \{ t' \mid s'(t') \neq 0 \} \); and
- rank(\( \{ H^f_\ell : \ell \in \mathcal{L}, s'(\ell) = 0 \} \)) = \( m - m' \).

Note that for an \( m \)-dimensional region \( R \), \( \mathcal{R} \) is an \( m \)-dimensional face of \( R \). 0-dimensional faces are called vertices.

**Theorem 1.** Let \( \mathcal{H} \) be an arrangement of \( N \) hyperplanes in dimension \( n \). Then the number of regions in \( \mathcal{H} \) is at most \( \sum_{k=0}^{n} \binom{N}{k} \).

**Remark 1.** Note that for a fixed dimension, \( n \), the bound \( \sum_{k=0}^{n} \binom{N}{k} \) grows like \( O(N^n) \), i.e. sub-exponentially.

### 3 MAIN RESULTS

#### 3.1 NN Verification Problem

In this paper, we take as a starting point the following verification problem, which we refer to as the verification problem for NNs.

**Problem 1.** Let \( \mathcal{N}_\Omega : \mathbb{R}^n \rightarrow \mathbb{R}^m \) be a NN with at least two layers. Furthermore, assume that there are two convex, bounded, full-dimensional polytopes \( P_X \subseteq \mathbb{R}^n \) and \( P_Y \subseteq \mathbb{R}^m \) with \( H \)-representations\(^2\) given as follows:

- \( P_X \triangleq \bigcap_{i=1}^{N_X} H^{-1}_{x,i} \subseteq \mathbb{R}^n \) where \( x_{i,i} : \mathbb{R}^n \rightarrow \mathbb{R} \) is an affine map for each \( i = 1, \ldots, N_X \); and
- \( P_Y \triangleq \bigcap_{i=1}^{N_Y} H^{-1}_{y,i} \subseteq \mathbb{R}^m \) where \( y_{i,i} : \mathbb{R}^m \rightarrow \mathbb{R} \) is an affine map for each \( i = 1, \ldots, N_Y \).

Then the verification problem is to determine whether the following formula is true:

\[
\forall x \in P_X \subset \mathbb{R}^n, (\mathcal{N}_\Omega(x) \in P_Y \subset \mathbb{R}^m).
\]

(16)

\(^2\)An \( H \)-representation of a polytope is (possibly non-minimal) representation of that polytope as an intersection of half-spaces.

If (16) is true, then we say that the problem is SAT; otherwise, we say that the problem is UNSAT.

#### 3.2 Main Theorems

As mentioned above, the main results of this paper demonstrate that Problem 1 can be solved in polynomial time complexity in the number of neurons for two classes of networks. In particular, the following two Theorems are the main results of this paper.

**Theorem 2.** Let \( \Theta = ((n, n), (n, m)) \) be a shallow network with \( n \) neurons. Now consider an instance of Problem 1 for this network: i.e. fixed dimensions \( n \) and \( m \), and fixed constraint sets \( P_X \) and \( P_Y \). Then there is an algorithm that solves this instance of Problem 1 in polynomial time complexity in \( n \). This algorithm has a worst case runtime of

\[
O \left( \left( n \cdot N^{n+2} \cdot \log N + N_Y \cdot N^n \cdot \text{Cplxty}(\text{LP}(N, n)) \right) + N^n \cdot m \cdot n \right)
\]

(17)

where \( N = n + N_Y \) and \( \text{Cplxty}(\text{LP}(N, n)) \) is the complexity of solving a linear program in dimension \( n \) with \( N \) constraints.

**Theorem 3.** Let \( \Xi_{N,n} \) be a multi-output TLL network. Now consider an instance of Problem 1 for this network: i.e. fixed dimensions \( n \) and \( m \), and fixed constraint sets \( P_X \) and \( P_Y \). Then there is an algorithm that solves this instance of Problem 1 in polynomial time complexity in \( N \) and \( M \) of these algorithms depends on the existence of polynomial-time solvers for linear programs, but such solvers are well known to exist (see e.g. [19]).

It is important to note that Theorem 2 and Theorem 3 both explicitly indicate that the difficulty in verifying their respective classes of NNs grows only polynomially in the complexity of the network, all other parameters of Problem 1 held fixed. Note also that the polynomial complexity of these algorithms depends on the existence of polynomial-time solvers for linear programs, but such solvers are well known to exist (see e.g. [19]).

In particular, Theorem 2 and Theorem 3 explicitly indicate that the difficulty in verifying their respective classes of NNs grows only polynomially in the complexity of the network, all other parameters of Problem 1 held fixed. Note also that the polynomial complexity of these algorithms depends on the existence of polynomial-time solvers for linear programs, but such solvers are well known to exist (see e.g. [19]).

Finally, it is essential to note that the results in Theorem 2 and Theorem 3 connect the difficulty of verifying a TLL NN (resp. shallow NN) to the size of the network not the expressivity of the network. The semantics of the TLL NN in particular make this point
especially salient, since each distinct affine function represented in the output of a TLL NN can be mapped directly to parameters of the TLL NN itself (see Proposition 9 in Section 6). In particular, consider the deep NNs exhibited in [18, Corollary 6]: this parameterized collection of networks expresses a number of unique affine functions that grows exponentially in the number of neurons in the network (i.e. as a function of the number of layers in the network). Consequently, the size of a TLL required to implement one such network would likewise grow exponentially in the number of neurons deployed in the original network. Thus, although a TLL NN may superficially seem “easy” to verify because of Theorem 3, the efficiency in verifying a TLL NN form could mask the fact that it is polynomial in the number of neurons for both types of NNs. Ultimately, this trade-off will not necessarily be universal, though, since TLL NNs also have mechanisms for parametric efficiency; for example, a particular local linear function need only be implemented once in a TLL NN, no matter how many disjoint regions on which it is activated (this could be especially useful in the case of networks implementing interpolated zero-order-hold functions, such as in [10]).

3.3 Proof Sketch of Main Theorems

3.3.1 Core Lemma: Polynomial-time Enumeration of Hyperplane Regions

The results in this paper all have the same broad proof structure:

Step 1: Choose a hyperplane arrangement with the following three properties:

(a) The number of hyperplanes is polynomial in the number of network neurons;
(b) \(P_x\) is the union of the closure of regions from this arrangement; and
(c) Problem 1 can be solved in polynomial time on the closure of any region, \(R\), in this arrangement – i.e. Problem 1 with \(P_x\) replaced by \(R\) can be solved in polynomial time.

Step 2: Iterate over all of the regions in this arrangement, and for each region, solve Problem 1 with \(P_x\) replaced by the closure of the current region.

The details of Step 1 will vary depending on the architecture of the network being verified (Theorem 2 and Theorem 3). However, no matter the details of Step 1, this proof structure depends on a polynomial time algorithm to traverse the regions in a hyperplane arrangement. Thus, the following Lemma establishes the complexity of just such a polynomial-time algorithm.

Lemma 1. Let \(L = \{f_1, \ldots, f_N\}\) be a set of affine functions, \(f_i : \mathbb{R}^n \to \mathbb{R}\), that can be accessed in \(O(1)\) time, and let \(H = \{H_i \mid i \in L\}\) be the associated hyperplane arrangement.

Then there is an algorithm to traverse all of the regions in \(H\) that has runtime

\[O(n \cdot N^{2n+2} \cdot \log N) \cdot \text{Cplxty}(LP(N,n))\]

(19)

where \(\text{Cplxty}(LP(N,n))\) is the complexity of solving a linear program in dimension \(n\) with \(N\) constraints.

It is crucial to note that there is more to Lemma 1 than just the sub-exponential bound on the number of regions in a hyperplane arrangement (see Theorem 1 in Section 2). Indeed, although there are only \(O(N^n)\) regions in an arrangement of \(N\) hyperplanes in dimension \(n\), it must be inferred which of the \(2^N\) possible hyperplane activations correspond to valid regions. That this is possible in polynomial time is the main contribution of Lemma 1, and hence the main facilitator of the other results in this paper.

3.3.2 Theorem 2 and Theorem 3. Given Lemma 1, the proofs of Theorem 2 and Theorem 3 depend on finding a suitable hyperplane arrangement, as described in Step 1 in the previous subsection.

In both cases, we note that the easiest closed convex polytope on which to solve Problem 1 is one on which the underlying NN is affine. Indeed, suppose for the moment that \(M(\Theta)\) is affine on the entire constraint set \(P_x\) with \(M(\Theta) = \ell_0\) on this domain. Under this assumption, solving the verification problem for a single output constraint, \(\ell_{y,i}\), entails solving the following linear program:

\[y_i = \max(\ell_{y,i} \circ \ell_0)(x)\]

s.t. \(\ell_{x,i}(x) \leq 0\) for \(i = 1, \ldots, N_x\). (20)

Of course if \(y_i > 0\), then Problem 1 is UNSAT under these assumptions; otherwise it is SAT for the constraint \(\ell_{y,i}\) and the next output constraint needs to be considered. Given the known (polynomial) efficiency of solving linear programs, it thus makes sense to select a hyperplane arrangement for Step 1 with the property that the NN is affine on each region of the arrangement. Although this is a difficult problem for a general NN, the particular structure of shallow NNs and TLL NNs allow just such a selection to be accomplished efficiently.

To this end, we make the following definition.

Definition 13 (Switching Affine Function/Hyperplane).

Let \(M(\Theta) : \mathbb{R}^n \to \mathbb{R}^m\) be a NN. A set of affine functions \(S = \{f_1, \ldots, f_N\}\) is said to be a set of switching affine functions for \(M(\Theta)\) if \(M(\Theta)\) is affine on every region of the hyperplane arrangement \(H \subseteq \{H_i \mid i \in S\}\). \(H \subseteq \{H_i \mid i \in S\}\) is then said to be an arrangement of switching hyperplanes of \(M(\Theta)\).

For both shallow NNs and TLL NNs, we will show that a set of switching hyperplanes is immediately evident (i.e. in polynomial complexity) from the parameters of those architectures directly; this satisfies Step 1(b). However it also further implies that this choice of switching hyperplanes has a number of hyperplanes that is polynomial in the number of neurons in either network; this satisfies Step 1(a). Identifying the affine function represented on a region from the arrangement we propose is a different procedure for a shallow NN and a TLL NN. Nevertheless, we show subsequently that it is polynomial in the number of neurons for both types of NNs. By these results, and the procedure outlined in the previous section, we will thus obtain the conclusions of Theorem 2 and Theorem 3.

4 POLYNOMIAL-TIME ALGORITHM TO TRAVERSE REGIONS IN A HYPERPLANE ARRANGEMENT

Our proof strategy for Theorem 2 and Theorem 3 is intended to exploit the sub-exponential scaling of the number of regions in a hyperplane arrangement (in a fixed dimension); see Theorem 1. However, since we ultimately seek a polynomial-time algorithm, it is essential that we exhibit an algorithm to traverse the regions in
a hyperplane arrangement without exhaustively searching over all $2^N$ possible combinations of half-spaces associated with $N$ hyperplanes.

The core of our region traversal algorithm is a particular poset on the regions in a hyperplane arrangement, which was introduced in [6] with other intentions. For our purposes, though, the essential feature of this poset is that given any region, we can compute its successors in polynomial time. Thus, this section first introduces the claimed poset, and then describes polynomial algorithm to traverse it.

### 4.1 A Poset of Regions in a Hyperplane Arrangement

We begin by defining the poset of interest from [6], which we dub the Region Adjacency Poset of a hyperplane arrangement.

**Definition 14 (Region Adjacency Poset of a Hyperplane Arrangement)** [6, PP. 618]. Let $\mathcal{H} = \{H^f | f \in \mathcal{L}\}$ be a hyperplane arrangement, and let $\mathcal{R}_H$ be its regions. Furthermore, let $B \in \mathcal{R}_H$ be a specific region of $\mathcal{H}$, and without loss of generality assume that $B = \cap_{f \in \mathcal{L}} H^f$. \hfill (21)

Furthermore, for a region $R = \cap_{f \in \mathcal{L}} H^f$, define the notation $\mathcal{J}(R) = \{f | f \in \mathcal{L} \land s(f) = -1\}$. \hfill (22)

Then the **region adjacency poset** of $\mathcal{H}$ based at $B$ is a partial order $\leq_{R} \subseteq \mathcal{R}_H \times \mathcal{R}_H$ defined as follows. Let $R_k = \cap_{f \in \mathcal{L}} H^f$, $k = 1, 2$ be two regions of $\mathcal{H}$. Then

$$ R_1 \leq_{R} R_2 \iff \mathcal{J}(R_1) \subseteq \mathcal{J}(R_2). \hfill (23) $$

Note that the definition of the region adjacency poset in terms of the special region $B = \cap_{f \in \mathcal{L}} H^f$ really is without loss of generality. For if we wish to take as a base some other region, $R$, then we can simply redefine those hyperplanes that don’t participate in $R$ by way of “positive” half-spaces. This alteration doesn’t affect the regions of the arrangement in any way.

No matter the choice of a base region $B$, though, for our purposes it is essential that every other region is a successor of $B$. This is more or less trivially true, but it is stated formally in Proposition 2, by way of Proposition 1.

**Proposition 1 ($\leq_{R}$ is ranked [6, Proposition 1.1]).** The function $\rho : R = \cap_{f \in \mathcal{L}} H^f \in \mathcal{R}_H \mapsto |\{ f \in \mathcal{L} | s(f) = -1\}|$ ranks the poset $\leq_{R}$. \hfill (24)

**Proposition 2.** Let $\leq_{R}$ be the region poset region associated with the base region $B = \cap_{f \in \mathcal{L}} H^f$, as described in Definition 14. Then for any region $R \in \mathcal{R}_H$ it is the case that $B \leq_{R} R$. Moreover, there exists a finite sequence of regions $R_k$, $k = 1, \ldots, K$ such that $R_1 = B$, $R_K = R$ and $\{R_k\}$ is totally ordered by $\leq_{R}$. \hfill (25)

**Proof.** Let $R = \cap_{f \in \mathcal{L}} H^f$ with $f : \mathcal{L} \to \{-1, 0, +1\}$ as usual. It follows from the choice of $B$ (without loss of generality) that $B \leq_{R} R$. The other claim follows directly from Proposition 1. \hfill (26)

Before we introduce the main facilitatory result for our algorithm, we need the following small proposition.

---

This poset is unnamed in [6]: we chose this name for notational convenience.

---

**Proposition 3.** Let $F$ be an $n$ - 1-dimensional face of any region $R = \cap_{f \in \mathcal{L}} H^f \in \mathcal{H}$, and let this face be described by the indexing function $s F : \mathcal{L} \to \{-1, 0, +1\}$. Then the set $\{ f \in \mathcal{L} | s F(f) = 0 \}$ is a singleton.

**Proof.** This follows immediately from Definition 12, since a set of distinct hyperplanes $\{H_1^f, \ldots, H_P^f\}$ with non-empty intersection has rank 1 if and only if $K = 1$ (otherwise, the hyperplanes are all parallel to each other). \hfill (27)

Now we are in a position to state the two most important results of this section. The first, Proposition 4 states that every $n - 1$-dimensional face of a region is associated with an adjacent region that is obtained by flipping the sign of a single hyperplane. In other words, this feature of the poset allows us to “move from one region [in a hyperplane arrangement] to another by ‘walking’ through one hyperplane at a time.” [6] This result thus forms the motivation for the second critical result of this section, Proposition 5. In particular, Proposition 5 states that the $n - 1$-dimensional faces of a region, $R$, can be obtained by computing one minimal H-representation of $\hat{R}$. Thus, Proposition 5 forms the basis for a polynomial region traversal algorithm, since minimal H-representations can be computed in polynomial time. \hfill (28)

**Proposition 4.** Let $F$ be an $n - 1$-dimensional face of any region $R = \cap_{f \in \mathcal{L}} H^f \in \mathcal{H}$, and let this face be described by the indexing function $s F : \mathcal{L} \to \{-1, 0, +1\}$, where $t^\prime \in \mathcal{L}$ is the unique affine map for which $s F(t) = 0$.

Then there is a unique region $R' = \cap_{f \in \mathcal{L}} H^f$ with indexing function $s F'$ that satisfies the property:

$$ s F'(t) = \begin{cases} s(F(t)), & t \neq t^\prime \\ -s(F(t)), & t = t^\prime. \end{cases} \hfill (29) $$

**Proof.** Regions are uniquely specified by their indexing functions (over the same set of hyperplanes), so if such a region $R'$ exists, it is unique. Thus, we only need to show that the claimed indexing function corresponds to a valid region. But the only way that the claimed $s F'$ can fail to correspond to a valid region is if the intersection of the associated half-spaces is empty. Thus, we must prove that $\cap_{f \in \mathcal{L}} H^f \neq \emptyset$. \hfill (30)

Let $U = \cap_{f \in \mathcal{L}} H^f = \cap_{f \in \mathcal{L}} H^f$, and note that $U \cap R \neq \emptyset$, so $U$ is itself a nonempty open set. Moreover, $\text{int}(F) = U \cap H_0^f$ is nonempty, since $F$ is of dimension $n - 1$ (the only faces with empty interior are vertices). In particular, there exists an $x_0 \in \text{int}(F) \subseteq U$. Hence, since $U$ is an open set, there exists a ball $B(x_0, \delta) \subseteq U$, and in particular, $x_0 \pm \frac{\delta}{2} \in \mathcal{L} H_0^f \subseteq U$. However, since $t^\prime(x_0) = 0$, by linearity it is clear that one these vectors belongs to $R = U \cap H^f$ and the other to $R' = U \cap H^{-s(F)}$. Thus, $R'$ is nonempty as claimed. \hfill (31)

---

**Proposition 5.** Let $F$ be the face of any region $R$ with dimension $n - 1$, and let this face be described by the indexing function $s F : \mathcal{L} \to \{-1, 0, +1\}$ with $\{ f \in \mathcal{L} | s F(f) = 0 \} = t^\prime$ (see Proposition 3). Then $t^\prime$ corresponds to a hyperplane in the minimal H-representation of $\hat{R}$. Likewise, every affine function in the minimal H-representation of $\hat{R}$ corresponds to an $n - 1$-dimensional face of $R$. \hfill (32)
Bounding the Complexity of Formally Verifying Neural Networks: A Geometric Approach

Figure 1: (Left) A hyperplane arrangement \( \{H_{t_1}^0, \ldots, H_{t_k}^0\} \) with positive half spaces, \( H_{t_{k-1}}^{t_{k-1}} \), denoted by red arrows and regions \( B, R_1, \ldots, R_9 \). (Right) The corresponding adjacency poset with base \( B \); changes in \( S(R) \) labeled on arrows. Example from [6].

Proof. First, we show the forward direction. Suppose that such an \( t' \) corresponds to an \( n - 1 \)-dimensional face of \( \tilde{R} \), but \( H_{t'}^0 \) is not in the minimal H representation of \( \tilde{R} \); in particular,

\[
\tilde{R} = \bigcap_{t \in \mathcal{L}, t \neq t'} H_{t'}^{\mathcal{S}(t)}.
\]

But this means that

\[
F = \bigcap_{t \in \mathcal{L}, t \neq t'} H_{t'}^{\mathcal{S}(t)} \subseteq \bigcap_{t \in \mathcal{L}, t \neq t'} H_{t'}^{\mathcal{F}(t)}.
\]

for the same indexing function \( \mathcal{S}' \). Let \( L \triangleq \{ t \in \mathcal{L} \mid \mathcal{S}'(t) = 0 \} \). Since are taking only finite intersections and \( H_{t'}^0 \subset H_{t'}^{\mathcal{F}(t)} \) for any \( t \), we can write

\[
F = \bigcap_{t \in \mathcal{L}, t \neq t'} H_{t'}^{\mathcal{S}(t)} \subseteq \bigcap_{t \in \mathcal{L}, t \neq t'} H_{t'}^{\mathcal{F}(t)}.
\]

Thus, we also have that

\[
F \cap H_{t'}^0 = \bigcap_{t \in \mathcal{L}, t \neq t'} H_{t'}^{\mathcal{S}(t)} \cap H_{t'}^0 \subseteq \bigcap_{t \in \mathcal{L}, t \neq t'} H_{t'}^{\mathcal{F}(t)} \cap H_{t'}^0 = F.
\]

This implies that \( F \subset H_{t'}^0 \), and in particular

\[
\bigcap_{t \in L} H_{t'}^0 \cap H_{t'}^0 \neq \emptyset.
\]

However, by the above argument, this implies that rank(\( L \cup \{ t' \} \)) > 1, which contradicts our assumption that \( F \) is a face of dimension \( n - 1 \) (in particular, that it is the closure of an \( n - 1 \)-dimensional region). Thus, every \( n - 1 \)-dimensional face of \( \tilde{R} \) corresponds to a hyperplane in the minimal H-representation of \( \tilde{R} \).

Finally, let \( M_{\tilde{R}} = \{ t_1, \ldots, t_k \} \) be the minimal H-representation of \( \tilde{R} \). It is enough to show that

\[
\bigcap_{t \in M_{\tilde{R}}} H_{t'}^{\mathcal{S}(t)} \neq \emptyset
\]

for any \( \mathcal{S}_k : M_{\tilde{R}} \to \{-1, 0, +1\} \) such that \( \mathcal{S}_k(t) = 0 \) if and only if \( t = t_k \). Thus, fix \( k \) and suppose not. However, this assumption implies that the set \( \cap_{t \in M \setminus \{ t_k \}} H_{t'}^{\mathcal{S}(t)} \) must lie entirely in \( H_{t_{k-1}}^{t_{k-1}} \) or \( H_{t_{k+1}}^{t_{k+1}} \); since the aforementioned set is an open, convex set. Of course this directly implies that the affine function \( t_k \) is redundant, thus contradicting the assumption that \( M_{\tilde{R}} \) is the minimal H-representation of \( \tilde{R} \).

Remark 2. In [6], hyperplanes that contain (what we refer to as) an \( n - 1 \)-dimensional face of a region are referred to as boundary hyperplanes of that associated regions, presumably for reasons related to Proposition 5.

4.2 A Polynomial Time Algorithm to Traverse the Regions in a Hyperplane Arrangement

Proposition 5 is the basis for a polynomial-time algorithm that visits each region in a hyperplane arrangement, since it directly establishes that the \( \lesssim R \) successors of any region \( R \) can be obtained by a polynomial algorithm (a minimal H-representation computation). Thus, we exhibit Algorithm 1, a polynomial-time algorithm to list the successors of a hyperplane region, \( R \), given an binary encoding of the half-spaces describing it. The correctness of Algorithm 1 follows directly from Proposition 5.

Thus, it only remains to show that we can effectively use Algorithm 1 to traverse the poset efficiently. However, this can be done by traversing the poset level-wise: recall that the region adjacency poset is ranked by the cardinality of the set \( \mathcal{S}(R) \) (Proposition 1). Thus, we propose Algorithm 2 to traverse the poset level by level, using a max heap (over the binary region encoding) to ensure that the same region isn’t traversed multiple times. The correctness of Algorithm 2 then follows from the arguments above and the correctness of Algorithm 1.

Remark 3. Using a heap in Algorithm 2 is somewhat extravagant computationally. We employ it here only because it has a straightforward worst-case runtime.

Now we are in a position to state the proof of Lemma 1.

Proof. (Lemma 1) Together, the correctness of both Algorithm 1 and Algorithm 2 is an existential proof that such an algorithm is possible, so we just need to account for the claimed runtime. But this follows from the fact that there are \( O(N^n) \) regions in a hyperplane arrangement. For each of these regions, we need to compute one minimal H-representation, which has cost \( O(N) \cdot \text{Cplxty}(LP(N, n)) \), and we need to do at most \( O(N^n) \) heap operations per region, each of which we assume is logarithmic in the size of the heap (in this case, the size of the heap is itself bounded by the number of regions).

\( \square \)
Algorithm 1: FindSuccessors.

Algorithm 2: TraverseHyperplaneRegions.

5 POLYNOMIAL-TIME ALGORITHM TO VERIFY SHALLOW NN

This section will consist of a sequence of propositions that address the various aspects of Step 3, as described in Subsection 3.3.1. Then the section will conclude with a formal statement of the proof of Theorem 2.

Proposition 6. Let $\Theta = ((W_1^1, b_1^1), (W_2^2, b_2^2))$ be a shallow NN with Arch$(\Theta) = ((n, n), (n, m))$. Then the set of affine functions $\Theta(S(\Theta) = \{L_i^\Theta \mid i = 1, \ldots, n\}$ is a set of switching affine functions for $\Theta$, and $H(\Theta) = \{H_i^\Theta \mid i \in S(\Theta)\}$ is a set of switching hyperplanes.

Proof. A region in the arrangement $H(\Theta)$ exactly assigns to each neuron a status of strictly active or strictly inactive – i.e. the output of the neuron is strictly greater than zero or strictly less than zero. But forcing a particular activation status on each neuron a status of strictly active or strictly inactive – i.e. the $\Theta$ is a set of switching affine functions for $(\section{3.3.1}). Then the section will conclude with a formal statement of the proof of Theorem 2.

Proposition 6. Let $\Theta = ((W_1^1, b_1^1), (W_2^2, b_2^2)) be a shallow NN with Arch$(\Theta) = ((n, n), (n, m))$, and let $H(\Theta) be as in Proposition 6. Then the complexity of determining the active linear function on a region of $H(\Theta)$ is at most $O(n \cdot m \cdot n)$. (32)

Proof. This runtime is clearly dominated by the cost of doing the matrix multiplication $W_2^2 \cdot W_1^1$. Given that Arch$(\Theta) = ((n, n), (n, m))$, this operation has the claimed runtime. □

Proposition 7. Let $\Theta = ((W_1^1, b_1^1), (W_2^2, b_2^2)) be a shallow NN with Arch$(\Theta) = ((n, n), (n, m))$, and let $H(\Theta) be as in Proposition 6. Then the complexity of determining the active linear function on a region of $H(\Theta)$ is at most $O(n \cdot m \cdot n)$. (32)

Proof. This runtime is clearly dominated by the cost of doing the matrix multiplication $W_2^2 \cdot W_1^1$. Given that Arch$(\Theta) = ((n, n), (n, m))$, this operation has the claimed runtime. □

Proposition 8. The arrangement $\mathcal{H} \equiv \mathcal{H}(\Theta) \cup \{H_i^\Theta \mid i = 1, \ldots, N_X\}$ has the property that $P_X$ is the union of the closure of regions from $\mathcal{H}$, and each region in $\mathcal{H}$ is strictly contained in a region from $\mathcal{H}(\Theta)$. Hence, $\mathcal{H}$ is also a switching hyperplane arrangement and Propositions 6 and 7 apply just as well to regions of $\mathcal{H}$ with run times the same as for $\mathcal{H}(\Theta)$.

Proof. This follows trivially by definition of a region and the fact that we are merely adding hyperplanes to the arrangement $H(\Theta)$. □

Now we can finally state the proof of Theorem 2.

Proof. (Theorem 2) We need to traverse the hyperplane arrangement $\mathcal{H}(\Theta) \cup \{H_i^\Theta \mid i = 1, \ldots, N_X\}$, which has $n + N_X$ hyperplanes. By Theorem 1, this arrangement has $O((n + N_X)^2)$ regions, so by Lemma 1, we need at most $O(n \cdot (n + N_X)^2 \cdot \log(n + N_X))$ calls to an LP solver to traverse all of these regions – i.e. we need $n + N_X$ LP calls per region to find the minimal H-representation of that region.
using Algorithm 1, in addition to the overhead associated with Algorithm 2. Then, on each region, we need to access the active linear function, so we add the run time described in Proposition 7 times the number of regions, i.e. \( O((n + N)^m/n \cdot n \cdot n) \). Finally, we need to run one linear program per region per output constraint. This comes at a total cost of \( N \cdot (n + N)^m/n \) calls to the LP solver. This explains the runtime expression claimed in the Theorem. \( \square \)

6 POLYNOMIAL-TIME ALGORITHM TO VERIFY TLL NN

This section will consist of a sequence of propositions that address the various aspects of Step 1, as described in Subsection 3.3.1. Then the section will conclude with a formal statement of the proof of Theorem 3.

Proposition 9. Let \( \Xi_{N,M}^{(m)} \) be a TLL NN as described in Definition 6. Then define

\[ S(\Xi_{N,M}^{(m)}) \triangleq \{ L^j(W_{f_t}^k, b_f^j) - L^j(W_{f_t}^k, b_f^j) | i, j \in \{1, \ldots, N\} \} \]

and \( HS(\Xi_{N,M}^{(m)}) \triangleq \{ H^0_b | \ell \in S(\Xi_{N,M}^{(m)}) \} \). Furthermore, define \( S(\Xi_{N,M}^{(m)}) \triangleq \cup_{k=1}^m S(\Xi_{N,M}^{(m)}) \) and \( HS(\Xi_{N,M}^{(m)}) \triangleq \cup_{k=1}^m HS(\Xi_{N,M}^{(m)}) \).

Then \( S(\Xi_{N,M}^{(m)}) \) is a set of switching affine functions for \( \Xi_{N,M}^{(m)} \), and the \( k \)-th component of \( \Xi_{N,M}^{(m)} \) is an affine function on each region of \( HS(\Xi_{N,M}^{(m)}) \) and is exactly equal to \( L^j(W_{f_t}^k, b_f^j) \) for some \( i \).

Proof. Let \( R \) be a region in \( HS(\Xi_{N,M}^{(m)}) \). It is obvious that such a region is contained in exactly one region from each of the component-wise arrangements \( HS(\Xi_{N,M}) \), so it suffices to show that each component TLL is linear on the regions of its corresponding arrangement.

Thus, let \( R_k \) be a region in \( HS(\Xi_{N,M}^{(m)}) \). We claim that \( \Xi_{N,M}^{(m)} \) is linear on \( R_k \). To see this, note by definition of a \( (n,m) \)-dimensional region, there is an indexing function \( s : S(\Xi_{N,M}^{(m)}) \rightarrow \{-1, +1\} \) such that

\[ R_k = \bigcup_{\ell \in S(\Xi_{N,M}^{(m)})} H^s(\ell). \]  

(33)

Thus, \( R_k \) is a unique order region by construction: each such half-space identically orders the outputs of two linear functions, and since \( R_k \) is \( n \)-dimensional it is contained in just such a half space for each and every possible pair. That is

\[ \forall x \in R_k : \| W_{f_t}^k x + b_f^k \|_{i_k} < \cdots < \| W_{f_t}^k x + b_f^k \|_{N_k} \]  

for some sequence \( i_k \subset \{1, \ldots, N\} \).

Thus, for each \( j = 1, \ldots, M \), there exists an index \( i_j \in \{1, \ldots, N\} \) such that

\[ \forall x \in R_k : \{ M(\Theta_{\min N_k})(S_j(W_{f_t}^k x + b_f^j)) = \| W_{f_t}^k x + b_f^j \|_{i_j} \} \]  

(35)

That is each of the min terms in \( \Xi_{N,M}^{(m)} \) is exactly equal to one of the linear functions \( \| W_{f_t}^k x + b_f^k \|_{i_j} \) on \( R_k \). Therefore,

\[ \forall x \in R_k : .\mathcal{A}(\Xi_{N,M}^{(m)})(x) = .\mathcal{A}(\Theta_{\max M})( \begin{bmatrix} \| W_{f_t}^k x + b_f^k \|_{i_1} \\ \vdots \\ \| W_{f_t}^k x + b_f^k \|_{i_M} \end{bmatrix} ). \]  

(36)

But applying the unique ordering property of \( R_k \) to the above further implies that there exists an index \( x \in \{1, \ldots, N\} \) such that

\[ .\mathcal{A}(\Xi_{N,M}^{(m)})(x) = \| W_{f_t}^k x + b_f^k \|_{i_j}, \]  

for all \( x \in R_k \). \( \square \)

Proposition 10. Let \( \Xi_{N,M}^{(m)} \) be a TLL NN as described in Definition 6, and let \( HS(\Xi_{N,M}^{(m)}) \) be the set of switching hyperplanes defined in Proposition 9.

Then for any region \( R \) of \( HS(\Xi_{N,M}^{(m)}) \) the affine function of \( \Xi_{N,M}^{(m)} \) that is active on \( R \) can be determined by a polynomial algorithm with runtime

\[ O(m \cdot N^2 + m \cdot (M + 1) \cdot N \cdot \log N). \]  

(37)

Proof. From the proof of Proposition 9 we know that a region in \( HS(\Xi_{N,M}^{(m)}) \) is a unique order region for the linear functions \( (W_{f_t}^k, b_f^j) \) of each component. In other words, the indexing function of the region \( R \) specifies a strict ordering of each pair of linear functions from each component of \( \Xi_{N,M}^{(m)} \). That is the region \( R \) by way of its indexing function \( s_R \) effectively “sorts” the component-wise linear functions on \( R \).

These pairwise comparisons can be turned into a sorted list of linear functions for each component at the cost of \( O(m \cdot N^2) \), which explains the first term in the claimed runtime. Thus, it remains only to check each of the selection sets against these component-wise sorted lists of linear functions to see which affine function is active for each min term; this is then followed by checking which of the active functions from each min term survives as the active function after the max operation. A procedure for doing this involves at most \( O(N \cdot \log N) \) operations per component per min term (using a binary search of the sorted list), followed by another \( O(N \cdot \log N) \) comparisons per component to see which of the (unique) linear functions expressed by min terms survives the final max term. \( \square \)

Proposition 11. The arrangement \( \mathcal{H} \triangleq \{ HS(\Xi_{N,M}^{(m)}) \} \cup \{ H^0_b \} \) has the property that \( P_\mathcal{H} \) is the union of the closures of regions from \( \mathcal{H} \), and each region in \( \mathcal{H} \) is strictly contained in a region from \( HS(\Xi_{N,M}^{(m)}) \). Hence, \( \mathcal{H} \) is also a switching hyperplane arrangement and Propositions 9 and 10 apply just as well to regions of \( \mathcal{H} \) with run times the same as for \( HS(\Xi_{N,M}^{(m)}) \).

Proof. This follows trivially by definition of a region and the fact that we are merely adding hyperplanes to the arrangement \( HS(\Xi_{N,M}^{(m)}) \).

Now we can finally state the proof of Theorem 3.

Proof. (Theorem 3) We need to traverse the hyperplane arrangement \( HS(\Xi_{N,M}^{(m)}) \cup \{ H^0_b \} \), which has \( m \cdot N^2 + N_k \) hyperplanes. By Theorem 1, this arrangement has \( O((m \cdot N^2 + N_k)\cdot n) \) regions, so by Lemma 1, we need at most \( O(n \cdot (m \cdot N^2 + N_k)^{2n+2} \cdot \log(m \cdot N^2 + N_k)) \) calls to an LP solver to traverse all of these regions – i.e. we need \( m \cdot N^2 + N_k \) LP calls per region to find the minimal H-representation of that region using Algorithm 1, in addition to the overhead associated with Algorithm 2. Then, on each region, we need to access the active linear function, so we add the run time described in Proposition 10 times the number of regions, i.e. \( O((m \cdot N^2 + N_k)^m \cdot (N^2 + M \cdot N \cdot \log N)). \) Finally, we need to run one linear program per region per output constraint. This comes at a total cost of \( N \cdot (m \cdot N^2 + N_k)^m \) calls to the LP solver. This explains the runtime expression claimed in the Theorem. \( \square \)
7 APPENDIX

Definition 15 (Input Replicator NN). Let \( n < m \) be two integers. An input replicator NN of size \((n, m)\) is a single-layer NN with the following parameter list:
\[
\Gamma_{n,m} \triangleq \left( \begin{array}{c}
I_n, \ldots, I_n \\
\vdots \\
1, \ldots, 1
\end{array} \right)
\]
(38)
where \( I_n \) represents the \((n \times n)\) identity matrix, and the \( n^{th} \) row thereof, \( I_n \), is repeated enough times so that \( \text{Arch}(\Gamma_{n,m}) = (n, m) \). That is \( \Gamma_{n,m} \) has \( n \) inputs and \( m > n \) outputs, with the final \( m - n \) outputs exact copies of the \( n^{th} \) input.

Definition 16 (Two element min NN). A two element min NN is given by parameter list
\[
\Theta_{\min} \triangleq \left( \begin{array}{cc}
1 & 0 \\
1 & 1 \\
0 & 1
\end{array} \right)
\]
(39)
This network presents at its output the minimum value of its two inputs.

Definition 17 (Two element max NN). A two element max NN is given by parameter list
\[
\Theta_{\max} \triangleq \left( \begin{array}{cc}
1 & 1 \\
1 & 0 \\
0 & 0
\end{array} \right)
\]
(40)
This network presents at its output the maximum value of its two inputs.

Definition 18 (Pairwise min/max NNs). A pairwise min NN of size \( n \) is a NN defined by the following parameter list:
\[
\Theta_{\min}^{n-2} \triangleq (\Theta_{\min} \mid \cdots \mid \Theta_{\min}) \circ I_{2·\lceil n/2 \rceil}
\]
(41)
where the parallel composition includes \( \lceil n/2 \rceil \) copies of \( \Theta_{\min} \). Note that \( \Theta_{\min} \) has exactly \( \lceil n/2 \rceil \) outputs. Also note that \( \Theta_{\min}^{n-2} \equiv \Theta_{\min} \).

A pairwise max NN of size \( n \) is defined as above, but with min replaced by max.

Definition 19 (n-element min/max NNs). An \( n \)-element min network is defined by the following parameter list:
\[
\Theta_{\min} \triangleq \Theta_{\min}^{2 \times 2} \circ \Theta_{\min}^{4 \times 4} \circ \cdots \circ \Theta_{\min}^{\lceil n/2 \rceil \times 2} \circ \Theta_{\min}^{n \times 2}
\]
(42)
\( \Theta_{\min} \) outputs minimum from among its \( n \) inputs using a divide and conquer approach.

An \( n \)-element max network, denoted by \( \Theta_{\max} \), is defined as above, only with all occurrences of min replaced by max. Analogously, \( \Theta_{\max} \) outputs the maximum element from among its \( n \) inputs.

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